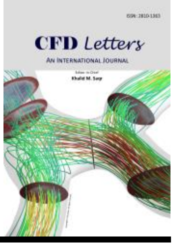

CFD Letters

Journal homepage:
https://semarakilmu.com.my/journals/index.php/CFD_Letters/index
ISSN: 2180-1363

CFD Simulation of CO_2 and Methane Adsorption at Various Temperature for MOF-5 using Dual-site and Single-site Langmuir Model

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ARTICLE INFO

Article history:
Received 14 August 2021
Received in revised form 13 September 2021
Accepted 14 September 2021
Available online 31 October 2021

Keywords:
CFD; carbon capture; temperature swing adsorption; MOF-5

ABSTRACT

The annual increase in energy demand has led to an increase in greenhouse gas emissions, in particular CO_2 emissions from the power generation industry. Carbon Capture and Utilization are technologies applied to capture CO_2 gases and transform the gases into a different energy source. The adsorption technology to capture CO_2 gases was chosen due to the minimum energy consumption and low costs required for an industrial application for sustainability. Metal-Organic Framework (MOF) has a reasonably high CO_2 adsorption capability. It has been applied as an adsorbent for capturing and storing CO_2. In this study, a comparison of CFD simulation with experimental CO_2 and methane adsorption values in solid adsorbent beds containing MOF-5 at various temperatures was presented. The simulation was performed using 2D and 3D models from 0℃ at STP to 130℃ for CO_2 and methane gas molecules. In addition, the isothermal and kinetic adsorption model was added to the simulations. This includes Single- and Dual-Site Langmuir adsorption isotherm and Linear Driving Force. The porous media model was then activated to imitate packed bed adsorbent and measured the pressure drop from the simulation. The results showed that the CO_2 adsorption values of MOF-5 decrease as the adsorbent temperature increases. There was a decline of 0.002 mmol/g of adsorbed CO_2 molecules per 10-kelvin difference. The CO_2 adsorption value was 0.53 mmol/g at STP and 1.15 mmol/g for CH4 at STP. Both CO_2 and CH4 adsorption were used to suggest optimal CO_2 adsorption for the Pressure Swing Adsorption cycle.

1. Introduction

The growing demand for energy from various industries has negative impacts on the world. Most energy production is based on fossil fuels such as coal, gas and oil which caused excessive greenhouse gases emitted such as carbon dioxide, methane, carbon monoxide, and other harmful substances. Global temperature has also risen by approximately 0.74% over the last 100 years and is expected to

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https://doi.org/10.37934/cfdl.13.10.110

rise by 6.4% by the end of the century. However, an international initiative to mitigate the issue was taken in the Paris agreement to strengthen the global response to maintain the below 2℃ global temperature rise for this century [1].

Since most carbon dioxide gases were the major contributor to greenhouse gases [2]. Carbon Capture and Utilization (CCU) methods have been considered the best option to reduce CO_2 gas emissions mainly caused by industrial power plants. Besides saving the environment from climate change, this method also contributes to economic gains by profiting from selling CO_2 gases for other uses. Adsorption is one of the processes of gas separation method to capture and store the emitted gases by adhering gas molecules to the surface of the adsorbents. Selecting suitable adsorbent materials is essential to maintain the maximum efficiency of CO_2 adsorption. An adsorbent with a high surface area Metal Organic Framework (MOF), is one of the most used adsorbents for the gas adsorption process. MOF-5 was chosen in this study due to its extensive research into gas adsorption processes [3].

Numerous experiments and simulations were conducted to investigate various methods for improving CO_2 storage [4–9]. Despite abundance of studies in CO_2 adsorption, there is still gap in explaining the effects of temperature in CO_2 adsorption in MOF-5. Therefore, the purpose of this study was to simulate the CO_2 and methane adsorption in solid sorbent beds containing MOF-5 at various temperatures. In this study, a CFD simulation method was conducted to measure CO_2 adsorption for MOF-5 at various gas inlet temperatures. The findings provide insight into the modelling of the dynamic adsorption process in a fixed bed [10–12]. This study is important as there are lack of study on MOF-5 adsorption in packed bed using simulation approach and to study the effects of temperature on CO_2 and CH_4 adsorption amount.

2. Methodology

2.1 Model Geometry

The 2D and 3D physical model for simulation was developed with the help of a design modeller, an application embedded in the ANSYS Fluent. Meanwhile, a plug flow model was used to model the adsorption bed to forecast the dynamic behaviour of an adsorption process [13]. As part of this study, the length of the cylinder is 70mm and its diameter is 4mm. The 2D and 3D design for the fixed bed adsorption model is illustrated in Figure 1 and 2, respectively. Similar geometrical model was widely used to measure the adsorption inside a packed bed reactor and achieved similar result with experimental study [14–18].

Fig. 1. Model of 2D adsorbent bed used for CFD simulation

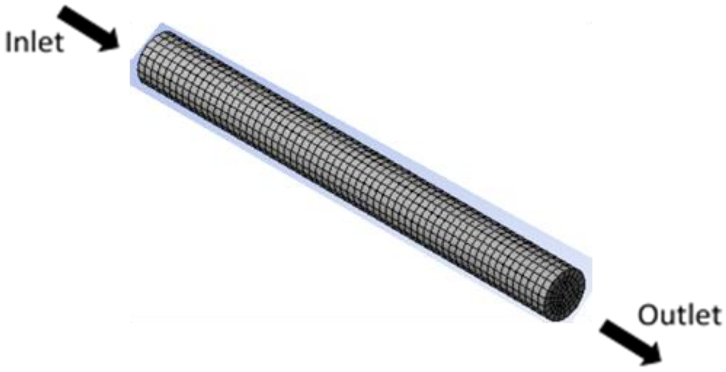


Fig. 2. Model of 2D adsorbent bed used for CFD simulation

2.2 Governing Equations

The mass, momentum and energy conservation equation were determined within ANSYS Fluent to predict the hydrodynamic behaviour of fluids within the adsorption column. The amount of adsorption was determined from the adsorption isotherm from the experimental value carried out for CO_2 and CH_4 adsorption. The inlet of CO_2/CH_4 was set from 0 to 1.3 bar. The adsorption isotherm and kinetic models were written in expression.

2.2.1 Gases mass balance equation

The mass continuity equation for the fixed bed adsorption column is shown in Eq. (1) [19,20].

$$-D_{z,i}\frac{\partial^2 C_i}{\partial x_i^2}+\frac{\partial u_i C}{\partial x_i}+\frac{\partial C_i}{\partial t}+\left[\frac{1-\varepsilon}{\varepsilon}\right]\frac{\partial q_i}{\partial t}=0 \tag{1}$$

Here, $D_{z,i}$ is the column 3D dispersion coefficient at depth z(m), C_i is the inlet concentration (kg m^{-3}), C is the bed concentration (kg m^{-3}), u is the gas velocity in x-direction (m sec^{-1}), t is time, ε is bed voidage fraction or porosity, and q_i is the adsorbent capacity.

The momentum balance for this study was referred to general momentum equation for porous media using Darcy's Law equation where $\vec{v}$ is the velocity vector (m s^{-1}), ρ is the gas density, P is the operating pressure (Pa), $\bar{\bar{\tau}}$ is the stress tensor (N m^{-2}), $\vec{g}$ is the gravity acceleration vector, and S is the momentum source term in porous media in (N m^{-3}).

$$\varepsilon\frac{\partial(\rho\vec{v})}{\partial t}+\nabla.(\rho\vec{v}\vec{v})=-\nabla P+\nabla\bar{\bar{\tau}}+\rho\vec{g}+S \tag{2}$$

$$S_i=-\left(\frac{\mu}{K}v_i+C_2\frac{1}{2}\rho|\vec{v}|v_i\right) \tag{3}$$

Ergun equations was applied to calculated the component of i -direction including viscous and inertial resistances as shown in Eq. (3). μ is the gas dynamic viscosity (Pa s), $\frac{1}{K}$ is the porous media viscous resistance (m^{-2}), C_2 is the inertial resistance (m^{-1}), $|\vec{v}|$ is the modulus value of the velocity vector, $v_i$is the velocity magnitude in i-direction.

2.2.2 Energy balance equation

The CO_2 separation energy equation shows the balance between the energy in the adsorbent bed and the energy transition of convective flow, and the energy emitted by the adsorption bed where $\rho_g$is the fluid density, $C_{pg}$is the specific heat capacity, $\Delta H_i$is the heat of adsorption [8,9].

$$\rho_g C_{pg} \frac{\partial T}{\partial z} - K_L \frac{\partial^2 T}{\partial Z^2} + \varepsilon \rho_g C_{pg} \left(u \frac{\partial T}{\partial z} \right) = -\rho_B (\Delta H_i) x \sum_{i=1}^{n} \frac{\partial q_i}{\partial t} \tag{4}$$

Based on Eq. (1) the adsorption rate for bulk flow is based on the Linear Driving Force (LDF) model as shown in Eq. (5) [21]. Where, $C_i^{pellet}$is the pellet concentration (kg m^{-3}), C_B is bulk concentration, k_i is the average mass transfer for each species, and a is the surface area of pellet per volume of bed.

$$\rho_s \partial q_i / \partial t = \left(C_B - C_i^{pellet} \right) * k_i a \tag{5}$$

For transient analysis of adsorption column data, The LDF was frequently applied because it is simple and physically consistent [10,22]. Based on Eq. (5) C_i^{pellet} is the pellet concentration (kg m^{-3}), C_b is the bulk concentration (kg m^{-3}), a is the surface area of pellet per volume of bed.

2.2.3 Dual site Langmuir model

$$q^* = (q_{m1}\, K_{eq1}\, P/1 + K_{eq1}\, P) + (q_{m2} K_{eq2} P/1 + K_{eq2}\, P) \tag{6}$$

Dual site Langmuir model was studied back in the early 1992 to express the concept of multilayer adsorption. The idea of one-site occupancy adsorption overlooks the influence of an adsorbate molecule's chemical structure on its mode of adsorption, instead relying on a single adsorption energy averaged over all possible sites of an adsorbed molecule [23]. The dual site Langmuir adsorption was developed to explain observed and absolute energy of adsorption at a high pressure at assume that the values of the adsorbed phase varies continually with the number of adsorbed molecules [24]. Based on the Dual site Langmuir model, q_{m1} (mmol g^{-1}) Equilibrium adsorption uptake for the first site, q_{m2} (mmol g^{-1}) Maximum adsorption uptake for the second site, and P (Pa) is the current pressure. Meanwhile, K_{eq} were denoted as follows

$$K_{eq,i} = \ k_0 exp^{-(\Delta H/RT)} \tag{7}$$

K_{eq} (Pa^{-1}) is the adsorption isotherm constant, while K_0 (Pa^{-1}) is the temperature-independent constant, ΔH (J mol−1) Heat of adsorption, R (J mol^{-1} K^{-1}) Universal gas constant, and T(K) current temperature.

A specific boundary condition was set to obtain high accuracy of the simulation, and the properties were defined by referring to the previous study [4]. The density for the stainless steel was set as 7941 kgm^{-3} and k value as 15.14 $Wm^{-1}k^{-1}$. The effects of CO_2 with the stainless-steel wall were taken as polynomial functions of temperature. The gas mixture density was calculated using the ideal gas law. The thermal heat capacity was estimated from the mixing law, and the thermal conductivity and viscosity were evaluated from the mass-weighted mixing law. Table 1 shows the thermal properties used to simulate the properties of CO_2. The following equations describe the thermal properties of a single gas.

$$C_{p,i} = A_{cp} + B_{cp}T + C_{cp}T^2 + D_{cp}T^3 + E_{cp}T^3 (Jkg^{-1}K^{-1}) \quad (8)$$

$$k_i = A_k + B_kT + C_kT^2 + D_kT^3 + E_kT^3 (Wm^{-1}K^{-1}) \quad (9)$$

$$\mu_i = A_\mu + B_\mu T + C_\mu T^2 + D_\mu T^3 + E_\mu T^3 (Pas) \quad (10)$$

Table 1
Thermal properties for CO_2

Thermal Properties	Constant Cp equation	Constant of k equation	Constant of μ equation
CO_2	A_k = 491.702	A_k = - 0.00694154	A_μ = -1.1 x 10^{-6}
	B_k= 1.43603	B_k = 7.53746 x 10^{-5}	B_μ = 5.89863 x 10^{-8}
	C_k= - 0.0007742	C_k = 7.53746 x 10^{-5}	C_μ = -1.74847 x 10^{-11}
	D_k = 0	D_k = 0	D_μ = 0
	E_k = 0	E_k = 0	E_μ = 0

The determination of q_m, maximum equilibrium adsorption and K_{eq}, adsorption isotherm constant was done using experimental fittings [25]. Two adsorption models were compared by fitting the breakthrough experimental adsorption isotherm using single-site Langmuir and dual-site Langmuir models, as shown in Figure 3 and 4. The different between both models are single site Langmuir model is limited to analysing the adsorption energy for each local chemistry and structure which is different for each site. The experimental adsorption isotherm was gained from gas sorption analyser data plotting. MOF-5 was used in this study due to its widely research in gases storage field and excellent structure properties. In addition, MOF-5 is suitable for different types of gases adsorption such as carbon dioxide, hydrogen, and other gases[6,26]

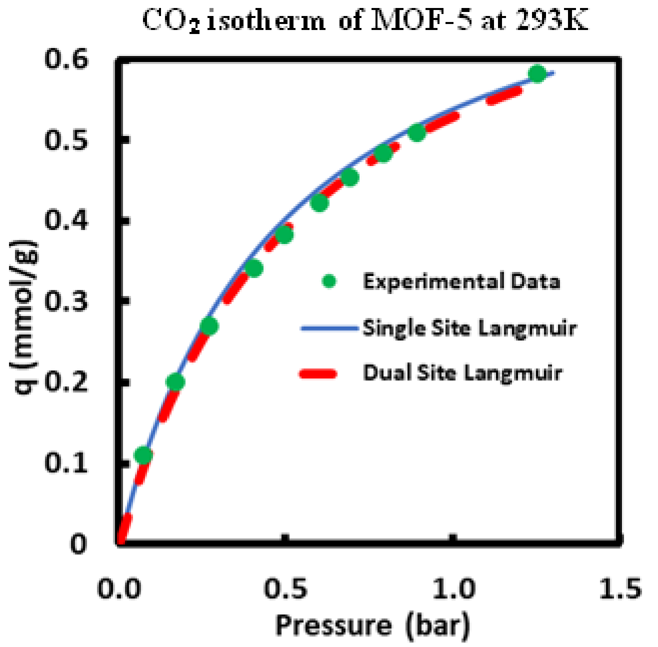


Fig. 3. A comparison of experimental data and simulation result of CO_2 adsorption for MOF-5

Next, the preparation of MOF-5 was made by degassing the adsorbent overnight for 150°C. After that, the packed bed adsorbent was weighted before transferred to different port for adsorption analysis. The gas properties for CO_2 gas adsorption were at ambient temperature with a maximum pressure of 1.3 bar. To ensure that the equilibrium point was reached, the holding time was set for each pressure range. The final pressure and amount of adsorbed gas were plotted at the point of equilibrium to obtain the adsorption isotherm. Origin 2020 was utilised to perform non-linear fitting to determine the isotherm parameters. Based on Figure 3, the higher value of the residual sum of squares for the single-site Langmuir model is 0.0016849. Meanwhile, the value for dual-site Langmuir is 0.0002812.

The same fitting method was applied to CH_4 adsorption by comparing the experimental data with dual-site and single-site Langmuir Isotherm, as shown in Figure 4. The maximum pressure of CH_4 was at 293 K at 35 Bar. Based on Figure 4, the residual sum of squares for single-site Langmuir fits is 0.4141, and the residual sum of squares for dual-site Langmuir is 0.0687. Based on both non-linear fittings results, we can summarize that dual-site Langmuir has better fits for equation better than the standard Langmuir equation. This may be due to dual-site Langmuir has more fitting parameters compared to single-site Langmuir

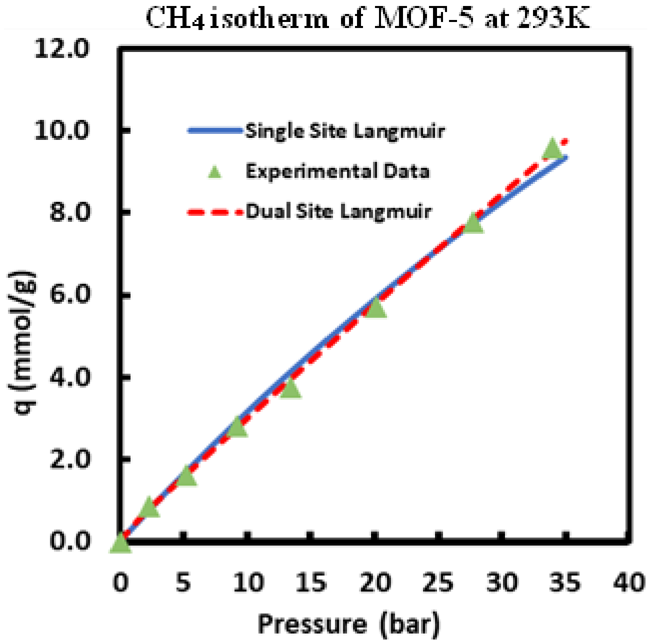


Fig. 4. A comparison of experimental data and simulation result of CH_4 adsorption for MOF-5

2.3 Flow Domain and Boundary Conditions

The boundary conditions and material properties (see Table 2) were based on the numerical model set up by Qasem [13]. This model assumed laminar flow model and the porous media is homogenous in the flow domain. For pressure velocity coupling, SIMPLE algorithm was applied [27]. Using second-order upwind systems, the convection terms in the conservation equations were discretized [28]. Lastly, the convergence criterion is 10^{-4} for continuity and velocity residual. For energy convergence criterion, the residual is 10^{-6}. The model was discretized using hexahedral elements and the number of hexahedral elements is 40095. The number of nodes are 42400 and elements are 4451

Table 2
Properties and solution setup

Parameters		Value
Materials	Adsorption column	Stainless Steel
Boundary Conditions	Inlet	Mass Flow Rate, 0.046 kg/s Initial Gauge Pressure, 101300 Pa Temperature, 323 K
	Outlet	Pressure, 0 Pa
	Bed Porosity	0.6

3. Result and Discussion

3.1 Effects of Temperature in Equilibrium Adsorption

To monitor the CO_2/CH_4 adsorption behaviour at a different temperature, simulation data of CO_2 and CH_4 average adsorption at porous media was plotted at 16 different temperatures from 253 K to 403 K as shown in Figure 5 and 6. Figure 5 shows the CO_2 adsorption at different temperatures as the pressure increases, the breakthrough curve becomes steeper. This was due to more gases adsorption can occupy empty site and the gas can be distributed effectively along the bed. Table 3 shows the difference in CO_2 adsorption value at 1.2 Bar for each temperature gap. As demonstrated, at temperature difference 263 K, the adsorption value is 0.04 mmol/g. The amount is higher than the different in adsorption value for 403 K at 0.017 mmol/g. A decreasing trend of difference in adsorption value from 253 K to 403 K was observed. This result exhibit that rises in temperature of CO_2 adsorption results in a more negligible difference in CO_2 adsorption amount for each 10 Kelvin rise in temperature. The trend may due to effects of high energy consumed in term of heat which reflected into lesser gas adherence in adsorption process.

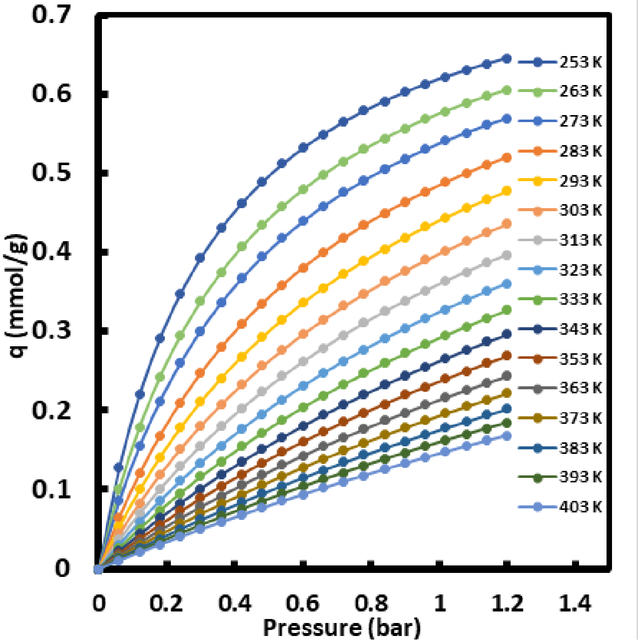
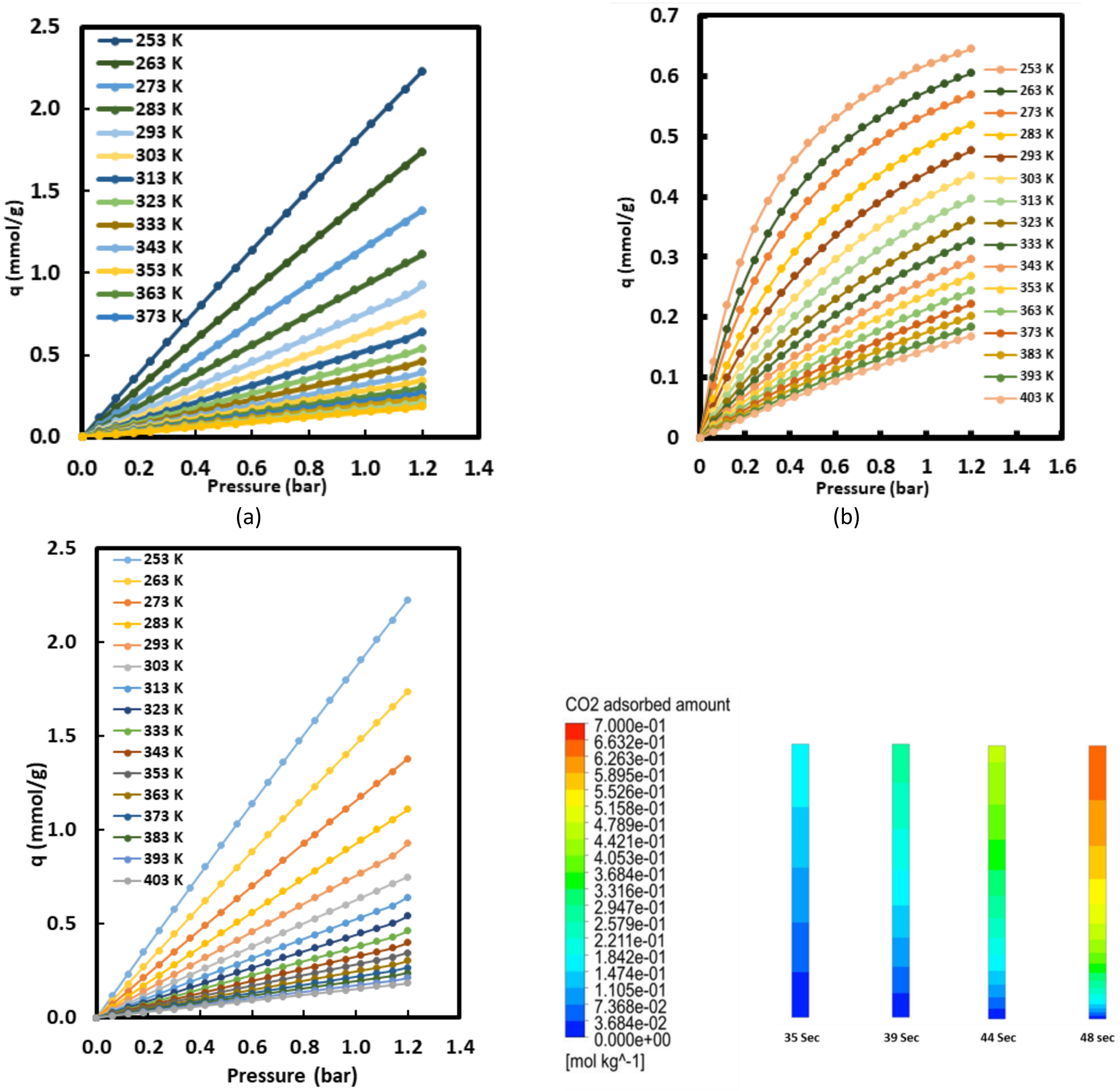


Fig. 5. A comparison of experimental data and simulation result of CH_4 adsorption for MOF-5

Table 3
Different in adsorption value at 1.2 Bar

Temperature (K)	263	283	303	323	343	363	383	403
Different in adsorption value at 1.2 Bar (mmol/g)	0.040	0.050	0.041	0.036	0.034	0.028	0.020	0.016

Figure 6(a) shows the simulated CH_4 adsorption from 0 to 1.2 Bar at 16 different temperatures. The adsorption value for CH_4 at 273 K 1.2 Bar is 1.38 mmol/g. Meanwhile, as shown in Figure 6, CO_2 adsorption value at 273 K 1.2 Bar is 0.57 mmol/g. This shows MOF-5 has 58.7% higher CH_4 adsorption compared to CO_2 at 273K 1.2 Bar. Meanwhile, Figure 6(b) and 6(c) shows dual-site Langmuir isotherm for MOF 5 CO_2 and CH_4 adsorption from 0 to 1.2 Bar. The result indicates that 0.5619 mmol/g of CO_2 was adsorbed at 1.2 Bar 273 K. Meanwhile, the adsorption value for CH_4 adsorption based on dual-site Langmuir at 1.2 Bar 273 Kelvin is 1.3787 mmol/g. For dual-site Langmuir, CH_4 has a higher adsorption value with 59.24% increase in adsorption value. Figure 6(d) shows the adsorption value of the adsorption column at 35, 39, 44, and 48 seconds. The highest adsorbed amount of CO_2 at 48 seconds. The adsorption value at the inlet region at 48 seconds was maximized at 0.7 mmol/g. However, for adsorption value at 35, 39, and 44 seconds the adsorption value increases uniformly overtime.



(a) (b)

(c) (d)

Fig. 6. Comparison of average adsorption amount at different operating pressure for (a) CH_4 adsorption using Singe Site Langmuir (b) CO_2 adsorption using Dual Site Langmuir (c) CH_4 adsorption using Dual Site Langmuir and CO_2 adsorbed amount contour at different time

4. Conclusions

In this study, the effects of different temperatures of CO_2 and CH_4 on MOF-5 adsorption amount from 0 to 1.2 Bar was studied based on single-site Langmuir and dual-site Langmuir isotherm model. Simulation results for CO_2 and CH_4 adsorption for MOF-5 based on Dual site Langmuir and Single Site Langmuir showed a good agreement with the experimental results with dual-site Langmuir led better fittings compared to single-site Langmuir. CH_4 shows a higher adsorption rate at 1.2 Bar than CO_2 for MOF-5 at 273K with a difference of 0.81mmol/g. Besides that, increasing the temperature gradually from 253 K to 403 K decreased the adsorbed amount for every 10 Kelvin increase from 0.04 mmol/g to 0.17 mmol/g. The results may influence by the higher operating pressure of CH_4 compared to CO_2. Despite the fact that higher CH_4 adsorption was attained, further study needs to be considered to study the selectivity between both gases using MOF-5 and using finned design adsorbent bed to improve heat distribution to the adsorbent [29,30].

Acknowledgement

This research was funded by Internal Research Grant OPEX (J5100D4103-BOLDREFRESH2025-CENTRE OF EXCELLENCE).

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