



# Muthanna Journal of Engineering and Technology

## MJET

Submitted 25 August 2026, Accepted in revised form 25 Sept 2026, Published online 07

October 2026



## Rapid Pressure Swing Adsorption Unit Operation Optimization for Improved Biogas Purity

Hind Shabbani<sup>a</sup>

<sup>a</sup>Chemical Engineering Department, College of Engineering, University of AL Qadisiyah, Iraq  
Corresponding author E-mail: [hind.shabbani@qu.edu.iq](mailto:hind.shabbani@qu.edu.iq)

### Abstract

Biogas is an emerging energy source. This work focuses on purifying biogas from CO<sub>2</sub> utilizing modeled dynamic and rapid pressure swing adsorption RPSA mediated by ZnO@ZIF-8 composite. The model was validated against published literature showing validity of  $R^2=0.943$ . four parameters (Adsorption pressure, temperature, feed flowrate, and feed composition) were studied to investigate their effect on four responses (breakthrough time, adsorption capacity, asymmetry, and front velocities) across 30 simulative runs. Adsorption pressure was shown to be the most influential across the main studied responses. The breakthrough adsorption capacity and breakthrough time increased significantly from 5.76 to 29.79 mmol/g and from 218.4 to 1125.0 s, respectively, as the pressure increased from 1 to 8 bar. On the other hand, the saturation and stoichiometric front velocities dropped by 76.4 % and 78.5 %, respectively. Furthermore, the creation of sharper and more advantageous concentration fronts is suggested by the 44.7 % decrease in curve asymmetry, showing enhanced adsorption performance and mass-transfer characteristics at higher pressures. Minimal effect was shown by feed temperature on convective transport opposite to the feed flowrate. For the duration of 14 cycles the biogas showed enhanced purity of 76.76 % compared to the feed biogas purity of 50 %. This study shows the potential of breakthrough analysis as a useful tool for optimizing cycle conditions and pressure settings in RPSA and emphasizes the significance of balancing numerous response factors.

**Keywords:** biogas; unit operation; adsorption column; adsorbent composite; metal organic frameworks.

### 1. Introduction

Biogas is considered to be a promising carrier; however, the presence of carbon dioxide (CO<sub>2</sub>) in biomethane can adversely affects it heating value [1]. Added to that, the depleting CO<sub>2</sub> emissions from the climate seems to be the most important task [2]. For biogas produced from anaerobic digestion process it consists of approximately 40 % CO<sub>2</sub> [3].

In addition to being environmentally beneficial, adsorption technology is a low-energy method that effectively separates carbon dioxide. As a result, it has drawn a lot of attention lately for its uses in biogas upgrading and carbon capture and storage [3]. Recently, a lot of work has been done to develop sustainable sorbents for carbon capture, optimize the carbon dioxide adsorption process, and lower energy consumption, which in turn lowers operational costs. Zeolites, activated carbons, metal–organic frameworks, covalent organic frameworks, and silicates are only a few of the samples that have been produced for carbon capture and sequestration through the evolution of adsorbents [3]. To improve adsorption



This is an open access article under the terms of the Creative Commons Attribution License, which permits use, distribution and reproduction in any medium, provided the original work is properly cited. © 2025 The Authors

<https://www.muthuni-ojs.org/index.php/mjet/index>

performance, researchers have been actively examining a variety of mesoporous structures. By combining graphene and ZIF-8 to create a Graphene/ZIF-8 hybrid aerogel, for instance, a review reported hierarchical porous structure was created with the goal of increasing CO<sub>2</sub> adsorption efficiency by combining microporous and mesoporous characteristics [1]. ZIF-8 has been previously reported to achieve methane purity of 99.93 % under non-isothermal 4 step pressure swing adsorption process [4]. MODs ZIF-8 was also reported for its efficient CO<sub>2</sub> capture abilities and its promising ability to be deployed in on industrial scale [5].

The most effective adsorption performance can be obtained the breakthrough curve is as sharp as possible and hence understanding the curve dynamic behavior becomes important. Breakthrough and saturation times can't be predicted by the breakthrough models exactly due to asymptotic form of the breakthrough curve. Forecasting and creating fixed bed column utilizing mathematical models that help explain dynamic adsorption behaviors are essential for the process design [6]. There is a need for fast and straightforward techniques because the experimental determination of these thermodynamic functions is difficult and time-consuming. Methods that assess measured breakthrough curves are very appealing [7,4]. It was reported that a reduced mass transfer zone (MTZ) width for the concentration profile, which corresponds to the breakthrough profile, is indicative of a good adsorbent [2]. According to a literature, the adsorption stage needs to coincide with the mass-transfer zone's development. If adsorption is stopped too soon, bed capacity is wasted, and if it is continued too long, the adsorbed component may break through and contaminate the product [8]. A biomethane purity greater than 97 % was reported when utilizing pressure swing adsorption (PSA) with only limitations attributed to high energy demand of the compressor [9]. It was reported that dual stage pressure swing adsorption process performs better than single stage when tested for biomethane purification from CO<sub>2</sub> [10].

The use of short cycle times is referred to as rapid pressure swing adsorption RPSA. The processes consist of mainly two cycles fast high-pressure adsorption and depressurization to regenerate the adsorbent [11]. When the mass-transfer kinetics and valve response are quick enough, it also lowers the quantity of adsorbent needed for a given feed rate. However, shorter cycles are not always preferable. Fast cycles make it possible to employ adsorbents more frequently, which boosts productivity as long as the process's performance is unaffected. Additionally, this method works very well for modular separators and downsizing [12]. Dynamic simulation is consequently central to rapid-PSA design. It was also reported that simulated RPSA is suitable for achieving high ammonia purity for small scale productions and suggested future subtility for CO<sub>2</sub> capture [13].

This work will focus on the performance of dynamic breakthrough curves under four different operational conditions of adsorption pressure, feed flowrate, feed composition, feed temperature, and feed flowrate. The key responses investigated were the curve mass transfer asymmetry, breakout time, stoichiometric and front velocities. Furthermore, single bed rapid pressure swing adsorption process was investigated to elucidate the cyclic stability of the adsorbent sample. Although the ZnO@ZIF-8 sample showed promising separation performance in reported literature [1], however their dynamic breakthrough curve across systemically varied multi factors and their cyclic RPSA haven't previously reported. This work provides validated model that investigated the breakthrough curve responses under four different operating conditions and then extending the evaluation to cyclic RPSA operations to elucidate CH<sub>4</sub> purity and recovery which hasn't been reported previously for this adsorbent.

## 2. Simulation Section

The simulation model of mesoporous ZnO@ZIF-8 composites generated was validated against actual experimental values that are published previously in literature [1]. The validations conditions were provided in table 1.

After validation the effect of adsorption pressure, feed flowrate, feed temperature and feed composition on breakthrough time ( $t_b$ ), curve Asymmetry, dynamic breakthrough capacity ( $q_b$ ), and front velocities ( $v_{sat}$ ,  $v_{stoich}$ ) were calculated. 30 runs were investigated to study the effect of these parameters in the range shown in Table 1. The simulated column was of 15 cm height loaded with 600 mg of the adsorbent sample. It is important to distinguish between dynamic breakthrough capacity (the amount adsorbed at the moment effluent stream to the feed stream reaches 0.1), working capacity (referring to adsorbent loading at the adsorption conditions remaining after regeneration), and saturation capacity (the adsorbate equilibrium loading when the bed is fully saturated and in thermal equilibrium with the feed).

The choice of the 30 runs was based on central composite design to rather than selecting the runs manually to ensure unbiased and systematic investigation of the operation conditions. Centre composite design ensures the investigation since it captures linear and nonlinear curvatures. All the simulation models were performed using Aspen Adsorption V11. All the investigated conditions were varied around the experimental validated ranges. The feed flowrate was varied around the validated conditions to capture fast and slow superficial velocities relevant for rapid cycling operation. As for feed conditions the values were varied based on the validated operational conditions and the ranges of biogas feedstock from anaerobic digestion sources. While operational pressure tested was based on industrial compression range from ambient to standard industrial compressors. The feed temperatures are based on ambient to moderate temperatures typically encountered in biogas upgrading feed streams. Combined together these feed conditions ensure the chosen conditions are within the validated range while extending to cover practical RPSA implementation for biogas upgrading.

**Table 1:** Feed conditions of validation, and investigation model

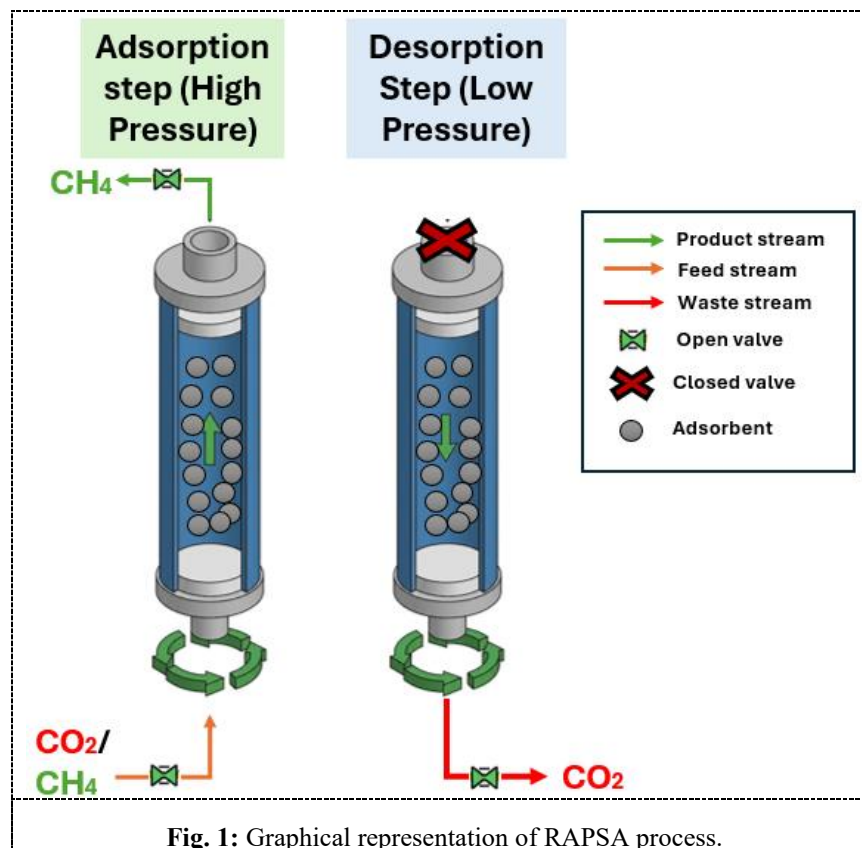
| Parameter | Feed flowrate (kmol/s)                  | Composition (v/v) | Feed Pressure (bar) | Temperature (K) | Type of study |
|-----------|-----------------------------------------|-------------------|---------------------|-----------------|---------------|
| Value     | $7.44 \times 10^{-9}$                   | 50:50             | 1                   | 298             | Validation    |
| Range     | $1.5 \times 10^{-8} - 6 \times 10^{-8}$ | 0.35-0.5          | 1-8                 | 298-323         | Investigation |

The parameters calculated, and model equations are provided in Table 2. The model assumes ideal gas behaviour, isothermal, and the axial dispersion is assumed to be in plug flow reactor with negligible dispersion coefficient (infinite Peclet number). Isotherms parameters of the validated model were best fit to Langmuir 1 pressure dependent. No reaction takes place within this process. Although the isothermal model is limited in terms of its release capture local thermal effects of temperature rise during adsorption due to heat release, it doesn't prevent global temperature dependence entering through equilibrium isotherm. The boundary conditions of the mathematical model were set at  $t=0$  the  $c_{CO_2}=0$ ,  $C_{CH_4}=1$ ; and at  $z=0$  the  $dc_i/dt$  term would equal zero.

**Table 2:** Utilized Equations

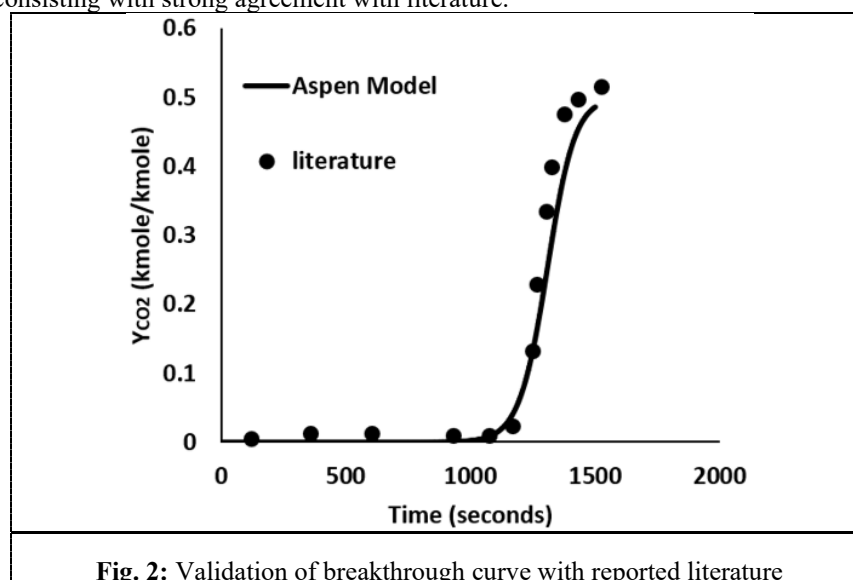
|                       | Equation       | Mathematical representation                                                                                                                                                                       | Ref. |
|-----------------------|----------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------|
| Material balance      | Total          | $\frac{d(vg C)}{dz} + [\epsilon b + (1 - \epsilon b)\epsilon p] \frac{dci}{dt} + p_s(1 - \epsilon b) \frac{dq}{dt} = 0$                                                                           | [8]  |
| Momentum              | Ergun equation | $\frac{\partial p}{\partial z} = -\left(\frac{1.5 \times 10^{-3} (1 - \epsilon_i)^2}{(2rp \psi)^2}\right) \mu vg + 1.75 \times 10^{-5} Mpg \frac{(1 - \epsilon_i)}{2rp^2 \psi \epsilon_i^3} vg^2$ |      |
| Isotherms             | Langmuir 1     | $q = q_m \frac{k_L P}{1 + k_L P}$                                                                                                                                                                 | [1]  |
| Asymmetry             | Clark model    | $\frac{c}{co} = [1 + A e^{-rt}]^{\frac{-1}{(n-1)}}$                                                                                                                                               | [6]  |
| The adsorption uptake | $q_b$          | $qb = \frac{co F}{w} \int_0^{tb} Cad dt$                                                                                                                                                          |      |

It is important to note that all the values of Langmuir isotherms and bed specifications are provided in the reported literature [1]. The values of physical characteristics are built-in in aspen adsorption physical property. Detailed calculations of the Clark model is available in supplementary materials. After the detailed analysis of the mentioned parameters earlier, a two steps rapid pressure swing adsorption (RPSA) was employed to investigate the adsorbent performance in terms of purity and recovery. the first step is the adsorption step and would last for 8 sec. followed by blowdown step that lasts until the pressure reaches 1.5 bar. The cyclic steady state was tested between cycle 13 and 14 ensuring a difference less than 1% difference in purity and recovery. Based on optimization analysis performed for the results the choice of feed conditions will depend on it. The graphical representation of the RPSA is presented in Fig. 1.



### 3. Results and discussion

Fig. 2 illustrates the validation experiment for adsorbent sample. The reported coefficient of determination was reported to be  $R^2 = 0.943$  showing consistency with the model presented. The mean absolute error (MAE) across the full data set was reported to be 0.0345, while the root mean square error (RSME) was 0.0488. the mean absolute percentage absolute error (MAPE) across the breakthrough region to be 23.8%. Breakthrough time error was quantified to show excellent agreement less than 1% relative error for both breakthrough and saturation times. A relative error of 3.7% was observed for the adsorption capacity consisting with strong agreement with literature.



To identify the dominant operating variables governing column performance, the linear correlation between each of the four design factors and the five breakthrough response variables was examined across all 30 experimental runs as illustrated in Fig. 3.

In line with the anticipated equilibrium relationship between adsorbate loading and partial pressure under a favourable isotherm, adsorption pressure emerged as the main factor influencing system behaviour, exhibiting a very strong positive association with breakthrough capacity. Local equilibrium between the fluid and adsorbent is reached instantly in a favourable isotherm system, resulting in a shock-like stoichiometric front whose position and the ensuing dynamic

adsorption capacity are directly controlled by the inlet partial pressure driving the equilibrium loading [2]. Although the response was clearly non-linear, increasing pressure from 1 to 8 bar increased breakthrough capacity by 417.6 % (from 5.76 to 29.79 mmol/g) and breakthrough time by 415.0 % (from 218.4 to 1125.0 s). Capacity increased by 264.6 % from 1 to 4.5 bar but only by 42.0 % from 4.5 to 8 bar, which is consistent with approaching isotherm saturation. Additionally, saturation and stoichiometric front velocities decreased by 76.4 % and 78.5 %, respectively, as the increased adsorption capacity slowed wavefront propagation. Due to gas law ( $PV=nRT$ ), the volumetric flowrate, and hence interstitial flowrate is reduced at increased pressure leading to increased breakthrough time and reduced front velocity. These results were reported at fixed flowrate and composition and only the pressure was changed.

Additionally, there was an inverse relationship between pressure and curve asymmetry, suggesting that although lower-pressure runs resulted in more dispersive, tailed profiles, higher operating pressures encourage sharper, more self-sharpening breakthrough fronts. Curve asymmetry dropped by 44.7 % (from 1.839 to 1.017) over the same pressure range, indicating a change from dispersive, tailed breakthrough fronts at low pressure to sharper, self-sharpening fronts at high pressure. For systems with favourable Type I isotherms, favourable Langmuir and Freundlich isotherms may initially broaden before rapidly achieving a constant-pattern front, an asymptotic shape in which the mass transfer zone remains constant with respect to both position and time. This constant-pattern behaviour has been extensively established theoretically and verified experimentally. While lower-pressure operation keeps the system closer to a less-favourable, more linear response, resulting in the broader, tailed profiles seen at 1 bar, pushing the system to higher pressure pushes it further into the strongly favourable region of the isotherm, further sharpening the front [14].

The coupling between capacity and front propagation speed suggested by fixed-bed mass-balance theory is further reflected in a moderately inverse relationship between pressure and both the saturation and stoichiometric front velocities. Since the adsorption isotherm, flow rate, mass transfer rate to the particles, and diffusion in the pores all affect the mass-transfer-zone breadth and shape, the stoichiometric front inevitably moves more slowly for a given feed rate as pressure increases capacity [2]. The interplay between convective mass transport and the lumped mass transfer resistance captured by linear driving force (LDF) is attributed to the pressure dependent change in the breakthrough curve. Sharp, narrow mass transfer zone, and more symmetric fronts observed in the as pressure increased due to that under LDF, the rate of adsorption is governed by the solid phase loading from local equilibrium where higher pressure leads to greater equilibrium driving force while lower pressures lead to broader mass transfer zone and more dispersive and tailed breakthrough profile.

The second most important factor was feed flowrate, which had a moderately negative relationship with breakthrough time, a moderately positive relationship with both front velocities, and almost no relationship with capacity. The feed flowrate decreased breakthrough time by 60.2 % and increased both  $v_{\text{sat}}$  and  $v_{\text{stoich}}$  by about 149 % when flowrate was increased from  $1.5 \times 10^{-8}$  to  $3.75 \times 10^{-8}$  kmol/s. Capacity changed by less than 1% (−0.6%), indicating that flowrate controls convective transport timing rather than equilibrium loading. Capacity increased by 28.6 % throughout the studied range ( $y_F = 0.35$ – $0.50$ ), with feed composition having a relatively minor impact. Capacity and breakthrough time each changed by less than 0.4 % over the entire 298–323 K range tested, suggesting that thermal effects on adsorption equilibrium and mass transfer were essentially insignificant in comparison to the dominant influence of pressure and flowrate. Feed temperature had a negligible effect on all responses. This is consistent with flowrate controlling convective transport timing rather than equilibrium loading, a distinction that has been emphasized in recent correlation-based studies of PSA operating variables [12].

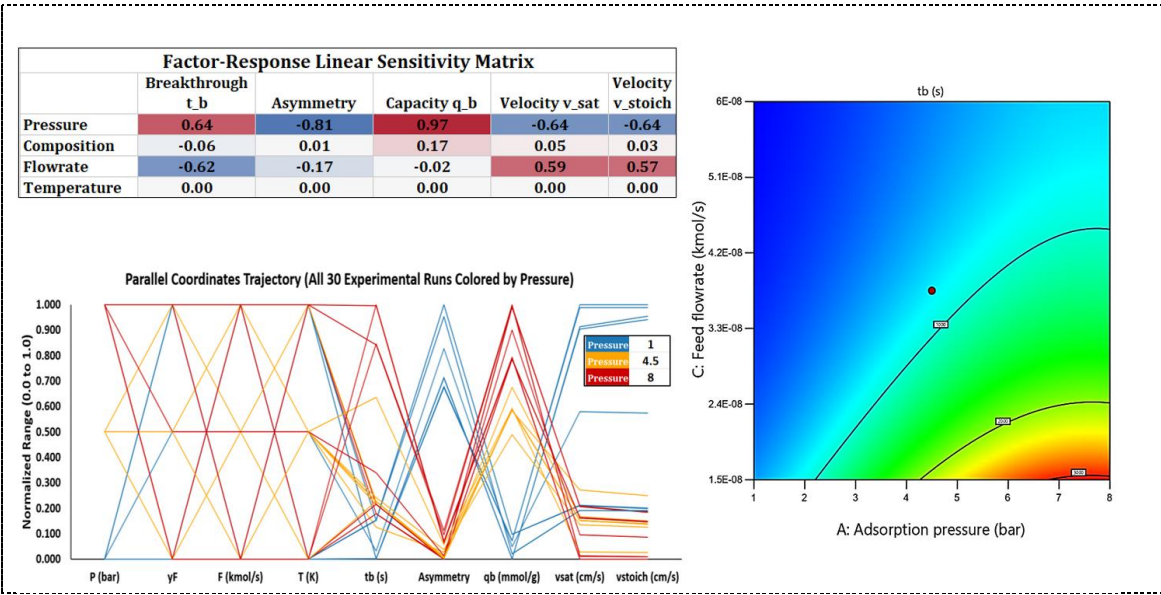
Since equilibrium loading is ultimately determined by the adsorbate partial pressure (composition  $\times$  total pressure) and an eight-fold swing in total pressure dominates a modest 0.35–0.50 swing in mole fraction, feed composition, on the other hand, showed only weak relationships with all responses. This is likely due to the relatively narrow range explored (0.35–0.50 mole fraction) in comparison to the eight-fold variation in pressure.

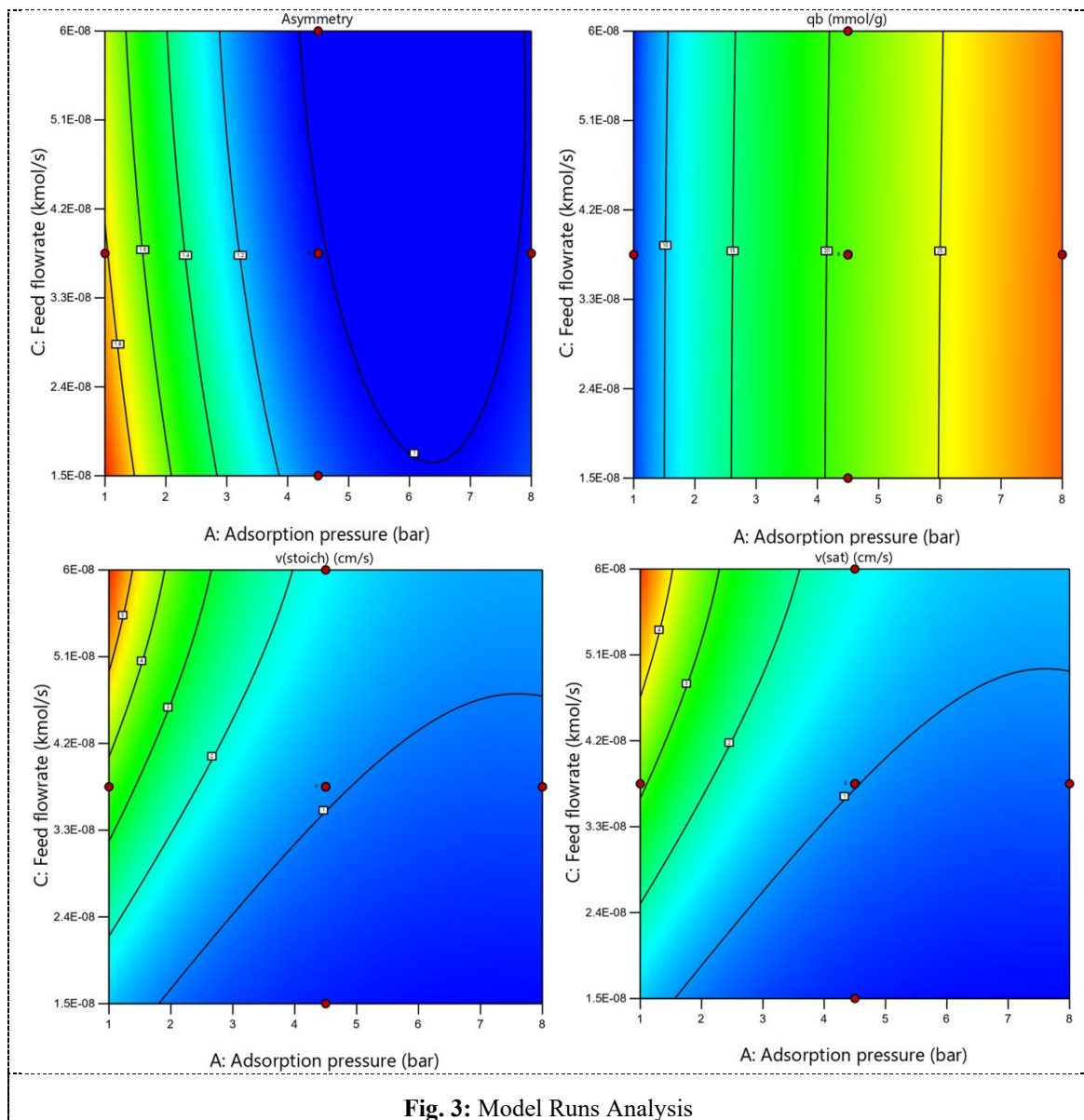
Opposite to the major effect of the adsorption pressure and feed flowrate, the feed temperature showed negligible effect across all reprocesses which is consistent with the model assumption of being isothermal. It is important to highlight that in the current study the insensitivity to feed temperature can be attributed to the isothermal model assumptions. However, it is important to note that in RAPSAs the adsorption step is very rapid and hence reducing the residence time available for heat propagation of the exothermic nature of the adsorption process. Added to that increased complexity would be associated with non-isothermal assumption. A summary of the pressure and flowrate on the reported responses is illustrated in Table 3.

**Table 3:** Effect of pressure and feed flowrate on breakthrough performance at 0.452 feed  $\text{CO}_2$  feed composition and 310.5 K.

| Factor         | value | tb (s) | Asymetry | qb (mmol/g) | $V_{\text{sat}}$ (cm/s) | $V_{\text{stoich}}$ (cm/s) |
|----------------|-------|--------|----------|-------------|-------------------------|----------------------------|
| Pressure (bar) | 1     | 218.4  | 1.839    | 5.76        | 3.14                    | 3.63                       |
|                | 8     | 1125.0 | 1.017    | 29.79       | 0.74                    | 0.78                       |

|                                                |     |        |       |       |      |      |
|------------------------------------------------|-----|--------|-------|-------|------|------|
| Feed Flowrate<br>× 10 <sup>8</sup><br>(kmol/s) | 1.5 | 1995.3 | 1.061 | 21.12 | 0.41 | 0.43 |
|                                                | 6   | 492.7  | 1.032 | 20.85 | 1.62 | 1.74 |





**Fig. 3: Model Runs Analysis**

The biomethane purity increased from 71.20 mol % to 76.76 mol % when increasing the pressure from 3 to 8 bar. This is consistent with previous data that showed that higher operating pressures had higher adsorption capacity  $q_b$  (approximately 6.4 mmol/g at 3 bars compared to 32.4 mmol/g at 8 bars). Also, the curves asymmetry and the sharpness of the mass transfer fronts was reduced at lower pressure at a value of approximately 3.01 compared to almost perfect asymmetry of 1 at 8 bars. The improved heavy retention of the adsorbent inhibits early slide into the raffinate stream and postpones  $\text{CO}_2$  breakthrough. It is important to note that these adsorption capacities are under different conditions of the values reported for the breakthrough investigation (5.76–29.79 mmol/g) which was obtained at reference centre point of flowrate of  $3.75 \times 10^{-8}$  kmol/s and feed composition of 0.425.

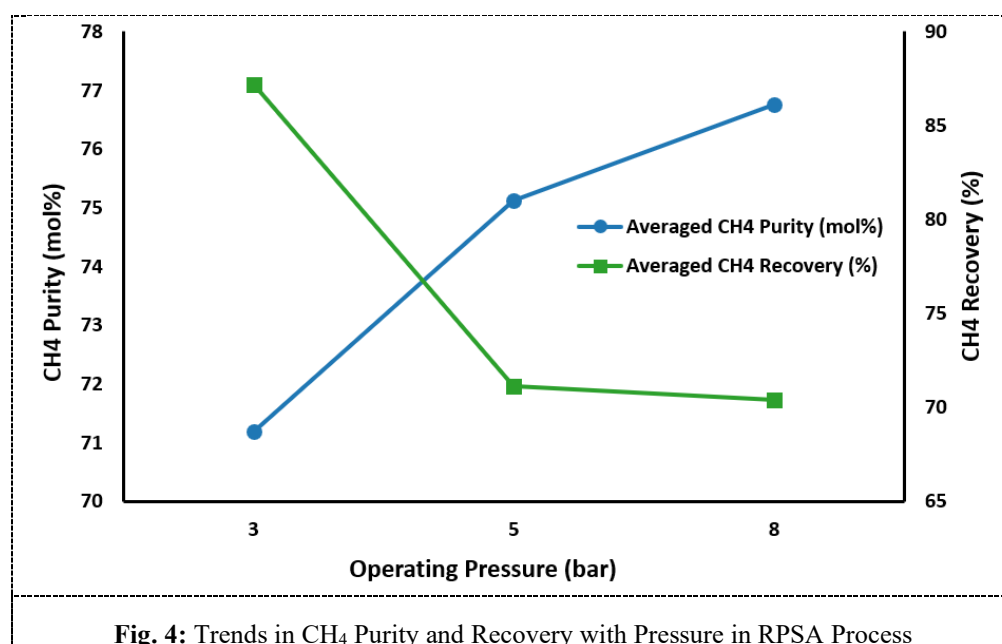
A trade-off to improved purity at higher pressures is reduced recovery. The biomethane recovery reduced from 87.16 % at 3 bars to 70.41 % at 8 bars. This is attributed to those higher operating pressures traps large inventory of undesorbed gas within the bed void space and encourages co-adsorption of the light component and causing the biomethane losses in the subsequent step of depressurization. This is a typical inverse relationship between purity and recovery inherent of the RAPSA process.

Since RAPSA is designed around short cycle times with cycle time in the range of 6-20 seconds, the adsorbent with high working capacity, quick and fast fronts are crucial characteristics of the adsorbent for process implementation. Reduced cycle time is essential for lowered system footprint, capital and operational cost. Optimizing RAPSA capacity, front sharpness, and cycle timing are hence essential [15,16]. An adsorption time of 8 seconds is consistent with prior reported RAPSA process times laying toward the lower end of the time window of 6-12 second reported earlier [15,16]. An 8 s time provides the benefits of a short adsorption time preserving low footprint, capital cost and high throughput. Added to that this time is sufficiently long than allows fast kinetics adsorption and sharp wavefronts characteristic achieving the meaningful working capacity utilization before breakthrough.

Although current results showing increased fronts at lower pressures (1 bar), lower pressures should be avoided for RAPSA since the adsorption capacity would be lowered by 75-80 %. Added to that dispersive fronts are also notable in lower pressure where the asymmetry increases substantially to value greater than 1.7. This will lead to reduced product purity and cycle efficiency. Although the results showed the best performance on high pressure of 8 bar, moderate pressures of 3, and 5 bars will be investigated for low-cost operational cost consideration without reaching the high-end target. Since the front sharpness at 4.5 bar and doesn't change significantly beyond the choice of the middle ranges and the majority of the sharpening effect is captured well before reaching 8 bar, the difference between moderate and large pressure values shouldn't change the results significantly and the asymmetry is expected to remain linear and ideal. Since RAPSA is a cyclic process, cumulative energy or wear penalty across the 14 cycles will compile over the continuous operation. Although the moderate ranges will be expected to show lower purity there would be a trade-off of maximum reduction in the demand of the compression energy demand and mechanical stress on valves seal since the compression work scales with the pressure ratio.

Fig. 4 shows biomethane purity and recovery utilizing RAPSA. The equilibrium mass transfer dynamics shown the breakthrough curve analysis is showing consistency and physical compatibility with the obtained purity of the 14 cycles of RAPSA runs. The biomethane purity increased from 71.20 mol % to 76.76 mol % when increasing the pressure from 3 to 8 bar. this considers with previous data that showed that higher operating pressures had higher adsorption capacity  $q_b$  (approximately 6.4 mmol/g at 3 bars compared to 32.4 mmol/g at 8 bars. Also, the curve's asymmetry and the sharpness of the mass transfer fronts was reduced at lower pressure at a value of approximately 3.01 compared to almost perfect (equals 1) asymmetry of 1 at 8 bars. The improved heavy retention of the adsorbent inhibits early slip into the raffinate stream and postpones  $\text{CO}_2$  breakthrough.

A trade-off to improved purity at higher pressures is reduced recovery. The biomethane recovery reduced from 87.16 % at 3 bars to 70.41 % at 8 bars. The 5.5 % increased purity when switching from 3 to 5 bars incurs larger decreased recovery of 18.4 % corresponding to the marginal trade off trend. On the other hand, increasing the pressure further to 8 bar results in 2.2 % while recovery declined only by 1 %. This indicates that most of the trade-off is mostly relevant at lower pressures while higher operating conditions showed a favourable balance achieving higher purity with minimal recovery losses. This is attributed to those higher operating pressures traps large inventory of undesorbed gas within the bed void space and encourages co-adsorption of the light component and causing the biomethane losses in the subsequent step of depressurization. This is a typical inverse relationship between purity and recovery inherent of the RAPSA process. Table 4 illustrates the summarized trends observed in purity and recovery.



**Table 4: CH<sub>4</sub> purity and recovery under different operating pressures.**

| Pressure (bar) | CH <sub>4</sub> Purity (%) | Purity trend | CH <sub>4</sub> recovery (%) | Recovery trend | Specific energy consumption (kJ/mol CH <sub>4</sub> recovered) | Specific energy consumption |
|----------------|----------------------------|--------------|------------------------------|----------------|----------------------------------------------------------------|-----------------------------|
| 3              | 71.20                      |              | 87.16                        |                |                                                                |                             |
| 5              | 75.16                      |              | 68.72                        |                |                                                                |                             |
| 8              | 76.76                      |              | 70.41                        |                |                                                                |                             |

|   |        |   |       |   |       |       |
|---|--------|---|-------|---|-------|-------|
| 3 | 71.197 | ↓ | 87.16 | ↑ | 7.59  | 0.094 |
| 5 | 75.13  | ↑ | 71.15 | ↓ | 13.58 | 0.168 |
| 8 | 76.76  | ↑ | 70.41 | ↓ | 18.79 | 0.233 |

The limitations associated with this research is related to the scale of the lab scale of the study and future research should delve into scaled study. Furthermore, a full overall RAPSA performance should be investigated for the operational conditions. Current work doesn't have a cost and energy analysis which could be important for future research.

#### 4. Conclusion

A ZnO@ZIF-8 composite was assessed utilizing modeled fixed bed adsorption bed. The model was validated with reported literature showing  $R^2$  of 0.943. the operational requirement of RAPSA can be connected with the breakthrough curve performance. Among the other factors investigated the pressure seemed to show the major effect on the curve duration. increasing the pressure from 1 to 8 bar leads to increased breakthrough time from 218.4 to 1125 seconds respectively. The dynamic adsorption capacity was also increased from 5.76 to 29.79 mmol/g under similar conditions. Similarly, the asymmetry reduced from 1.839 to 1.017. the higher stoichiometric and saturation velocities were higher at lower pressures. These results show that increased pressure promotes higher adsorbate uptake and sharper concentrations fronts. Increased flow rates led to decreased breakthrough time and increased front velocities. This is attributed to the concentration fronts and propagation are mainly affected by the feed flowrate. On the other hand, feed concentration and temperature had insignificant effects due to narrow range of the selected range and isothermal assumption. The RAPSA validated the findings of the dynamic breakthrough studies. However, a future overall performance criterion should be used to identify the optimum operating pressure for RAPSA. The purity reduced from 76.76 mol % at 8 bars to 71.20 mol % at 3 bars. This result shows that the adsorption capacity by itself can't determine optimal RAPSA conditions rather than sufficient working capacity, stable and sharp mass transfer front are necessary as well.

#### Nomenclature

| Symbol  | Description                           |
|---------|---------------------------------------|
| $r_p$   | Particle radius (m)                   |
| A, r, n | Clark model constants                 |
| $q_m$   | Langmuir saturation capacity (mmol/g) |
| $K_L$   | Langmuir isotherm constant (1/bar)    |
| $q_b$   | Breakthrough capacity                 |
| Co      | Feed composition                      |
| C       | Composition at time t                 |
| $p_s$   | Solid velocity (kg/m <sup>3</sup> )   |
| $p_g$   | Gas velocity (kg/m <sup>3</sup> )     |
| $v_g$   | Gas velocity (m/s)                    |
| M       | Mean molecular weight (kg/kmol)       |
| $\mu$   | Gas phase dynamic viscosity (kg/m.s)  |
| $\psi$  | Shape factor                          |

#### References

- [1] M. Essid et al., "One-step synthesis of mesoporous ZnO@ZIF-8 composites for CO<sub>2</sub>, CH<sub>4</sub>, N<sub>2</sub> adsorption and separation with potential application for industrial biogas," *J. Alloys Compd.*, vol. 1032, Jun. 2025, doi: 10.1016/j.jallcom.2025.181123.
- [2] M. K. Al Mesfer, M. Danish, M. I. Khan, I. H. Ali, M. Hasan, and A. El Jery, "Continuous fixed bed co<sub>2</sub> adsorption: Breakthrough, column efficiency, mass transfer zone," *Processes*, vol. 8, no. 10, pp. 1–16, Oct. 2020, doi: 10.3390/pr8101233.
- [3] M. Karimi, M. Shirzad, J. A. C. Silva, and A. E. Rodrigues, "Carbon dioxide separation and capture by adsorption: a review," *Environ. Chem. Lett.*, vol. 21, no. 4, pp. 2041–2084, 2023, doi: 10.1007/s10311-023-01589-z.
- [4] A. A. Abd, J. Kim, D. J. Jasim, and M. R. Othman, "Production of green methane by carbon dioxide capture from landfill biogas via pressure swing adsorption mediated by MOF ZIF-8," *Energy Convers. Manag.*, vol. 321, Dec. 2024, doi: 10.1016/j.enconman.2024.119090.
- [5] A. Farrukh et al., "ZIF-8 based materials for CO<sub>2</sub> capture: synthesis, functionalization, and adsorption performance," *Coord. Chem. Rev.*, vol. 563, art. no. 218015, Sep. 2026, doi: 10.1016/j.ccr.2026.218015.

- [6] Q. Hu, Y. Xie, and Z. Zhang, "Modification of breakthrough models in a continuous-flow fixed-bed column: Mathematical characteristics of breakthrough curves and rate profiles," *Sep. Purif. Technol.*, vol. 238, May 2020, doi: 10.1016/j.seppur.2019.116399.
- [7] S. Zarei, I. Harriehausen, J. W. Lee, and A. Seidel-Morgenstern, "Equilibrium loadings and adsorption isotherm model parameters estimated from multi-component breakthrough curves," *Adsorption*, vol. 30, no. 8, pp. 2295–2312, Dec. 2024, doi: 10.1007/s10450-024-00549-5.
- [8] Y. Chen and Y. Hu, "Aspen Adsorption simulation breakthrough curve to determine adsorption time in CH<sub>4</sub>/N<sub>2</sub> adsorption separation by activated carbon," *J. Taiwan Inst. Chem. Eng.*, vol. 171, Jun. 2025, doi: 10.1016/j.jtice.2025.106065.
- [9] S. Ganesan, R. L. S. Canevesi, and C. A. Grande, "Simplified and cost-effective pressure swing adsorption system for simultaneous production of bio-methane & biogenic CO<sub>2</sub> from biogas," *Energy Convers. Manag.*, vol. 325, Feb. 2025, doi: 10.1016/j.enconman.2024.119398.
- [10] S. Ganesan, R. L. S. Canevesi, and C. A. Grande, "Pressure Swing Adsorption Configurations for Simultaneous Production of High-Purity Biomethane and Carbon Dioxide from Biogas," *Ind. Eng. Chem. Res.*, vol. 63, no. 43, pp. 18497–18512, Oct. 2024, doi: 10.1021/acs.iecr.4c01555.
- [11] B. H. L. Betlem, R. W. M. Gotink, and H. Bosch, "Optimal operation of rapid pressure swing adsorption with slop recycling," *Comput. Chem. Eng.*, vol. 22, Suppl. 1, pp. S633–S636, 1998.
- [12] X. Zhu and X. Wang, "Experimental study of a rotary valve multi-bed rapid cycle pressure swing adsorption process based medical oxygen concentrator," *Adsorption*, vol. 26, no. 8, pp. 1267–1274, Nov. 2020, doi: 10.1007/s10450-020-00240-5.
- [13] B. Lin, I.-M. Hsieh, and M. Malmali, "Rapid pressure swing adsorption for small scale ammonia separation: A proof-of-concept," *J. Adv. Manuf. Process.*, vol. 3, no. 2, art. no. e10077, 2021, doi: 10.1002/amp2.10077.
- [14] J. C. Knox, A. D. Ebner, M. D. Levan, R. F. Coker, and J. A. Ritter, "Limitations of Breakthrough Curve Analysis in Fixed-Bed Adsorption," *Ind. Eng. Chem. Res.*, vol. 55, no. 16, pp. 4734–4748, Apr. 2016, doi: 10.1021/acs.iecr.6b00516.
- [15] D. A. Chisăliță, J. Boon, and L. Lücking, "Adsorbent shaping as enabler for intensified pressure swing adsorption (PSA): A critical review," Jan. 19, 2025, Elsevier B.V. doi: 10.1016/j.seppur.2024.128466.
- [16] S. Sircar and B. E. Hanley, "Production of oxygen enriched air by rapid pressure swing adsorption," 1995.