# Experimental and modeling study of fixed-bed CO<sub>2</sub> adsorption using Zeolite 13X

Durga Ramadas Nayanar\*, Swapna Singha Rabha

Department of Chemical Engineering, Indian Institute of Technology Madras

\*Corresponding author: ch21d041@smail.iitm.ac.in

### Highlights

- Zeolites have immense potential as solid sorbents for CO<sub>2</sub> capture
- CO<sub>2</sub> adsorption performance of zeolite 13X is investigated in a lab-scale packed-bed column
- Adsorption is also described by a 1D mathematical model and validated with experimental results
- Effect of feed flow rate and particle size on packed-bed CO<sub>2</sub> adsorption is studied

## 1. Introduction

 $CO_2$  emissions from human activities have contributed to global warming, with global surface temperatures increasing 1.1°C since pre-industrialization.[1] Fossil fuel combustion to meet the growing global energy demands account for 87% of anthropogenic  $CO_2$  emissions. Shifting to low-carbon and renewable energy sources is not feasible within the near future since a major part of the energy demand is still met through fossil fuels.[2] In this scenario, Carbon Capture and Storage (CCS) is necessary to tackle the rising  $CO_2$  emissions. Adsorption using dry solid sorbents is being explored as an alternative to conventional absorption using liquid amine solvents due to their lower regeneration energy requirements and better adsorption capacity.[3] Zeolite, activated carbon and amine functionalized silica and polymeric materials are commonly used sorbents for  $CO_2$  capture.

In this work, a parametric study of zeolite 13X for  $CO_2$  capture in a packed-bed column is performed. Experiments are conducted using zeolite 13X at different operating conditions, and the  $CO_2$  adsorption behaviour is studied. The work also aims to provide insights into the heat effects in the column during the exothermic adsorption process by studying the axial temperature profiles. The adsorption behaviour is also predicted using a detailed 1D axially dispersed plug flow model and has been validated with experimental results.

## 2. Methods

## 2.1. Experimental set-up and procedure

The packed-bed experimental set-up consists of a cylindrical acrylic column of height 0.5 m and diameter 0.05 m. The experimental set-up is shown in Figure 1a, and a schematic of the column is shown in Figure 1b. Experiments are conducted using zeolite 13X beads of various sizes ( $d_p = 0.5$  mm, 1.5 mm, and 3.5 mm) using a CO<sub>2</sub>-N<sub>2</sub> (20-80) gas mixture at different feed flow rates. The CO<sub>2</sub> concentration at the exit of the bed is continuously measured using a CO<sub>2</sub> gas analyser (Technovation Analytical Instruments), the bed temperature at the centre of the bed at three different axial positions was measured using K-type thermocouples. The pressure drops across the distributor and across the bed were measured using differential pressure transmitters (Yokogawa, EJA110E).

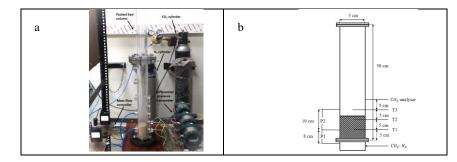


Figure 1. (a) Experimental set-up for packed-bed adsorption (b) schematic representation of the packed-bed column

### 2.2. Numerical model

Along with the experimental study, a detailed 1D axially dispersed plug-flow model is developed and solved using MATLAB under experimental conditions. The model considers mass and energy balances, the pressure drop across the bed, constitutive equations like the adsorption isotherm and the equation of state, and the Linear Driving Force (LDF) approximation for mass transfer. The mass balance:

$$\frac{\partial C}{\partial t} + \frac{\partial (uC)}{\partial z} = D_L \frac{\partial^2 C}{\partial z^2} - \frac{(1-\varepsilon)}{\varepsilon} \rho \frac{\partial q}{\partial t}$$
(1)

The gas-phase energy balance:

$$-\lambda \frac{\partial^2 T}{\partial z^2} + C_g \frac{\partial (uT)}{\partial z} + C_g \frac{\partial T}{\partial t} + \frac{(1-\varepsilon)}{\varepsilon} C_s \frac{\partial T_s}{\partial t} = \frac{(1-\varepsilon)}{\varepsilon} \left( -\Delta H \right) \frac{\partial q}{\partial t} - \frac{4h_w}{\varepsilon d_c} \left( T - T_w \right)$$
(2)

Pressure drop across the bed is expressed using the Ergun equation:

$$-\frac{\partial P}{\partial z} = 150 \frac{\mu_g (1-\varepsilon)^2}{\varepsilon^3 d_p^2} v_s + 1.75 \frac{(1-\varepsilon)}{\varepsilon^3 d_p} \rho_g {v_s}^2$$
(3)

#### 3. Results and discussion

The CO<sub>2</sub> breakthrough curve and temperature profile obtained from a packed-bed experiment using zeolite 13X beads of diameter 1.5 mm at  $U_G = 0.7 U_{mf}$  (N<sub>2</sub>:CO<sub>2</sub> = 80:20) is shown in Figures 2 (a) and 2 (b) respectively. The experimental and modeling results are found to be in good agreement.

It is observed that the  $CO_2$  adsorption capacity decreases with increase in feed flow rate, while it increases with increase in particle size.

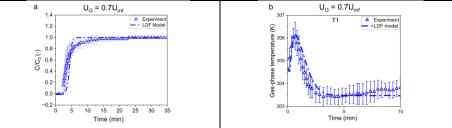


Figure 2. (a)  $CO_2$  breakthrough curve and (b) temperature profile from packed-bed experiments and simulation at  $U_G = 0.7U_{mf}$  using zeolite 13X of diameter 1.5 mm

### 4. Conclusion

In this work, the packed-bed  $CO_2$  adsorption performance of zeolite 13X beads of various sizes is investigated at different feed flow rates, and the  $CO_2$  adsorption capacity, temperature evolution, and pressure drop across the bed are studied. The adsorption behavior has also been studied using a 1D numerical model and the results have been validated with the experimental results.

The present work provides an understanding about the adsorption performance of zeolite 13X sorbent in a packed-bed column under various operating conditions. The results of this study will be valuable for the design and development of process intensification approaches for the sorbent-based  $CO_2$  capture technologies.

#### References

- K. Calvin et al., IPCC, 2023: Climate Change 2023: Synthesis Report. Contribution of Working Groups I, II and III to the Sixth Assessment Report of the Intergovernmental Panel on Climate Change [Core Writing Team, H. Lee and J. Romero (eds.)]. IPCC, Geneva, Switzerland., 2023. https://doi.org/10.59327/IPCC/AR6-9789291691647.
- [2] Our Energy Needs: World Energy Consumption & Demand | CAPP, (n.d.). https://www.capp.ca/energy/world-energy-needs/ (accessed December 29, 2023).
- [3] A. Samanta, A. Zhao, G.K.H. Shimizu, P. Sarkar, R. Gupta, Post-combustion CO 2 capture using solid sorbents: A review, Ind. Eng. Chem. Res. 51 (2012) 1438–1463. https://doi.org/10.1021/ie200686q.

### Keywords

CO<sub>2</sub> capture; zeolite 13X; packed-bed; mathematical modeling