Journal of Advanced Research in Micro and Nano Engineering, 30, Issue 1 (2025) 48-57

SEMARAK ILMU
PUBLISHING
202103268166(003316878-P)

Journal of Advanced Research in
Micro and Nano Engineering

Journal homepage:
https://semarakilmu.com.my/journals/index.php/micro_nano_engineering/index
ISSN: 2756-8210

Prediction of Binary Adsorption Isotherms of Carbon Dioxide and Methane from Pure Adsorption Data

Marhaina Ismail[1], Mohamad Azmi Bustam[2,*], Yeong Yin Fong[1], Aqeel Ahmad[3]

[1] Carbon Dioxide Research Centre (CO_2RES), Universiti Teknologi PETRONAS, 32610 Bandar Seri Iskandar, Perak, Malaysia
[2] Centre of Research in Ionic Liquids (CORIL), Universiti Teknologi PETRONAS, 32610 Bandar Seri Iskandar, Perak, Malaysia
[3] Interdisciplinary Research Center for Refining and Advanced Chemicals, King Fahd University of Petroleum and Minerals, Dhahran 31261, Saudi Arabia

ARTICLE INFO

Article history:
Received
Received in revised form
Accepted
Available online

ABSTRACT

In the area of adsorption, experimental multicomponent data possess challenges in comparison to pure components. By solely relying on the pure adsorption experiment, a model known as Ideal Adsorbed Solution Theory (IAST) can predict binary adsorption isotherms without requiring any experimental multicomponent data. According to our previous work, Co-gallate exhibited higher CO_2 uptakes than CH_4 based on pure adsorption isotherms. However, there is a lack of study on the equilibrium isotherms of binary adsorption calculated by IAST for multi CO_2/CH_4 compositions at different temperature conditions. Therefore, the experimental CO_2 and CH_4 pure adsorption isotherms were fitted with six analytical models, in which Langmuir model yielded the highest goodness-of-fit. IAST calculations via the Python package were employed to predict the equilibrium isotherms of binary CO_2/CH_4 adsorption at different compositions and temperatures. The predicted binary adsorption isotherms revealed that CO_2 adsorption was more favourable on the surface of Co-gallate than CH_4, even though those uptakes were lower than pure adsorption data due to competitive co-adsorption behaviours. Moreover, IAST selectivity suggested that CO_2/CH_4 separation performed better as the CO_2/CH_4 compositions approached unity and at lower temperature condition. IAST approach evaluated that Co-gallate can be a promising solid material for CO_2/CH_4 mixed gas separations.

Keywords:

Carbon dioxide; methane; MOF; binary adsorption

1. Introduction

The mixed gas adsorption (binary adsorption) on porous solid materials (adsorbents) continues to gain attention, particularly in petrochemical and biochemical processes. The adsorption technology is an operation that is firmly established owing to its efficiency in addressing a wide range of procedures such as purification of gas, separation of recycled streams and removal of impurities [1]. Carbon dioxide (CO_2) and methane (CH_4) mixture separation and purification are among the most crucial processes for upgrading the natural gas and biogas. Natural gas and biogas consist of

---

[*] *Corresponding author.*
E-mail address: azmibustam@utp.edu.my

https://doi.org/10.37934/armne.30.1.4857

approximately 75-90 % and 50-70 % of methane respectively, in the presence of other components [2,3]. The CO_2 capture from these CH_4-rich streams is important to provide highly purified sources of methane to meet the sale gas specification and to prevent the pipelines and equipment corrosion.

Adsorption is one of the separation technologies by capturing molecules on the surface of adsorbents [4]. A fundamental procedure for adsorptive gas separation and purification involves allowing a gas mixture into a column packed with adsorbents, resulting in a product that is enriched with a component having weaker adsorption. The design of adsorption column requires multicomponent equilibrium adsorption data (equilibrium isotherm of binary adsorption). This equilibrium data involves extensive experimental work and is normally carried out using self-built equipment, which is time-consuming. Therefore, predicting multicomponent equilibrium data for binary adsorption is of great interest.

The equilibrium isotherms of binary adsorption can be predicted by a thermodynamic approach known as Ideal Adsorbed Solution Theory (IAST). Introduced by Myers and Prausnitz, IAST is an analogue of Raoult's law for vapor-liquid equilibria and the prediction depends solely on experimental pure adsorption isotherms, which need to be fitted first to a continuous function to allow for analytical or numerical solutions [5]. This approach assumes that the components in the mixed gas have an equivalent access to the internal surface of homogeneous adsorbent, and there is absence of adsorbate interactions in the ideal adsorbed phase [6]. IAST has been found to be a systematic and adequate approach for predicting the equilibrium isotherms of binary adsorption on metal-organic frameworks, activated carbon and zeolites (MOFs) [7-9]. MOFs have appeared as a prominent class of porous materials due to their distinctive properties including large surface area, great porosity, tailorable pore size, tunable geometry and structure, and stability [10,11].

Various biomass-based materials have been reported as effective adsorbents in a variety of applications [12-14]. Gallate-based metal-organic framework, made up of gallic acid and metal salt has revealed the remarkable performance in CO_2 and CH_4 adsorption, with cobalt gallate (Co-gallate) offering higher CO_2 adsorption capacity compared to CH_4 [15]. However, there is a scarcity of literature reported on the equilibrium isotherms of binary adsorption calculated by IAST for multi CO_2/CH_4 compositions using Co-gallate at different temperature conditions. Therefore, the purpose of this work is to carry out the prediction of equilibrium isotherms of binary CO_2/CH_4 adsorption through IAST calculations using Python Package. The predicted equilibrium isotherms of binary CO_2/CH_4 adsorption were presented at 75:25, 50:50, 25:75, 10:90 compositions at 273, 298 and 313 K. The predicted binary component data were then used to determine the IAST selectivity. These predicted equilibrium isotherms of binary CO_2/CH_4 adsorption are poised to offer valuable insights for the prospective design of CO_2/CH_4 mixed gas separation employing Co-gallate.

2. Methodology

The predicted equilibrium isotherms of binary CO_2/CH_4 adsorption were carried out by IAST calculation using Python Package (pyIAST) based on the experimental CO_2 and CH_4 pure adsorption isotherms conducted in our previous work [15]. The detailed explanations can be found in the previously reported works [16-18]. The calculation of spreading pressure can be conducted using the subsequent equation.

$$\frac{\pi A}{RT} = \int_0^{P_i^0} \frac{n_i}{P_i} dP_i \quad (1)$$

where the spreading pressure is denoted by π, T is the temperature (K), R represents the gas constant (8.314 J/K.mol), A is the specific surface area of adsorbent (m^2/g), and n_i is the adsorption of component i (mmol/g).

The experimental CO_2 and CH_4 pure adsorption isotherms were fitted to the analytical model, $n_i^o(P)$ using a least-squares loss function, resulting in an analytical formula for the spreading pressure [17]. The pyIAST has the capability to fit various established analytical models. It exclusively supports thermodynamically consistent isotherm models adhering to Henry's law at low coverage, as stated in the previous work and listed in Table 1 below [17].

Table 1
Analytical model and their spreading pressure corresponding to the model

Model	General form	Spreading pressure corresponding to the model
Langmuir	$n_i^o(P) = M\frac{KP}{1+KP}$	$\frac{A}{RT}\pi_i(P) = M\ log(1+KP)$
Quadratic	$n_i^o(P) = M\frac{(K_A+2K_BP)P}{1+K_AP+K_BP^2}$	$\frac{A}{RT}\pi_i(P) = M\ log(1+K_AP+K_BP^2)$
BET	$n_i^o(P) = M\frac{K_AP}{(1-K_BP)(1-K_BP+K_AP)}$	$\frac{A}{RT}\pi_i(P) = M\ log\frac{1-K_BP+K_AP}{1-K_BP}$
Henry	$n_i^o(P) = K_HP$	$\frac{A}{RT}\pi_i(P) = K_HP$
Approximated Temkin	$n_i^o(P) = M\left(\frac{KP}{1+KP}+\theta\left(\frac{KP}{1+KP}\right)^2\left(\frac{KP}{1+KP}-1\right)\right)$	$\frac{A}{RT}\pi_i(P) = M\left(\log(1+KP)+\theta\frac{2KP+1}{2(KP+1)^2}\right)$
Dual-site Langmuir	$n_i^o(P) = M_1\frac{K_1P}{1+K_1P}+M_2\frac{K_2P}{1+K_2P}$	$\frac{A}{RT}\pi_i(P) = M_1\log(1+K_1P)+M_2\log(1+K_2P)$

2.1 Root Mean Square Error (RMSE)

Root mean square error (RMSE) signifies a measure of the average magnitude of the errors between predicted and actual values. A lower RMSE designates better predictive performance, with zero being the ideal value. RMSE can be determined using the equation below [19].

$$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(x_i^{exp} - x_i^{cal})^2} \tag{2}$$

where x_i^{exp} is the experimental value of component *i*, x_i^{cal} represents the calculated value of component *i* and N is the number of data points.

2.2 IAST Selectivity

The adsorption selectivity determined through IAST is defined by the following equation [20].

$$S_{ij} = \frac{x_i/x_j}{y_i/y_j} \tag{3}$$

where x_i and x_j signify mole fractions of component *i* and *j* in the adsorbed phase, while y_i and y_j denote mole fractions of component *i* and *j* in the gas phase (dimensionless).

3. Results

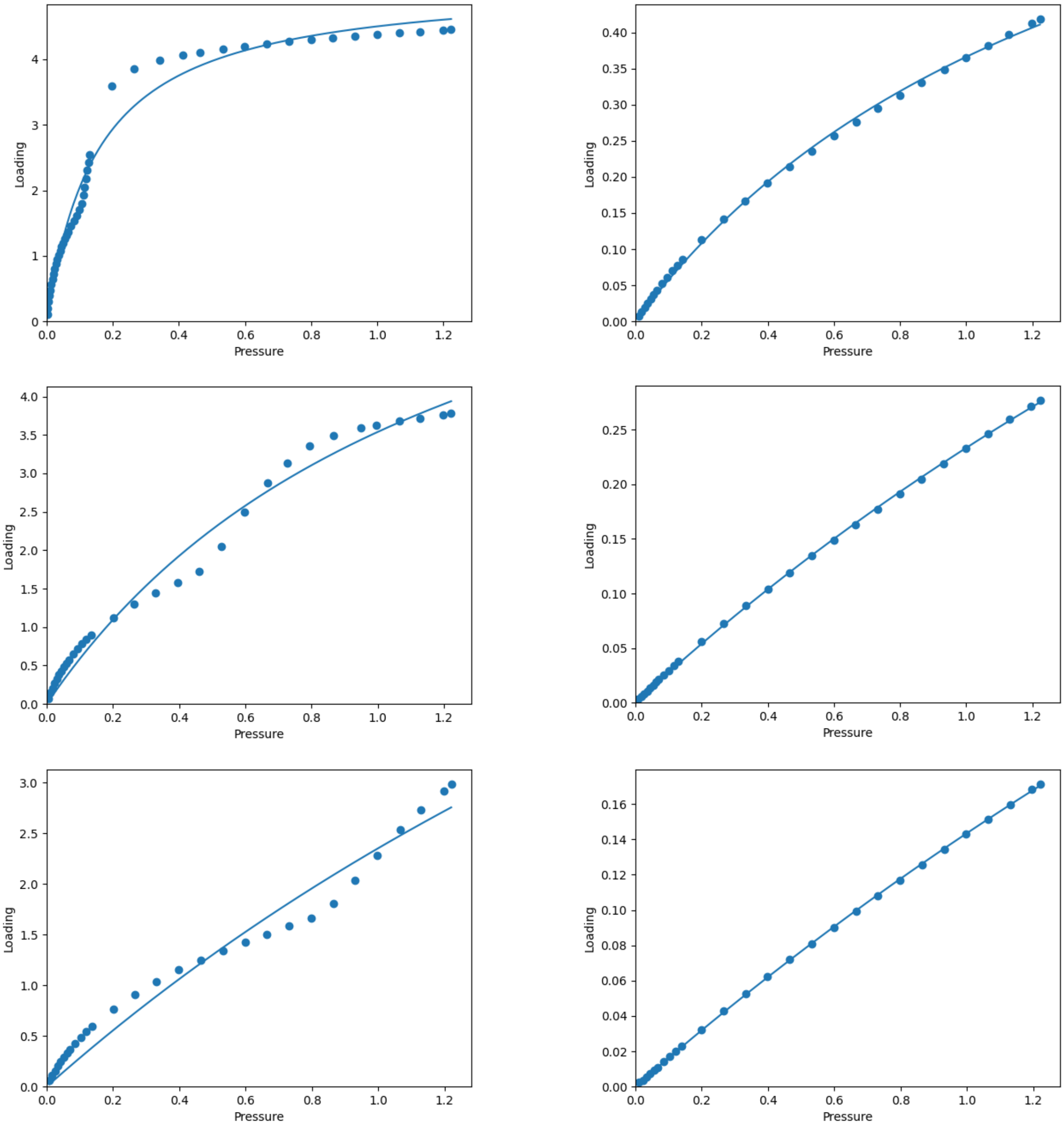
3.1 Analytical Model Fittings

The experimental CO_2 and CH_4 pure adsorption isotherms of Co-gallate were fitted using various models including Langmuir, Henry, approximated Temkin, BET, quadratic, and Dual-site Langmuir. Their model parameters are tabulated in Table 2.

Table 2
Analytical model parameters

Model	Parameter	CO_2			CH_4		
		273 K	298 K	313 K	273 K	298 K	313 K
Langmuir	M	5.1927	8.0105	12.3798	0.9082	1.3956	1.1382
	K_L	6.5122	0.7915	0.2347	0.6758	0.2008	0.1442
	RMSE	0.2065	0.1786	0.1645	4.72 x 10^{-3}	1.36 x 10^{-3}	4.67 x 10^{-4}
Quadratic	M	2.4351	4.7543	7.8109	0.5955	5.25 x 10^{-4}	5.25 x 10^{-4}
	K_A	9.8985	1.3728	0.3777	1.0554	5.0 x 10^{-4}	5.0 x 10^{-4}
	K_B	59.2289	0.3118	0.0218	0.1496	5.0 x 10^{-4}	5.0 x 10^{-4}
	RMSE	0.1892	0.1778	0.1639	4.14 x 10^{-3}	0.1443	0.0916
BET	M	8.1795	6.2152	5.25 x 10^{-4}	0.4034	5.25 x 10^{-4}	1.1493
	K_A	3.5494	1.0521	5.0 x 10^{-4}	1.7544	5.0 x 10^{-4}	0.1428
	K_B	−0.3482	0.0676	5.0 x 10^{-4}	0.2297	5.0 x 10^{-4}	−6.53 x 10^{-4}
	RMSE	0.1719	0.1784	1.4656	1.07 x 10^{-3}	0.1443	4.68 x 10^{-4}
Henry	K_H	5.1275	3.6559	2.3780	0.3769	0.2354	0.1444
	RMSE	1.2415	0.3335	0.1761	0.0270	6.41 x 10^{-3}	3.0 x 10^{-3}
Approximated Temkin	M	4.3152	9.6645	16.2138	0.9091	5.25 x 10^{-4}	1.1462
	K_T	5.2970	0.6837	0.1829	0.6751	5.0 x 10^{-4}	0.1432
	θ	−1.6099	0.4130	0.4780	1.84 x 10^{-3}	5.0 x 10^{-4}	8.63 x 10^{-3}
	RMSE	0.1777	0.1776	0.1638	4.72 x 10^{-3}	0.1443	4.66 x 10^{-4}
Dual-site Langmuir	M_1	2.5802	5.25 x 10^{-4}	5.25 x 10^{-4}	5.25 x 10^{-4}	5.25 x 10^{-4}	5.25 x 10^{-4}
	K_1	6.5122	5.0 x 10^{-4}	5.0 x 10^{-4}	5.0 x 10^{-4}	5.0 x 10^{-4}	5.0 x 10^{-4}
	M_2	2.6125	5.0 x 10^{-4}	5.0 x 10^{-4}	5.0 x 10^{-4}	5.0 x 10^{-4}	5.0 x 10^{-4}
	K_2	6.5122	5.0 x 10^{-4}	5.0 x 10^{-4}	5.0 x 10^{-4}	5.0 x 10^{-4}	5.0 x 10^{-4}
	RMSE	0.2065	2.1577	1.4656	0.2326	0.1443	0.0916

Based on the RMSE values, Langmuir model demonstrated the highest goodness-of-fit with relevant parameter values among the studied models for CO_2 and CH_4 pure adsorption isotherms of Co-gallate. Langmuir model, known for describing monolayer adsorption on a homogenous surface of adsorbent, provided a simple yet effective fit [21]. The Langmuir parameter denoted by M, representing the maximum adsorption capacity was observed to increase with temperature for CO_2 adsorption of Co-gallate. In contrast, CH_4 exhibited a fluctuating trend. Meanwhile, the Langmuir constant (K_L) values for CO_2 and CH_4 decreased from 273 to 313 K. The Langmuir constant is related to the affinity between the adsorbate and adsorbent [22]. The higher the constant value the greater interaction is, but it decreases with temperature. Consequently, this parameter contributes to the higher adsorption uptakes at lower temperature. The experimental CO_2 and CH_4 pure adsorption along with Langmuir-fitted isotherms are illustrated in Figure 1.

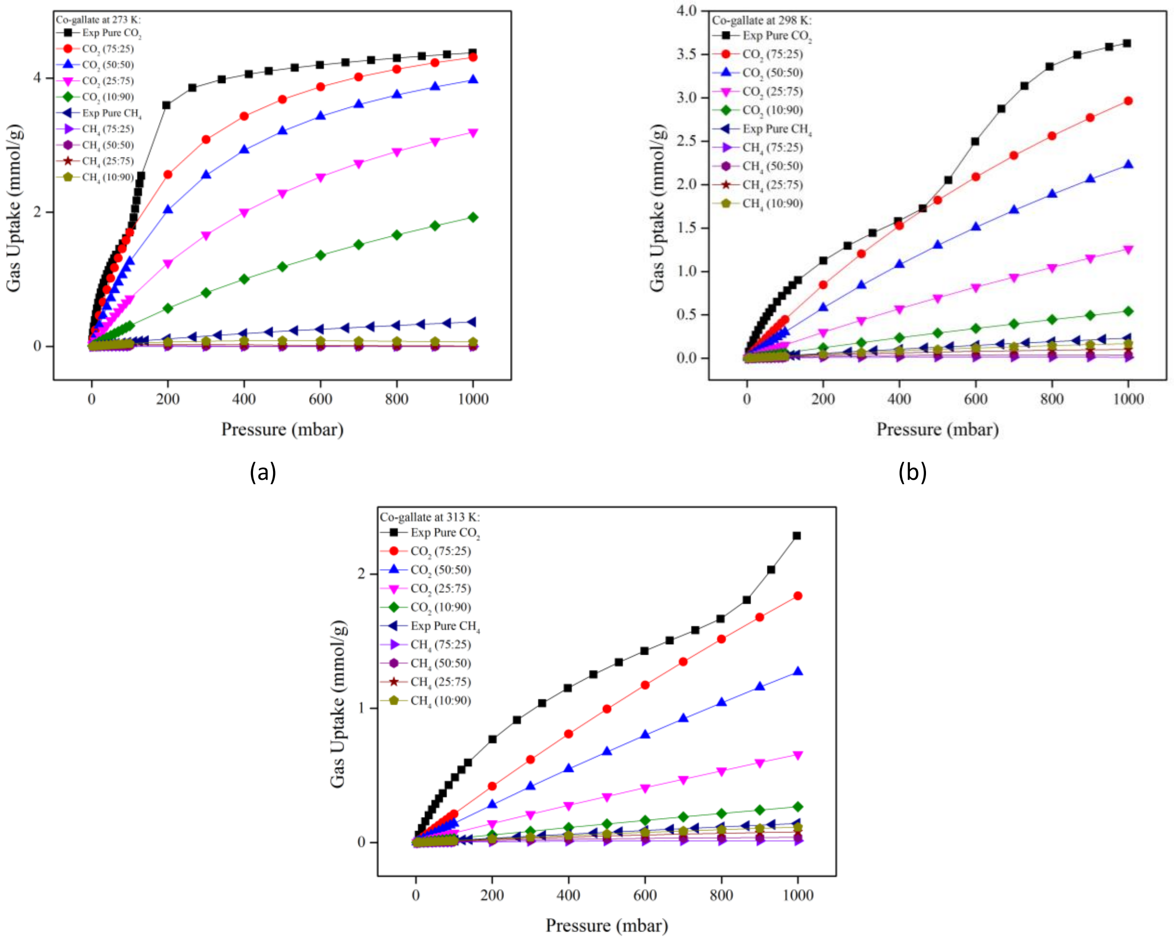


(a) (b)

Fig. 1. Experimental pure adsorption (dot) and Langmuir-fitted isotherms (line) for (a) CO_2 and (b) CH_4 at 273, 298 and 313 K. The experimental pure adsorption isotherms are re-plotted based on previous work [15]

3.2 Prediction of Equilibrium Isotherms of Binary CO_2/CH_4 Adsorption

The equilibrium isotherms of binary CO_2/CH_4 adsorption were predicted using IAST calculations at different compositions and temperatures (273, 298 and 313 K) as illustrated in Figure 2.



(a)

(b)

(c)

Fig. 2. Experimental (pure component) and predicted (binary component) CO_2 and CH_4 equilibrium adsorption isotherms of Co-gallate for 75:25, 50:50, 25:75 and 10:90 compositions at (a) 273, (b) 298 and (c) 313 K

The co-adsorption was found to impact gas uptakes on the surface of Co-gallate. The predicted CO_2 and CH_4 uptakes were observed to be lower than the experimental values. In all studied compositions, the presence of CH_4 in the mixed gas led to competitive adsorption, resulting in lower CO_2 uptakes compared to pure adsorption. During co-adsorption, the surface of Co-gallate was able to accommodate both CO_2 and CH_4 molecules. Consequently, the CO_2 molecules engaged in competition with CH_4 for the available adsorption sites, thus slightly reducing the accessible sites for CO_2 adsorption. However, despite this competition, CO_2 exhibited dominance and more favourable behaviour than CH_4, leading to higher CO_2 uptakes. This phenomenon is attributed to the thermodynamic equilibrium effect, indicating the stronger interactions between Co-gallate and CO_2 molecules. The thermodynamic equilibrium effect describes different adsorbent-adsorbate interactions, leading to the preferential adsorption of certain molecules over others on the surface of the adsorbent [23]. This preference is due to CO_2 exhibits greater polarizability (29.1×10^{-25} cm^3 for CO_2, 25.9×10^{-25} cm^3 for CH_4) and possesses a quadrupole moment (4.30×10^{-26} esu cm^2 for CO_2, 0 for CH_4) in comparison to CH_4 [24].

The predicted equilibrium isotherms of binary CO_2/CH_4 adsorption were observed to increase with both pressure and CO_2/CH_4 compositions. It means that Co-gallate can offer greater gas uptakes at higher pressure and CO_2/CH_4 compositions approached unity. Given that adsorption is classified as an exothermic process, it was noted that gas uptakes were higher at lower temperature condition.

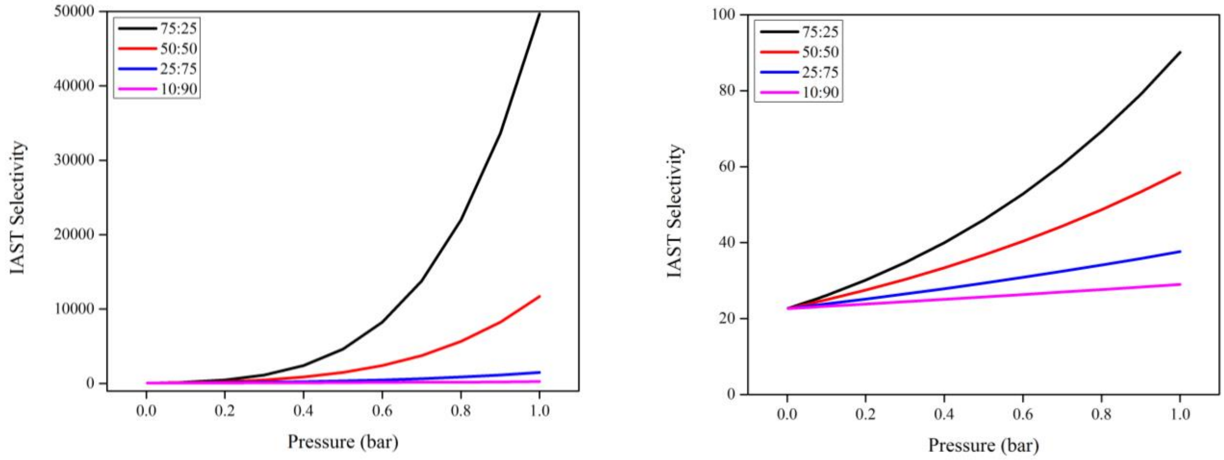
High temperature, being inversely proportional to adsorption, induces the release of adsorbate molecules from the surface of adsorbent. This phenomenon is denoted as desorption, elucidating the diminished adsorption uptake observed under high temperature conditions. The gas uptakes increase with pressure and decrease with temperature, aligns with Le Chatelier's principle [25].

As the CO_2/CH_4 composition approached unity, the predicted CO_2 isotherms shifted to Type I shape particularly at 273 K. The concave curve indicates a rapid increase in CO_2 uptake during initial stage of adsorption due to the accessibility of vacant active sites and gradually occupied until no further adsorption occurred, denoting the saturation was achieved. This corresponds to the completion of a surface monolayer, signifying the gas adsorption limit. Meanwhile, predicted CH_4 isotherms demonstrated plateau pattern with very low uptakes.

3.3 IAST Selectivity

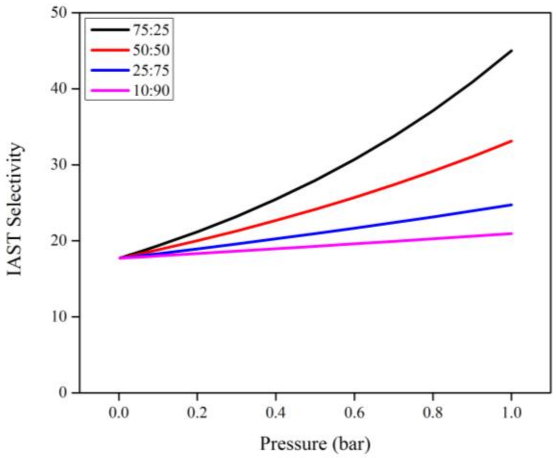
Adsorption selectivity stands as a crucial parameter for assessing the efficacy of an adsorbent in separating gas mixtures. It reflects the contrast in interaction between the different components of the gas mixture and how much the gas component attracted to the adsorbent. In this context, selectivity is straightforwardly explained as the preference of Co-gallate to adsorb CO_2 due to their stronger interaction compared to CH_4. IAST selectivity can be determined from the predicted equilibrium isotherms of binary CO_2/CH_4 adsorption as shown in Figure 3.

With a reduction in temperature, an augmentation in the IAST selectivity was observed, affirming superior performance of Co-gallate at lower temperature for CO_2/CH_4 mixed gas adsorption. IAST selectivity exhibited a rapid escalation as the CO_2/CH_4 compositions approached unity. These values highlight the robust adsorption behaviours of CO_2, indicating a more favourable adsorption affinity for Co-gallate compared to CH_4. In CO_2 capture applications, achieving high selectivity for CO_2 over other components in a gas mixture is imperative.



(a)

(b)



(c)

Fig. 3. IAST selectivity of Co-gallate for 75:25, 50:50, 25:75 and 10:90 compositions at (a) 273, (b) 298 and (c) 313 K

Nevertheless, an argument can be made that the IAST tended to overpredict the selectivity of the CO_2/CH_4 mixture, particularly at 273 K. This disparity commonly arises when there is a substantial contrast in the adsorption strength between the two components, with CO_2 exhibiting a notably stronger adsorption affinity than CH_4. Moreover, uncertainties emerged when applying IAST in regimes necessitating extrapolation beyond the available experimental data. As mentioned in the literature, IAST possesses one limitation in situations where there are huge differences in the adsorption capacity of components, requiring extrapolations to high pressures and resulting in predictions of multicomponent behaviour that may deviate significantly [26].

4. Conclusions

IAST is an approach used to predict the equilibrium isotherms of binary gas adsorption based on the pure adsorption isotherms. This method starts with the fitting of experimental pure adsorption isotherms using analytical models provided by a Python package. Langmuir model was observed to exhibit the best fit, leading to analytical formula for the spreading pressure. The predicted equilibrium isotherms of binary CO_2/CH_4 adsorption were found to be lower than the experimental data due to co-adsorption behaviours. Nevertheless, the stronger interactions between Co-gallate and CO_2 molecules resulted in higher uptakes compared to CH_4. IAST selectivity was calculated based on the predicted isotherms and demonstrated that the values increased as the CO_2/CH_4 compositions approached unity, indicating CO_2 adsorption was favourable. Therefore, IAST approach suggests that Co-gallate can be commercialized as an effective porous material for CO_2/CH_4 separation.

Acknowledgement

This funding for this research was provided through a grant from Yayasan Universiti Teknologi PETRONAS (015LC0-364). Additionally, the research received support from Carbon Dioxide Research Centre (CO_2RES) and Centre of Research in Ionic Liquids (CORIL) at Universiti Teknologi PETRONAS.

References

[1] Pullumbi, Pluton, Federico Brandani, and Stefano Brandani. "Gas separation by adsorption: technological drivers and opportunities for improvement." *Current Opinion in Chemical Engineering* 24 (2019): 131-142. https://doi.org/10.1016/j.coche.2019.04.008

[2] Jasim, Dheyaa, T. Mohammed, and Mohammad F. Abid. "A Review of the Natural Gas Purification from Acid Gases by Membrane." *Engineering and Technology Journal* 40, no. 03 (2022): 441-450. http://doi.org/10.30684/etj.v40i2.1983

[3] Vilardi, Giorgio, Claudia Bassano, Paolo Deiana, and Nicola Verdone. "Exergy and energy analysis of three biogas upgrading processes." *Energy Conversion and Management* 224 (2020): 113323. https://doi.org/10.1016/j.enconman.2020.113323

[4] Zulkifli, Mohd Zul Amzar, Azfarizal Mukhtar, Muhammad Faizulizwan Mohamad Fadli, Anis Muneerah Shaiful Bahari, Akihiko Matsumoto, and Halina Misran. "CFD Simulation of CO_2 and Methane Adsorption at Various Temperature for MOF-5 using Dual-site and Single-site Langmuir Model." *CFD Letters* 13, no. 10 (2021): 1-10. https://doi.org/10.37934/cfdl.13.10.110

[5] Yang, Yafan, Arun Kumar Narayanan Nair, and Shuyu Sun. "Adsorption and diffusion of carbon dioxide, methane, and their mixture in carbon nanotubes in the presence of water." *The Journal of Physical Chemistry C* 124, no. 30 (2020): 16478-16487. https://doi.org/10.1021/acs.jpcc.0c04325

[6] Edens, Samuel J., Kane T. Drake, Nathan C. Harvey-Reid, Ken R. Morison, Paul E. Kruger, and Matthew G. Cowan. "Experimental Measurement of Pure and Mixed-Gas Kinetics of Ethylene and Ethane Adsorption onto Mordenite, Zeolite 13X, and ZJU-74a: Insights into the Value of Single-vs Mixed-Gas Kinetics, Validity of IAST and Sips Isotherm Models, and Temperature/Pressure Relationships for Process Modeling." *Industrial & Engineering Chemistry Research* 62, no. 21 (2023): 8396-8409. https://doi.org/10.1021/acs.iecr.3c01085

[7] Sim, Allan HH, Xiu Liu, and Chunyan Fan. "Adsorptive separation of carbon dioxide at ambient temperatures in activated carbon." *Carbon Capture Science & Technology* 4 (2022): 100062. https://doi.org/10.1016/j.ccst.2022.100062

[8] Wang, Li, Jiaqi Liu, Caihong Lin, Hua Shang, Jiangfeng Yang, Libo Li, and Jinping Li. "Effects of different alkali metal cations in FAU zeolites on the separation performance of CO_2/N_2O." *Chemical Engineering Journal* 431 (2022): 134257. https://doi.org/10.1016/j.cej.2021.134257

[9] Wang, Jun, Yan Zhang, Yun Su, Xing Liu, Peixin Zhang, Rui-Biao Lin, Shixia Chen et al. "Fine pore engineering in a series of isoreticular metal-organic frameworks for efficient C2H2/CO_2 separation." *Nature communications* 13, no. 1 (2022): 200. https://doi.org/10.1038/s41467-021-27929-7

[10] Abid, Hussein Rasool, Aamir Hanif, Alireza Keshavarz, Jin Shang, and Stefan Iglauer. "CO_2, CH4, and H_2 adsorption performance of the metal–organic framework HKUST-1 by modified synthesis strategies." *Energy & Fuels* 37, no. 10 (2023): 7260-7267. https://doi.org/10.1021/acs.energyfuels.2c04303

[11] Li, Chen-Ning, Shi-Ming Wang, Zhi-Peng Tao, Lin Liu, Wei-Guo Xu, Xue-Jun Gu, and Zheng-Bo Han. "Green synthesis of MOF-801 (Zr/Ce/Hf) for CO2/N2 and CO2/CH4 separation." *Inorganic chemistry* 62, no. 20 (2023): 7853-7860. https://doi.org/10.1021/acs.inorgchem.3c00560

[12] Ho, Min Hui Julie, Yeu Yee Lee, Chin Voon Charlie Sia, and Kok Heng Soon. "Microcrystalline Cellulose Based Adsorbent Derived from Watermelon Rind for Dye Removal." *Journal of Advanced Research in Applied Mechanics* 122, no. 1 (2024): 130-146. https://doi.org/10.37934/aram.122.1.130146

[13] Nandiyanto, Asep Bayu Dani, Willy Cahya Nugraha, Intan Yustia, Risti Ragadhita, Meli Fiandini, Muksin Saleh, and Diana Rahayu Ningwulan. "Rice husk for adsorbing dyes in wastewater: literature review of agricultural waste adsorbent, preparation of Rice husk particles, particle size on adsorption characteristics with mechanism and adsorption isotherm." *Journal of Advanced Research in Applied Mechanics* 106, no. 1 (2023): 1-13. https://doi.org/10.37934/aram.106.1.113

[14] Nandiyanto, Asep Bayu Dani, Meli Fiandini, Risti Ragadhita, Hanifa Maulani, Muthia Nurbaiti, Abdulkareem Sh Mahdi Al-Obaidi, Jumril Yunas, and Muhammad Roil Bilad. "Sustainable biochar carbon biosorbent based on tamarind (Tamarindusindica L) seed: Literature review, preparation, and adsorption isotherm." *Journal of Advanced Research in Applied Sciences and Engineering Technology* 32, no. 1 (2023): 210-226. https://doi.org/10.37934/araset.32.1.210226

[15] Ismail, Marhaina, Mohamad Azmi Bustam, and Yin Fong Yeong. "Adsorption of Carbon Dioxide and Methane on Cobalt Gallate-Based Metal-Organic Framework (Co-Gallate): Equilibrium Isotherm, Thermodynamic and Kinetic Studies." *Journal of Advanced Research in Fluid Mechanics and Thermal Sciences* 108, no. 2 (2023): 151-163. https://doi.org/10.37934/arfmts.108.2.151163

[16] Walton, Krista S., and David S. Sholl. "Predicting multicomponent adsorption: 50 years of the ideal adsorbed solution theory." *AIChE Journal* 61, no. 9 (2015): 2757-2762. https://doi.org/10.1002/aic.14878

[17] Simon, Cory M., Berend Smit, and Maciej Haranczyk. "pyIAST: Ideal adsorbed solution theory (IAST) Python package." *Computer Physics Communications* 200 (2016): 364-380. https://doi.org/10.1016/j.cpc.2015.11.016

[18] Ismail, Marhaina, Mohamad Azmi Bustam, Nor Ernie Fatriyah Kari, and Yin Fong Yeong. "Ideal adsorbed solution theory (IAST) of carbon dioxide and methane adsorption using magnesium gallate metal-organic framework (Mg-gallate)." *Molecules* 28, no. 7 (2023): 3016. https://doi.org/10.3390/molecules28073016

[19] Ćalasan, Martin, Shady HE Abdel Aleem, and Ahmed F. Zobaa. "On the root mean square error (RMSE) calculation for parameter estimation of photovoltaic models: A novel exact analytical solution based on Lambert W function." *Energy conversion and management* 210 (2020): 112716. https://doi.org/10.1016/j.enconman.2020.112716

[20] Cessford, Naomi F., Nigel A. Seaton, and Tina Düren. "Evaluation of ideal adsorbed solution theory as a tool for the design of metal–organic framework materials." *Industrial & engineering chemistry research* 51, no. 13 (2012): 4911-4921. https://doi.org/10.1021/ie202219w

[21] Fernandez, David Cantador, David Suescum Morales, José Ramón Jiménez, and José María Fernández-Rodriguez. "CO2 adsorption by organohydrotalcites at low temperatures and high pressure." *Chemical Engineering Journal* 431 (2022): 134324. https://doi.org/10.1016/j.cej.2021.134324

[22] Chiang, Yu-Chun, Cheng-Yen Wu, and Yu-Jen Chen. "Effects of activation on the properties of electrospun carbon nanofibers and their adsorption performance for carbon dioxide." *Separation and Purification Technology* 233 (2020): 116040. https://doi.org/10.1016/j.seppur.2019.116040

[23] Li, Jian-Rong, Ryan J. Kuppler, and Hong-Cai Zhou. "Selective gas adsorption and separation in metal–organic frameworks." *Chemical Society Reviews* 38, no. 5 (2009): 1477-1504. https://doi.org/10.1039/B802426J

[24] Cui, Wen-Gang, Tong-Liang Hu, and Xian-He Bu. "Metal–organic framework materials for the separation and purification of light hydrocarbons." *Advanced Materials* 32, no. 3 (2020): 1806445. https://doi.org/10.1002/adma.201806445

[25] Li, Jinyi, Sen Yang, Zhenhui Du, Ruixue Wang, Liming Yuan, Hongyi Wang, and Zhichao Wu. "Quantitative analysis of ammonia adsorption in Ag/AgI-coated hollow waveguide by mid-infrared laser absorption spectroscopy." *Optics and lasers in engineering* 121 (2019): 80-86. https://doi.org/10.1016/j.optlaseng.2019.03.021

[26] Fraux, Guillaume, Anne Boutin, Alain H. Fuchs, and François-Xavier Coudert. "On the use of the IAST method for gas separation studies in porous materials with gate-opening behavior." *Adsorption* 24 (2018): 233-241. https://doi.org/10.1007/s10450-018-9942-5