Designs 2026 Conference
The 1st International Online Conference on Designs
9–10 February 2026 | Online
MDPI

Modelling and MATLAB –Based Optimization of Carbon Dioxide Adsorption Using Zn-MOF-5

Shonisani Salvation Muthubi, Dorcas Museme Mabulay, Pascal Kilunji Mwenge
Department of Chemical and Metallurgical Engineering, Vaal University of Technology, Vanderbijlpark 1900, South Africa

INTRODUCTION & AIM

The rapid growth of industrial activities has significantly increased atmospheric carbon dioxide (CO_2) concentrations, making CO_2 a major contributor to climate change, global warming, sea-level rise, and glacier melting. If current trends continue, atmospheric CO_2 concentrations are expected to exceed 570 ppm by the year 2100 [1]. Conventional CO_2 capture methods, particularly amine-based absorption processes, are widely applied but remain energy-intensive due to the high regeneration energy required for solvent [2].

These limitations have driven the development of adsorption-based separation technologies such as PSA, VSA, and TSA, which offer lower energy penalties than absorption methods [3]. Their performance strongly depends on the adsorbent used. Metal–Organic Frameworks (MOFs), particularly Zn-MOF-5, have shown high CO_2 uptake and rapid adsorption due to their high surface area and tunable pore structure [1,4].

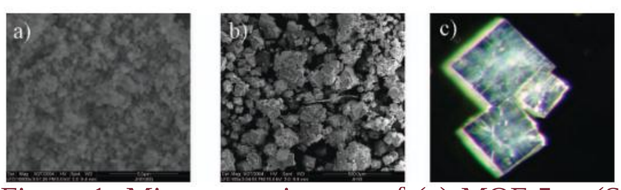

Figure 1: Microscopy images of (a) MOF-5_n (SEM), (b) MOF-5_m (SEM), and (c) MOF-5_m (light microscope) [5]

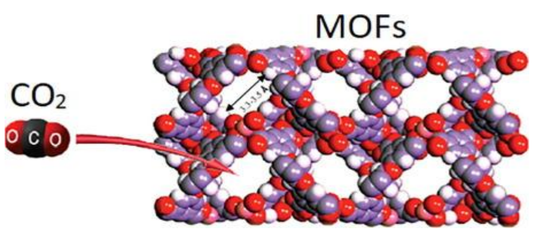

Figure 2: CO_2 adsorption mechanism in metal–organic frameworks (MOFs) [6]

Experimental investigation of CO_2 adsorption under varying operating conditions is often time-consuming, costly, and limited in its ability to systematically evaluate multiple interacting variables. While Zn-MOF-5 has demonstrated strong CO_2 adsorption potential, there is limited validated simulation-based analysis that simultaneously captures equilibrium behaviour, adsorption kinetics, and the combined effects of temperature, pressure, and flow rate.
This study addresses this gap by developing and validating a MATLAB–Excel simulation framework to model CO_2 adsorption on Zn-MOF-5 and to quantitatively evaluate the influence of key operating parameters on adsorption performance.

METHOD

CO_2 adsorption modelling was carried out using MATLAB for equilibrium and kinetic calculations, while Excel was used for regression and statistical analysis. Equilibrium adsorption was described using the Langmuir isotherm, which predicts the maximum adsorption capacity:

$$q_e = \frac{q_{sat}\, bP}{1+bP} \quad (1)$$

Adsorption kinetics were modelled using the Linear Driving Force (LDF) model, which describes the rate of CO_2 uptake by the adsorbent:

$$\frac{dq_t}{dt} = k_{LDF}(q_e - q_t) \quad (2)$$

with the integrated form:

$$q_t = q_e\left(1 - e^{-k_{LDF}t}\right) \quad (3)$$

The Langmuir and LDF models were implemented in MATLAB using iterative loops over the temperature–pressure range to generate equilibrium and transient adsorption data. This approach enabled evaluation of how temperature, pressure, and flow rate influence CO_2 adsorption behaviour on Zn-MOF-5.
MATLAB outputs were exported to Excel for regression and ANOVA analysis to quantify the effects of operating variables (temperature, pressure, and flow rate of 10–100 kmol/h) on adsorption performance. Statistical indicators such as R^2, Significance F, and p-values were used to validate the model and assess parameter significance.

Table 1: Simulation parameters

Parameter	Symbol	Value / Range
Temperature	T	280–320 K
Pressure	P	1–10 bar
Flow rate	F	10–100 kmol·h^{-1}
Maximum adsorption capacity	q_m	23 mmol·g^{-1}
Saturation capacity	q_{sat}	21.2 mmol·g^{-1}
Langmuir constant	b	1.0 × 10^{-6} Pa^{-1}
LDF mass transfer coefficient	$k_l df$	0.01 s^{-1}

RESULTS & DISCUSSION

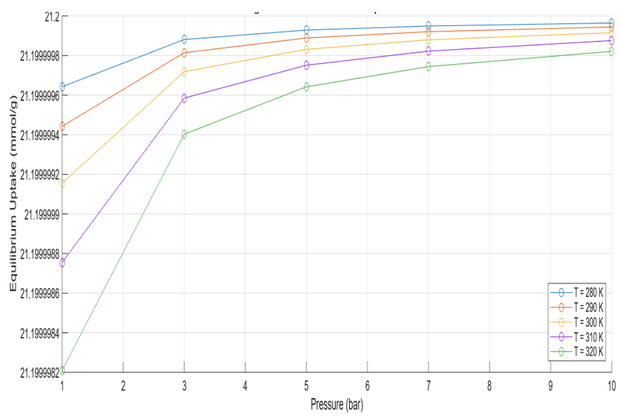

Figure 3: Langmuir Isotherm for CO_2 on MOF-5

CO_2 uptake increased with temperature from 280 to 320 K, contrary to equilibrium thermodynamic expectations for exothermic adsorption [8]. This behaviour indicates that kinetic effects dominated the process, as higher temperatures enhanced molecular mobility and mass transfer, leading to faster CO_2 uptake in the simulated system [9]. The results in Figure 4 highlight the importance of distinguishing between equilibrium-controlled and rate-controlled adsorption when interpreting simulation outcomes.

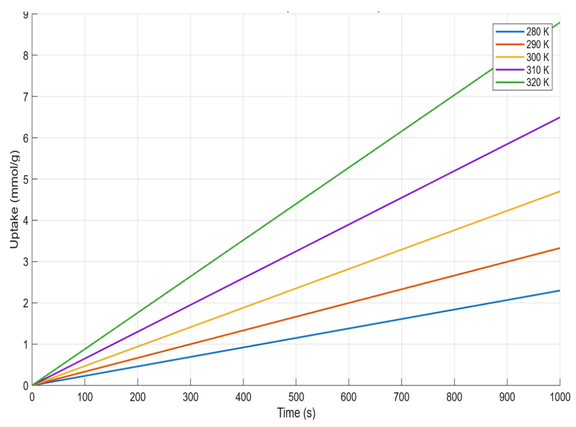

Figure 4: Temperature effect on CO2 adsorption

At constant temperature, CO_2 uptake increases with pressure and approaches a plateau, indicating Langmuir-type monolayer adsorption. Adsorption decreases with increasing temperature, confirming the exothermic nature of CO_2 adsorption on MOF-5. At higher pressures, saturation of adsorption sites occurs, leading to minimal changes in uptake. These trends in Figure 3 validate the suitability of the Langmuir model for describing CO_2 equilibrium adsorption on MOF-5 and are consistent with reported literature [7].

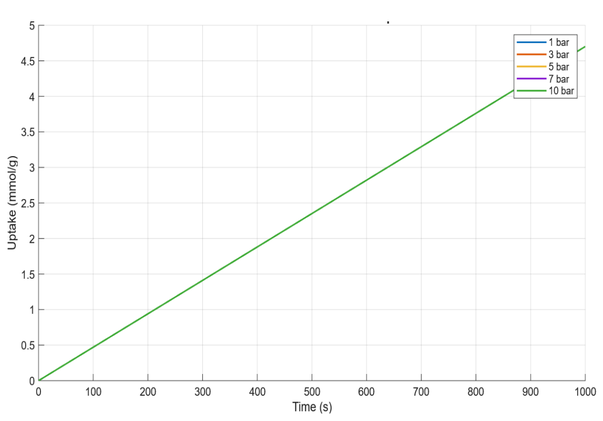

Figure 5: Effect of Pressure

CO_2 uptake in Figure 5 showed little variation across 1-10 bar, indicating low pressure sensitivity under the simulated conditions. Although Zn-MOF-5 typically exhibits increased adsorption with pressure [10], the observed trend suggests that kinetically limited adsorption is dominated by internal diffusion, with pressure effects potentially underestimated in simplified models [11].

The LDF kinetic profile in Figure 6 showed rapid CO_2 uptake within the first 200 s, followed by a gradual approach to equilibrium between 400–600 s. Beyond 600 s, adsorption plateaued at approximately 21.19 mmol·g^{-1}, indicating saturation of active sites and equilibrium adsorption under the studied conditions (10 bar, 300 K). This behaviour is consistent with LDF theory, where adsorption rate decreases as the driving force toward equilibrium diminishes.

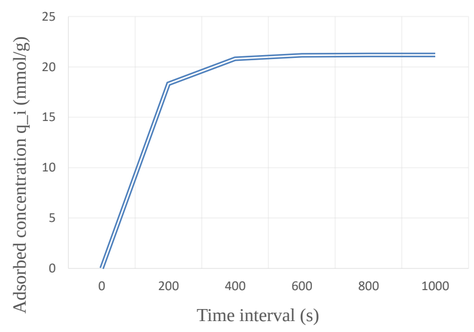

Figure 6: LDF evaluation of CO_2 adsorption using MOF-5

CONCLUSION

The simulation model successfully reproduced CO_2 adsorption behaviour on Zn-MOF-5, with a simulated uptake of 21.196 mmol·g^{-1}, deviating by only 0.59% from experimental data. Temperature was identified as the dominant parameter influencing adsorption, followed by pressure, while flow rate had negligible effect. The results confirm Zn-MOF-5 as an effective CO_2 adsorbent and demonstrate that MATLAB-based simulations combined with Excel validation provide a cost- and time-efficient approach for adsorption process modelling.

REFERENCES

[1] Yang, L., Xiao, Y., Chen, X., Zhang, W., Yang, X., Yang, H. and Fang, D., 2025. Research progress on CO_2 capture and catalytic conversion of metal–organic framework materials. *Catalysts*, 15(5), p.421. https://doi.org/10.3390/catal15050421
[2] Altintas, C., Avci, G., Daglar, H., Azar, A.N., Erucar, I. and Keskin, S., 2018. An extensive comparative analysis of MOFs for CO_2 capture using molecular simulations. *Energy & Environmental Science*, 11(1), pp.249–264.
[3] Wang, Z. and Zhou, T., 2025. Computer-aided metal–organic framework screening and design approaches toward efficient carbon capture processes. *Molecular Systems Design & Engineering*, Advance online publication. https://doi.org/10.1039/D5ME00075K
[4] Qasem, N.A.A., Ben-Mansour, R. and Habib, M.A., 2018. An efficient CO_2 adsorptive storage using MOF-5 and MOF-177. *Applied Energy*, 210, pp.317–326. https://doi.org/10.1016/j.apenergy.2017.11.011
[5] Hafizovic, J.; Bjørgen, M.; Olsbye, U.; Dietzel, P.D.C.; Bordiga, S.; Prestipino, C.; Lamberti, C.; Lillerud, K.P. The Inconsistency in Adsorption Properties and Powder XRD Data of MOF-5 Is Rationalized by Framework Interpenetration and the Presence of Organic and Inorganic Species in the Nanocavities. J. Am. Chem. Soc. 2007, 129, 3612–3620. https://doi.org/10.1021/ja0675447
[6] Ghanbari, T.; Abnisa, F.; Wan Daud, W.M.A. A Review on Production of Metal Organic Frameworks (MOF) for CO_2 Adsorption. Sci. Total Environ. 2020, 707, 135090. https://doi.org/10.1016/j.scitotenv.2019.135090
[7] Wang, J. and Guo, X., 2020. Adsorption isotherm models: Classification, physical meaning, application and solving method. *Chemosphere*, 258, p.127279. https://doi.org/10.1016/j.chemosphere.2020.127279
[8] Wang, J., Luo, J., Zhong, Z. and Borgna, A., 2020. CO_2 capture by solid adsorbents and their applications. *Energy & Environmental Science*, 4(1), pp.42–55.
[9] Gupta, M., Beniwal, V. and Singh, R., 2017. Kinetic modeling and breakthrough analysis for CO_2 adsorption in fixed-bed columns. *Journal of Environmental Chemical Engineering*, 5(5), pp.4824–4832.
[10] Saeed, R., Khan, M. and Bokhari, S., 2018. Pressure and temperature effects on CO_2 adsorption by metal–organic frameworks. *Microporous and Mesoporous Materials*, 272, pp.147–155.
[11] Zhao, L., Li, B. and Wang, T., 2021. Simulation of CO_2 adsorption dynamics in MOF-based systems. *Journal of CO_2 Utilization*, 48, p.101548.