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High-pressure adsorption isothermal on a novel microporous material from polyethylene terephthalate plastic waste in carbon dioxide capture applications

Awaludin Martin[1], Erman Taer[2], Nasruddin[3] and Nur Khotimah[1*]

[1] Department of Mechanical Engineering, Faculty of Engineering, Universitas Riau, **Indonesia**
[2] Department of Physics, Faculty of Mathematics and Natural Sciences, Universitas Riau, **Indonesia**
[3] Department of Mechanical Engineering, Faculty of Engineering, Universitas Indonesia, **Indonesia**

* Corresponding Author: nurkhotimah052@gmail.com

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Abstract: Carbon capture is a vital strategy for mitigating climate change by reducing industrial CO_2 emissions. Adsorption technology using microporous material shows significant promise. However, significant challenges persist in developing cost-effective and sustainable adsorbents. This study addresses this issue by simultaneously enabling CO_2 adsorption and plastic waste utilization through activated carbon derived from polyethylene terephthalate (PET). It was evaluated under isothermal conditions (27°C, 35°C, and 45°C) at pressures up to 3500 kPa. The maximum CO_2 adsorption capacity was 0.21313 kg/kg at 27°C and 3504.39 kPa, demonstrating the effectiveness of PET-derived activated carbon in capturing CO_2. The Toth isotherm model exhibited a strong fit with experimental data, with an R^2 of more than 99%. The Clausius-Clapeyron equation yielded an adsorption heat of 2223.66 kJ/kg using the Toth fitting, and the Chakraborty-Saha-Koyama model yielded a heat of 2383.65 kJ/kg, confirming strong adsorption potential. These results underline PET waste as a viable precursor for sustainable carbon capture adsorbents. Furthermore, the results provide essential data for developing numerical models to optimize adsorption-based carbon capture technologies.

Keywords: carbon capture; adsorption isotherm; heat of adsorption; isosteric adsorption

1. Introduction

Fossil fuels are still the primary energy source used worldwide [1]. However, the combustion of fossil energy is a major driver of environmental change, causing 86% of carbon dioxide emissions over recent years [2]. Due to its impact on climate change and environmental degradation, increasing carbon emissions are a major global threat and source of concern for both developed and developing countries [3]. According to data from the Global Monitoring Laboratory, atmospheric carbon dioxide (CO_2) concentrations are predicted to be 426.03 ppm (parts per million) in January 2025. This exceeds the safe threshold of 350 ppm, beyond which accelerated melting of Antarctic ice caps and subsequent sea-level rise become likely [4].

Utilization of non-renewable energy sources, land use change, and deforestation increase fossil fuel emissions that trigger environmental change in Indonesia [5]. Indonesia must develop more rigorous procedures and responsibilities for reducing emissions that drive climate change. From the description of these problems, there is an urgent need for energy-efficient, cost-effective, and environmentally safe solutions to reduce CO_2 emissions [6]. Because the accumulation of CO_2 continues to increase, the amount of emissions produced can have a significant impact on climate change and ecological sustainability [7]. To address this challenge, the development and implementation of carbon capture and reduction technologies are urgently required to mitigate emissions. Carbon capture technology is one of the most promising innovations for reducing CO_2 emissions [8].

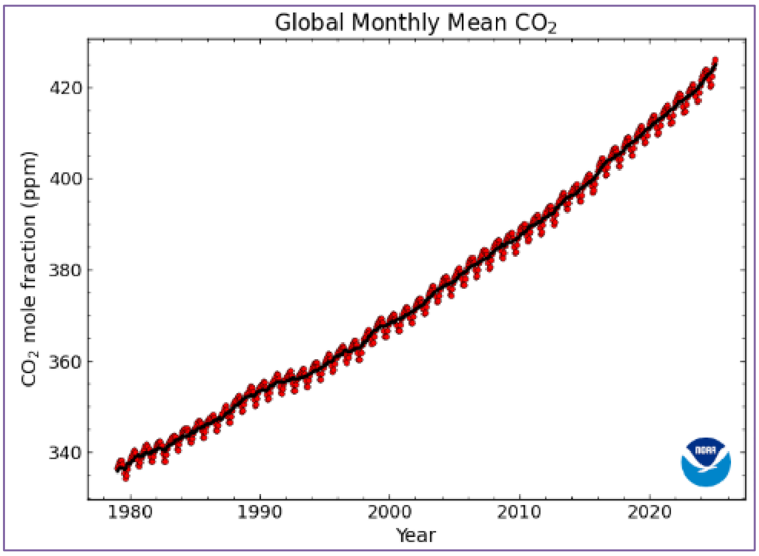

Figure 1. Trends in atmospheric carbon dioxide (CO_2) [9]

It works by capturing CO_2 emissions directly from major industrial sources, such as petroleum power plants, and sequestering them to prevent atmospheric release [10]. The development and implementation of effective carbon capture technologies are essential for reducing CO_2 emissions and mitigating global climate change impacts [11]. A critical component of these technologies are activated carbon (AC) adsorbent [12]. Among microporous materials, AC is one of the most common forms, widely used due to its availability, cost-effective production, and high adsorption capacity.

Adsorption using solid adsorbents such as AC represents a promising CO_2 capture technology [13]. The adsorption process involves the adhesion of gas molecules (adsorbate) to a solid surface (adsorbent) due to unbalanced surface forces [14]. An adsorbent is a substance or material that can bind and hold liquids or gases within it [15]. AC is the most widely used type of adsorbent in adsorption systems, because AC has a relatively large volume of micropores and mesopores, so it has a large surface area and total pore volume, thus it is possible to adsorb a large amount of adsorbate [16]. The basic source of AC is carbon-containing materials, both derived from organic and inorganic waste [17]. AC serves as an effective adsorbent for CO_2 capture due to its high surface area and tunable pore structures. Polyethylene terephthalate (PET) plastic waste, a persistent environmental pollutant, serves as a sustainable feedstock for AC production, concurrently solving plastic pollution while producing effective CO_2 adsorbents. This study focuses on experimentally evaluating the adsorption performance of PET-AC under varying temperatures and pressures.

2. Material and methods

The basic material used in this research is PET plastic waste. The physical and chemical properties of PET are listed in Table 1. PET plastic waste is collected and separated from other types of plastic. Before processing, rigorous material sorting ensures the purity of the PET feedstock. The sorted flakes are then thermally treated in a furnace at a high temperature [18]. It breaks down the PET polymer chains into carbon and volatile gases. PET was carbonized under N_2 (400°C, 240 minutes, 3°C/min) to maintain an inert atmosphere. Subsequently, physical activation was conducted using carbon dioxide (CO_2) as the activating agent at the setting condition (800°C, 240 minutes, 10°C/min). Parameters such as temperature and holding time for carbonization and physical activation are detailed in Figure 2.

Table 1. Physical and chemical properties of PET

Property type	Property	Value/Characteristic
Physical	Density	1.38 – 1.40 g/cm³
	Melting point	250 – 260°C
	Glass transition temperature	~70 – 80°C
	Tensile strength	55 – 75 MPa
	Crystallinity	Semi-crystalline
	Water absorption	Very low (hydrophobic)
Chemical	Chemical structure	$(C_{10}H_8O_4)_n$
	Resistance to Chemicals	weak acids, oils, and alcohol
	Susceptibility	Degraded by strong acids/bases at high temperature
	Oxidation resistance	High at room temperature
	Polymer type	Thermoplastic

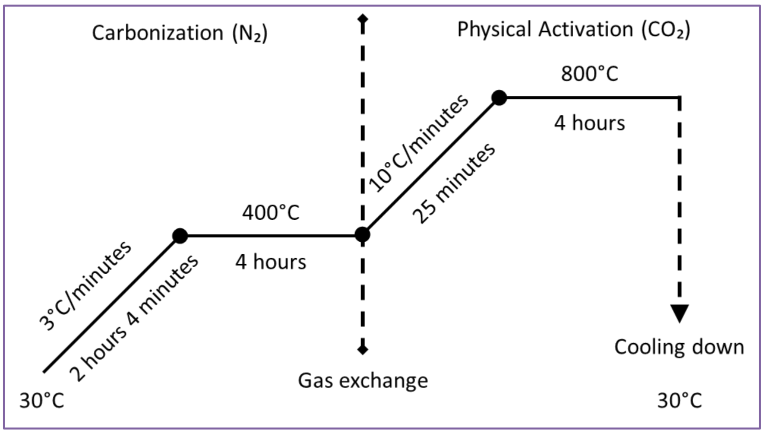

Figure 2. Carbonization process profile and physical activation

This activation process aims to increase the surface area and number of pores on the carbon, thus increasing its adsorption ability [19]. The effectiveness of the physical activation used in this experiment can essentially be observed from the characteristics of the adsorbent in the iodine adsorption test of the AC. This study demonstrated an iodine adsorption capacity of 895.78 mg/g for the synthesized AC, exceeding the minimum quality standard (750 mg/g) specified in SNI 06-3730-1995. The high iodine adsorption capacity (895.78 mg/g) reflects a larger pore surface area of the AC [20]. It correlates well with the characterization of microporous PET-AC by Khotimah et al. [21], showing a surface area of 428.141 m^2/g, pore volume of 0.4083 cm^3/g, and an average pore size of 19.07 Å (micropore classification).

This testing phase was designed to assess the adsorption capacity of PET-AC under varying temperature and pressure conditions, simulating practical scenarios in gas separation and carbon capture applications. The primary objective of this stage was to determine the quantity of CO_2 that could be effectively adsorbed per unit mass of the AC.

2.1 Adsorption isothermal

The adsorption process will occur at equilibrium. In the adsorbate-adsorbent system, the amount of adsorbate when equilibrium conditions are reached is a function of temperature and pressure [22], calculated from Eq. (1):

$$\frac{x}{m} = f(\mathrm{P}, \mathrm{T}) \tag{1}$$

Where x/m is the amount of adsorbate adsorbed per unit mass of adsorbent at equilibrium pressure and adsorption temperature. Adsorption isothermal is an adsorption process maintained at constant temperature, where the adsorption capacity varies as a function of pressure, calculated from Eq. (2):

$$\frac{x}{m} = f(\mathrm{P}) \quad [\mathrm{T} = \text{constant}] \tag{2}$$

Adsorption was performed under isothermal conditions at varying temperatures and pressures. The volumetric method measures pressure, volume, and temperature as the adsorbate is introduced into the adsorption chamber containing the adsorbent [23]. The amount of CO_2 adsorbed is calculated using the ideal gas law based on the equilibrium pressure and temperature measurements [24]. The isothermal adsorption apparatus features a stainless-steel adsorption chamber comprising two interconnected cells: a charging cell and a measuring cell [25]. These cells are connected via stainless steel tubing and immersed in a temperature-controlled water bath.

The temperature of the fluid is controlled by a circulating thermal bath (CTB). The temperature in both cells is measured using a type K thermocouple. The pressure on the two cells is measured using a pressure transmitter. Pressure and temperature data were recorded via a National Instruments data acquisition system and processed in LabVIEW to calculate the adsorption capacity [26]. The schematic diagram of the isothermal adsorption apparatus is shown in Figure 3.

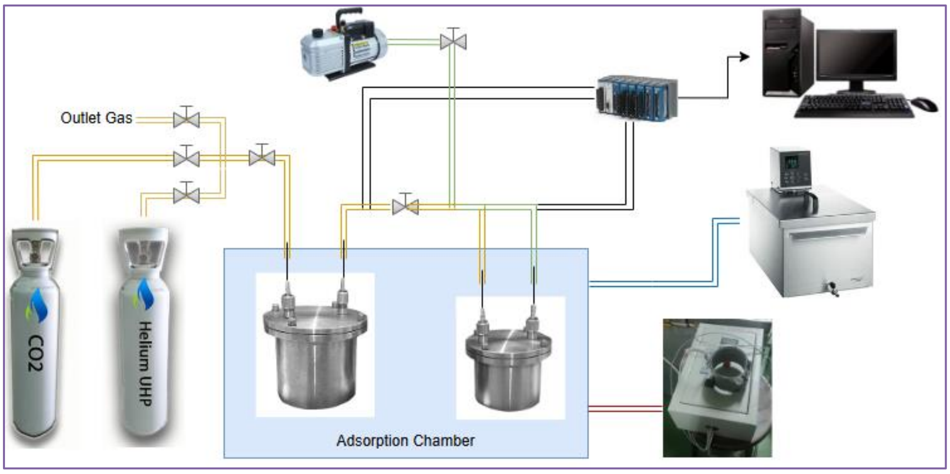

Figure 3. Schematic diagram of the isothermal adsorption apparatus

Samples underwent vacuum degassing (120°C, 2 h) to remove residual gases and adsorbed contaminants. Post-degassing void volume calibration preceded CO_2 adsorption measurements. Triplicate measurements provided statistically validated data. Adsorbate density was calculated from the CO_2 adsorption isothermal using Refprop software at experimentally measured absolute temperatures and pressures. The resulting adsorption represents excess adsorption, as they are determined volumetrically from the CO_2 density difference between two cells [27]. Refprop automatically provides the CO_2 gas density (ρ) in units of kg/m^3. However, for manual data processing or preliminary validation, gas density can be approximated using the ideal gas law as an initial estimate. The equation is referred to as Eq. (3):

$$\rho = \frac{P\,.\,M}{R\,.\,T} \tag{3}$$

Where ρ is the gas density. P is the gas pressure. M is the molar mass of CO_2. R is the universal gas constant, and T is the temperature. Gas density varies with observed temperatures and pressures due to the molecular kinetic effect. Increased temperature elevates molecular velocity, expanding intermolecular distances within a fixed volume [28].

2.2 Toth model

The Toth model is an isotherm model used to describe adsorption on heterogeneous solid surfaces by non-uniform adsorption energies. It is widely recognized as an advancement over the Langmuir and Freundlich models due to its higher flexibility in characterizing heterogeneous surfaces and diverse adsorbate-adsorbent interactions. It can be used to analyze across both low and high pressures [24], as defined by Eq. (4):

$$Q_e = Q_{max}\frac{K\ .\ C_e}{(1+(K\ .\ C_e)^n)^{1/n}} \tag{4}$$

Where Q_e is the amount of adsorbate adsorbed per unit mass of adsorbent at equilibrium. Q_{max} is the maximum adsorption capacity. K is the adsorption equilibrium constant. C_e is the equilibrium concentration of adsorbate in solution, and n is the Toth model exponent, indicating the degree of surface heterogeneity. In this study, the Toth isothermal provides the optimal correlation for calculating the heat of adsorption. The heat of adsorption represents the enthalpy change during adsorbate binding to or release from an adsorbent surface. The isosteric heat of adsorption was calculated using the Clausius-Clapeyron approach [29], defined by Eq. (5):

$$H_{ads} = -R\ .\ ln\left(\frac{P_2}{P_1}\right).\left(\frac{(T_1\ .\ T_2)}{(T_2-T_1)}\right) \tag{5}$$

Where H_{ads} is heat adsorption and R is the ideal gas constant.

The Chakraborty-Saha-Koyama (CSK) model and Clausius-Clapeyron equation are used for different purposes in adsorption and thermodynamic studies. CSK model excels in describing adsorption isotherms on heterogeneous surfaces for industrial applications, while the Clausius-Clapeyron equation serves fundamental thermodynamic analyses, particularly for calculating isosteric heat of adsorption and phase-change enthalpies [30]. The general form of the Chakraborty-Saha-Koyama (CSK) equation is given by Eq. (6) [31]:

$$W = W_0\ .\ exp\left(\frac{-\Delta H_{ads}}{R\ .\ T}\right).\ \left(\frac{P}{P_0}\right)^n \tag{6}$$

Where W is the weight or amount of adsorbate adsorbed at equilibrium. W_0 is the maximum adsorption capacity, and ΔH_{ads} is the enthalpy of adsorption, indicating the energy released during adsorption. Parameters W_0, ΔH_{ads}, and n must be determined experimentally for a particular adsorbent and adsorbate. These two approaches complement each other in providing a comprehensive understanding of adsorption and phase change processes.

3. Results and discussion

The following section presents the CO_2 adsorption performance of polyethylene terephthalate-derived activated carbon (PET-AC), including PET-AC as adsorbent, CO_2 adsorption comparison, Toth model for CO_2 adsorption, heat of adsorption, and isosteric adsorption.

3.1 PET-AC as adsorbent

CO_2 adsorption performance of PET-AC was evaluated to assess its viability for carbon capture applications under controlled isothermal conditions at 27°C, 35°C, and 45°C across a pressure range (100 - 3500 kPa). CO_2 adsorption on AC is an exothermic process, where increasing the temperature generally reduces the adsorption capacity. Therefore, testing at lower temperatures (27°C) maximizes adsorption capacity due to the exothermic nature of CO_2 physisorption, while elevated temperatures (35 - 45°C) reveal the effect of temperature on adsorbent performance. Adsorption at pressures up to 3500 kPa confirms the suitability of this range for high-pressure adsorption studies [32]. Elevated pressure enhances CO_2 adsorption capacity. Studies across a pressure range of 1 to 35 bar provide insight into pressure-dependent capacity trends and identify optimal carbon capture conditions. The uptake results are expressed in units (kg/kg), which describe the uptake of kilograms of CO_2 for every kilogram of PET-AC (kg adsorbate/kg adsorbent). Initial testing at 27°C. These results validate theoretical predictions that elevated pressure improves CO_2 adsorption capacity [33].

Maximum adsorption capacity at 27°C (0.21313 kg/kg) occurred at 3504.39 kPa, with a standard error of regression (SER) of 0.00366 kg/kg. This minimal deviation is relatively low compared to the range of uptake values. This indicates that the regression model provides an excellent fit to the experimental data, with minimal deviation between predicted and observed values. The high R^2 value (0.9976) and the statistically significant p-value (4.31×10^{-13}) further confirm the robustness and reliability of the linear model in describing the relationship between pressure and CO_2 adsorption capacity at 27°C.

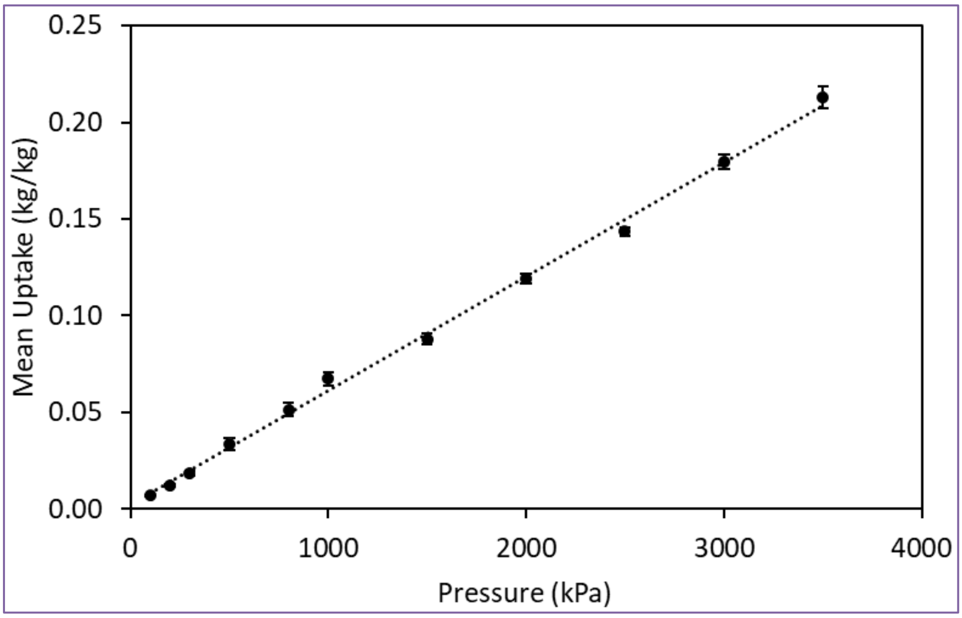

Figure 4. CO_2 adsorption capacity at 27°C

Adsorption testing at 35°C (Figure 5) and 45°C (Figure 6) confirmed the consistent result observed at 27°C that capacity increased proportionally with pressure. As shown in Figure 5, maximum adsorption capacity at 35°C (0.15585 kg/kg) occurred at 3481.08 kPa, with SER 0.00258 kg/kg, a high R^2 value (0.9979), and a significant p-value (1.97×10^{-13}).

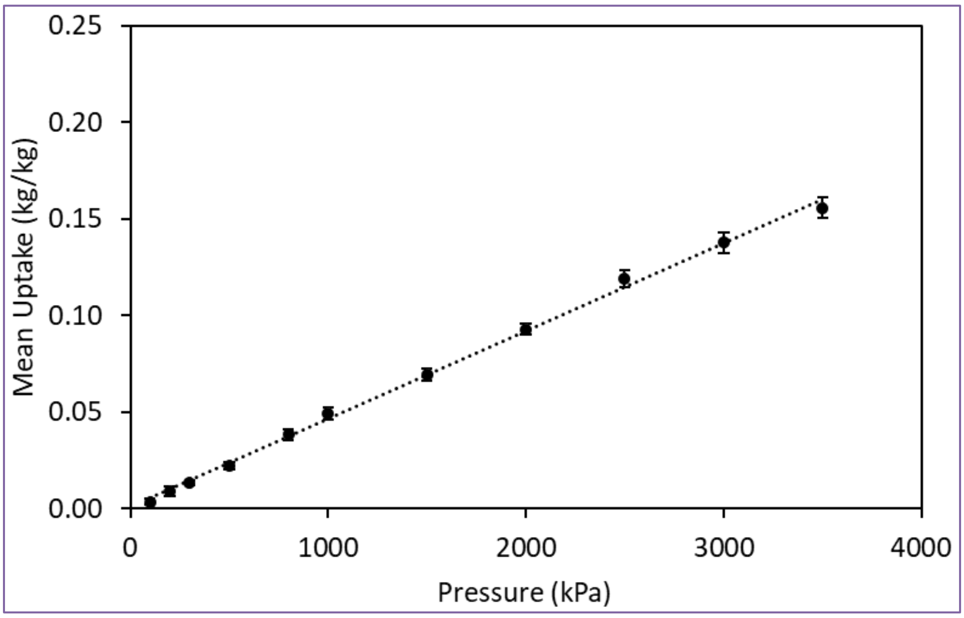

Figure 5. CO$_2$ adsorption capacity at 35°C

As shown in Figure 6, maximum adsorption capacity at 45°C (0.09951 kg/kg) occurred at 3483.79 kPa, with SER 0.00184 kg/kg, a high R^2 value (0.9974), and a significant p-value (5.79×10^{-13}). At 45°C and elevated pressures, error bars increase. It indicates greater uncertainty and variability under these conditions. This trend quantitatively confirms that CO$_2$ adsorption is thermodynamically favored at lower temperatures, where consistently minimal error bars reflect robust reproducibility across replicates. These results confirm that CO$_2$ adsorption on activated carbon is fundamentally pressure-dependent, with PET-derived AC demonstrating excellent capture performance and robust experimental reproducibility across the investigated pressure range.

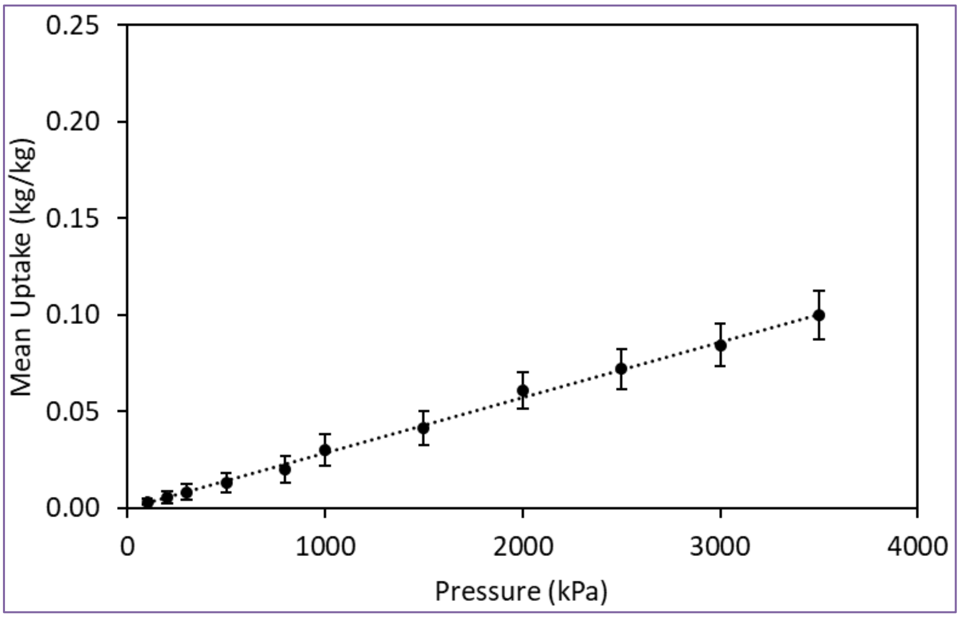

Figure 6. CO$_2$ adsorption capacity at 45°C

Several studies reported that PET-AC exhibits superior CO$_2$ adsorption capacity compared to biomass-derived counterparts. This is primarily attributed to the effectiveness of the physical activation method employed, typically involving high-temperature CO$_2$ or steam treatment, which selectively develops microporous nd avoids chemical contamination from activating agents. Upcycling PET waste into high-performance adsorbents simultaneously addresses dual environmental concerns: plastic pollution and greenhouse gas emissions. Therefore, PET-AC not only offers enhanced adsorption efficiency but also aligns with the principles of sustainable materials development and circular economy practices.

3.2 CO_2 adsorption comparison

The CO_2 adsorption process observed in this study using PET-AC aligns unequivocally with the characteristics of physisorption, as supported by both experimental and theoretical studies. Consistent with established mechanisms, CO_2 physisorption occurs with an adsorption enthalpy is more than 40 kJ/mol. It indicates weak van der Waals interactions between the adsorbate and the surface of the adsorbent [34]. In this study, CO_2 adsorption on PET-AC occurred at moderate temperatures (27°C to 45°C) and a pressure (100 to 3500 kPa), with no indication of chemical bonding or irreversible uptake.

The reversibility of the process, coupled with capacity enhancement at lower temperatures and higher pressures, unequivocally aligns with physisorption behavior. These trends confirm a physical interaction mechanism, distinct from chemisorption, which involves stronger bonds and higher adsorption energies. Comparative analysis across the three temperature regimes is presented in Figure 7.

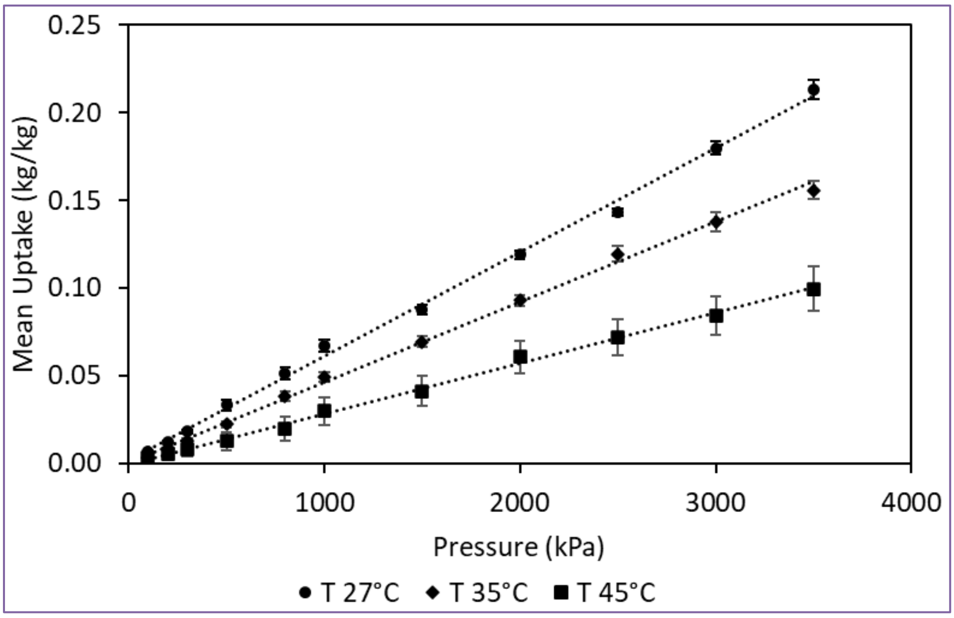

Figure 7. CO_2 adsorption capacity of PET-AC at elevated temperatures

Furthermore, PET-AC achieves exceptional CO_2 uptake (0.213 kg/kg at 27°C), demonstrating its high surface area and well-developed microporous structure, which are critical parameters for effective physisorption. The consistency and reproducibility of the results, with low standard errors and narrow error bars across multiple replicates, confirm that PET-AC operates effectively via physisorption mechanisms, validating its potential for scalable CO_2 capture applications. Subsequently, the sorption capacity of PET-AC was compared to similar adsorbents in previous studies (Table 2). While PET-AC demonstrates favorable adsorption capacity, its performance is lower compared to Commercial-AC.

The lower CO_2 uptake of PET-AC compared to Commercial-AC is attributable to differences in pore structure, surface area, and surface chemistry. Commercial-AC usually features more micropores and greater surface area, resulting in superior CO_2 adsorption. It arises because PET-AC relied solely on physical activation, a process that may limit pore optimization. To improve its performance, PET-AC can be chemically activated, surface-functionalized, or treated with combined activation methods to improve pore quality and CO_2 adsorption capacity.

Table 2. Comparison of activated carbon CO_2 adsorption

Adsorbent	T (°C)	P (kPa)	Uptake (kg/kg)	Uptake (mmol/g)	References
Commercial-AC	27	3500	0.322	7.318	[24]
ACPX-76	25	400	0.28996	6.590	[35]
PET-AC	27	3504.39	0.21313	4.844	This study
PET6KN	25	101.32	0.20152	4.580	[36]
AC P628K7063	25	100	0.18581	4.223	[37]
AC-PET	25	100	0.176	4.00	[38]
AC PET	30	100	0.05764	1.310	[39]

3.3 Toth model for CO_2 adsorption

The Toth model robustly describes adsorption on heterogeneous surfaces over broad adsorbate concentration ranges. It offers a more realistic and accurate description than the Langmuir and Freundlich models, with the flexibility to handle a wide range of temperatures and pressures. Parameters derived from the Toth model guide the design, optimization, and scaling of adsorption systems. The Toth model was used to correlate CO_2 adsorption results on activated carbon (AC). From the modeling results, the lowest deviation (1.412%) occurred at 27°C and a coefficient of determination of 99.28%. Figure 8 shows the Toth model correlation.

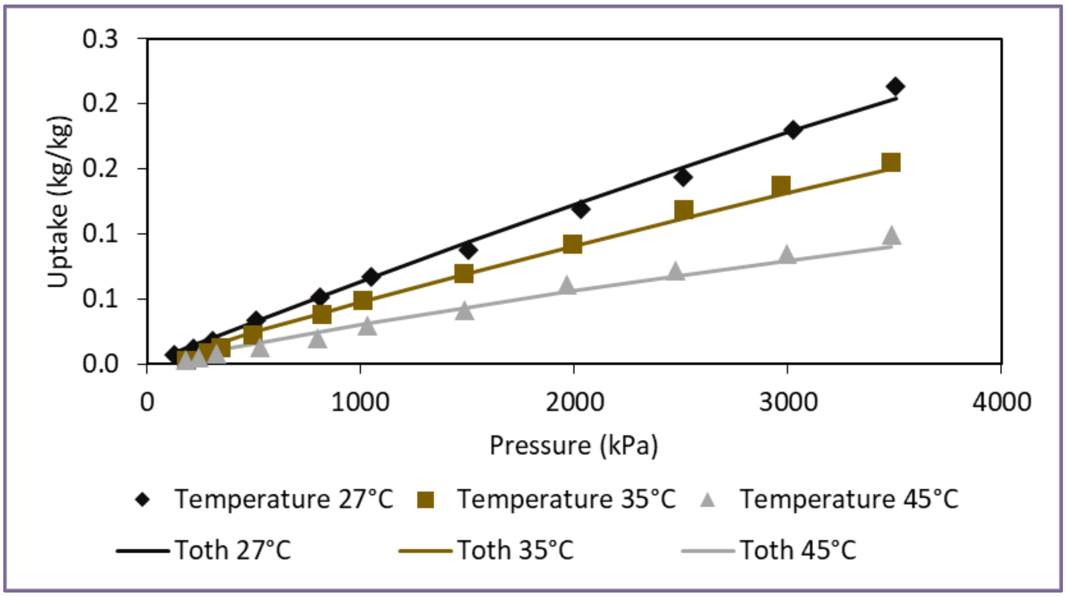

Figure 8. Isothermal adsorption correlation with the Toth model

The Toth model best describes the CO_2 adsorption on PET-AC because it accounts for the adsorbent's heterogeneous surface properties. This model assumes adsorbent surface heterogeneity and applies across low-to-high pressure ranges. Thus, it is suitable for analyzing adsorption processes under broad pressure conditions, as experimentally validated.

3.4 Heat of adsorption

The heat of adsorption reveals the nature of PET-AC's adsorption processes and quantifies adsorbent-adsorbate interactions as a function of temperature. Moreover, isosteric heat of adsorption typically decreases with increasing sorption capacity at constant temperature. It arises due to weakening adsorbate-adsorbent molecular interactions, which reduce the heat of adsorption. As shown in Figure 9, the adsorption heat calculated via the Clausius-Clapeyron equation, using Toth fittings from CO_2 adsorption test on PET-AC, was 2223.66 kJ/kg. In contrast, the CSK model yielded 2383.65 kJ/kg. The heat of adsorption obtained for PET-AC appears significantly higher than typical CO_2 physisorption for activated carbons in the literature (generally 15–40 kJ/mol).To enable direct comparison, these were converted to a molar basis, 2223.66 kJ/kg (97.84 kJ/mol) and 2383.65 kJ/kg (104.88 kJ/mol). These results exceed the expected range for physical adsorption, suggesting either a stronger interaction mechanism or the influence of experimental/modeling inaccuracies. Possible contributing factors include deviations in isotherm fitting, unaccounted chemisorption contributions, or overestimation due to limited data resolution. Therefore, further validation, either through alternative thermodynamic methods or enhanced isotherm modeling, is recommended to confirm the nature and accuracy of the adsorption energy observed in PET-AC.

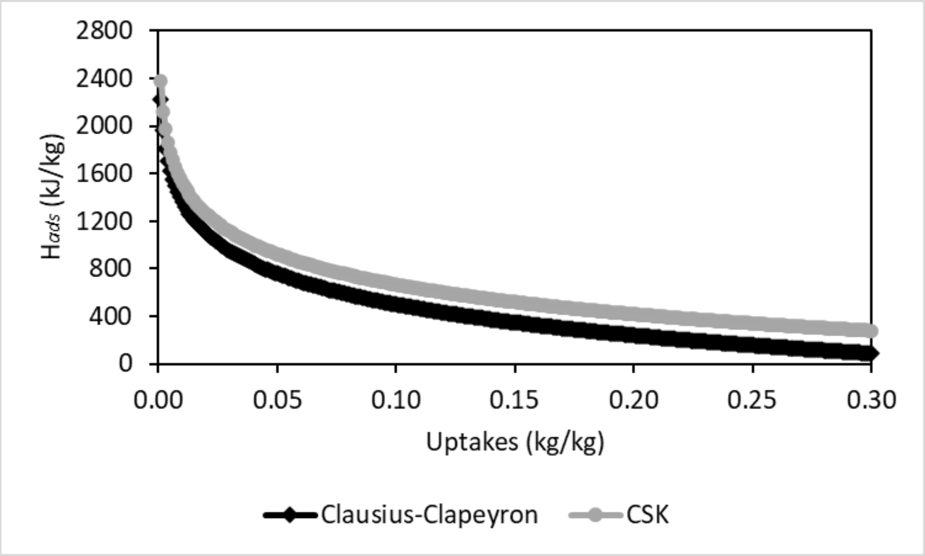

Figure 9. Heat of adsorption for CO_2 on PET-AC

3.5 Heat of adsorption and phase-chage enthalpies

Isosteric adsorption calculations use parameters obtained from the Toth equation. The equation was chosen because it has the best fitness among other models. The isosteric adsorption data are shown in Figure 10. The graph serves critical design parameters for adsorption systems utilizing activated carbon (AC), providing a foundational dataset for process optimization. The microporous characteristics of PET-AC strongly influence its CO_2 adsorption performance. PET-AC characterization falls within the microporous range (<2 nm), which is ideal for capturing small gas molecules like CO_2. Micropores deliver high-density adsorption sites and intensify van der Waals interactions—essential mechanisms for efficient physisorption. The isosteric adsorption graph further supports this, showing that CO_2 uptake is favored at lower temperatures and higher pressures, consistent with micropore filling mechanisms. Thus, the pore structure directly contributes to the material's capacity and affinity for CO_2, validating its suitability as a CO_2 adsorbent.

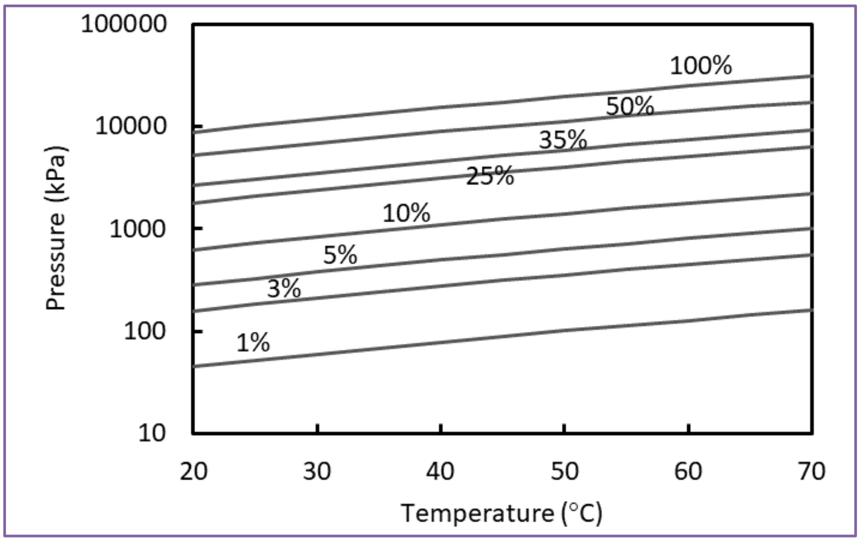

Figure 10. Isosteric adsorption of CO_2 gas on AC

4. Conclusion

This study demonstrates the feasibility of utilizing PET-AC as a sustainable adsorbent for CO_2 capture. Systematic adsorption experiments mechanistically linked thermodynamic parameters to adsorption behavior, establishing PET-AC as a circular alternative to conventional sorbents through plastic waste utilization and emission mitigation. However, several limitations should be acknowledged. The adsorption experiments employed pure CO_2 under idealized laboratory conditions, potentially diverging from real-world flue gas complexities (e.g., humidity, multicomponent gases, and impurities). Furthermore, the anomalously high isosteric heats of adsorption suggest potential methodological inconsistencies—either in unit conversion or model application, necessitating rigorous validation. Future research should focus on testing under mixed-gas conditions, exploring the effects of humidity, and conducting cyclic adsorption–desorption tests to assess material stability. Moreover, integrating advanced surface analysis techniques and optimizing post-activation treatments may further enhance the adsorption capacity and selectivity of PET-AC for industrial-scale applications.

Author's declaration

Author contribution

Awaludin Martin: Research conceptualization, writing review, supervision and funding acquisition. **Erman Taer**: Conceptualization, methodology, writing review. **Nasruddin**: Software, validation, visualization. **Nur Khotimah**: Gathering data, writing - result analysis, data analysis, visualization.

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Data Availability

The raw data of this study is available. If anyone wishes to use it as a basis for further research, please contact the corresponding author.

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Competing interest

We declare that we have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Ethical clearance

This research did not involve human or animal subjects.

AI statement

This article is the original work of the authors without using AI tools for writing sentences and/or creating/editing tables and figures in this manuscript. The manuscript underwent professional grammatical review by subject-matter experts to ensure linguistic precision.

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