

CO₂ Capture Exploration on Potassium Hydroxide Employing Response Surface Methodology, Isotherm and Kinetic Models

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ABSTRACT: *In this research, KOH has been evaluated as a solid adsorbent for carbon dioxide (CO₂) capture. The effect of pressure, temperature, and KOH loading on CO₂ adsorption in a fixed-bed reactor were investigated. Response Surface Methodology (RSM) based on the central composite design (CCD) was used to evaluate the effects of operating parameters on adsorption capacity in order to achieve the optimum conditions. The experimental values of the responses were in decent agreement with the predicted result of regression models. Techniques such as Fourier Transform InfraRed (FT-IR) spectroscopy and X-ray diffraction (XRD) were used to study the consider KOH sorbent. The results show that CO₂ adsorption is improved with the loading of 0.5 g of KOH. The maximum CO₂ adsorption capacity was acquired for KOH at temperature 45°C and pressure 6 bars. The Freundlich model was found to be the best for fitting the adsorption of CO₂ owing to the closeness of the R² to unity. Furthermore, the kinetic study specified that the first-order model is well-fitted with the experimental data. Overall, the very high surface area of KOH adsorbent makes this adsorbent new promising material for CO₂ capture.*

KEYWORDS: *CO₂ adsorption; KOH sorbents; Response Surface Methodology (RSM); Isotherm; Kinetics*

INTRODUCTION

The rise in carbon dioxide (CO₂) emissions is considered as the central cause of the climate change in the 21st century [1-8]. Fourth report of Intergovernmental

Panel on Climate Change (IPCC) shows that the growth of 0.74 °C on average global temperature during 1906-2005[9-14]. The temperature is also projected

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to increase up to 6.4 °C till 2100 that leads to an increase in sea level up to 59 cm [15, 16]. Several technologies have been proposed to reduce and eliminate carbon dioxide emissions, which comprise a development in energy efficiency, shift to lower carbon-fuel material and renewable energy [16-21]. Commonly used approaches to capture CO₂ from flue gas are adsorption, absorption, cryogenic distillation, and membrane separation. However, the current commercial CO₂ capture technologies are expensive and energy intensive. Improving the technologies for CO₂ adsorption is essential in order to reach low energy rewards [19-24]. CO₂ adsorption is typically exploited as a final polishing step in the hybrid CO₂ capture organization. Ideal CO₂ adsorbents should have the following characteristics: a high specific surface area, well-developed micro and mesopores, and many active sites on the surfaces, such as amine functional groups and basic metal oxide [15-24]. Till today, several adsorbents such as zeolites, alumina, mesoporous silica, CaO, and porous carbons have been used for CO₂ adsorption (Table 1, Fig. 1) [3-7]. The studies in Table 1 show that the correction of adsorbents is accomplished with two objectives: structural modification and the addition of functional groups on the adsorbent surface. Fig. 1 shows that carbon dioxide is absorbed by two techniques of physical adsorption and chemical adsorption in the post-combustion method. In the physical adsorption, the adsorbents are including mineral absorbers, zeolites, and metal-organic frames. In the chemical adsorption, the adsorbents are modified with amines and react with carbon dioxide. Also, lithium and calcium base adsorbents are also chemical adsorbents.

Furthermore, potassium hydroxide (KOH), a solid adsorbent, can adsorb considerable amount of CO₂ and can be simply regenerated. Likewise, the separated CO₂ stream from the regeneration column is of excessive purity [25]. KOH has been engaged as a sorbent in order to capture CO₂ from flue gas stream. It increases profits by lowering operating temperature as well as reduced heat consumption. According to Lee et al. (2014) [26], an activation of specific KOH caused a growth of specific surface area and total pore volume, which caused in the improvement of CO₂ adsorption capacity. A similar conclusion was drawn by de Andres et al. (2013) [27]. Wei et al. (2012) [28] stated a high surface area and CO₂ uptake at high pressure (3.57MPa) with KOH. A biological material (Ubago-Perez et al., 2006) [29] was also

employed for construction of different granular and powder achieved by KOH activation. In the design and statistical evaluation of experiments, Response Surface Methodology (RSM) can be used for process modeling and optimization [11, 17]. Consequently, in the current study, RSM based on central composite design was exploited to design experiments, build models and measure the optimum modification circumstances for desirable responses. The main impartial of current study was to explore the influence of modification parameters (temperature, pressure, and amount of adsorbent) on the CO₂ adsorption/desorption performance of the modified adsorbents in a batch fixed-bed reactor. These models presented the significance of variables and the interactions among them on the CO₂ adsorption process.

EXPERIMENTAL SECTION

Apparatus and chemicals

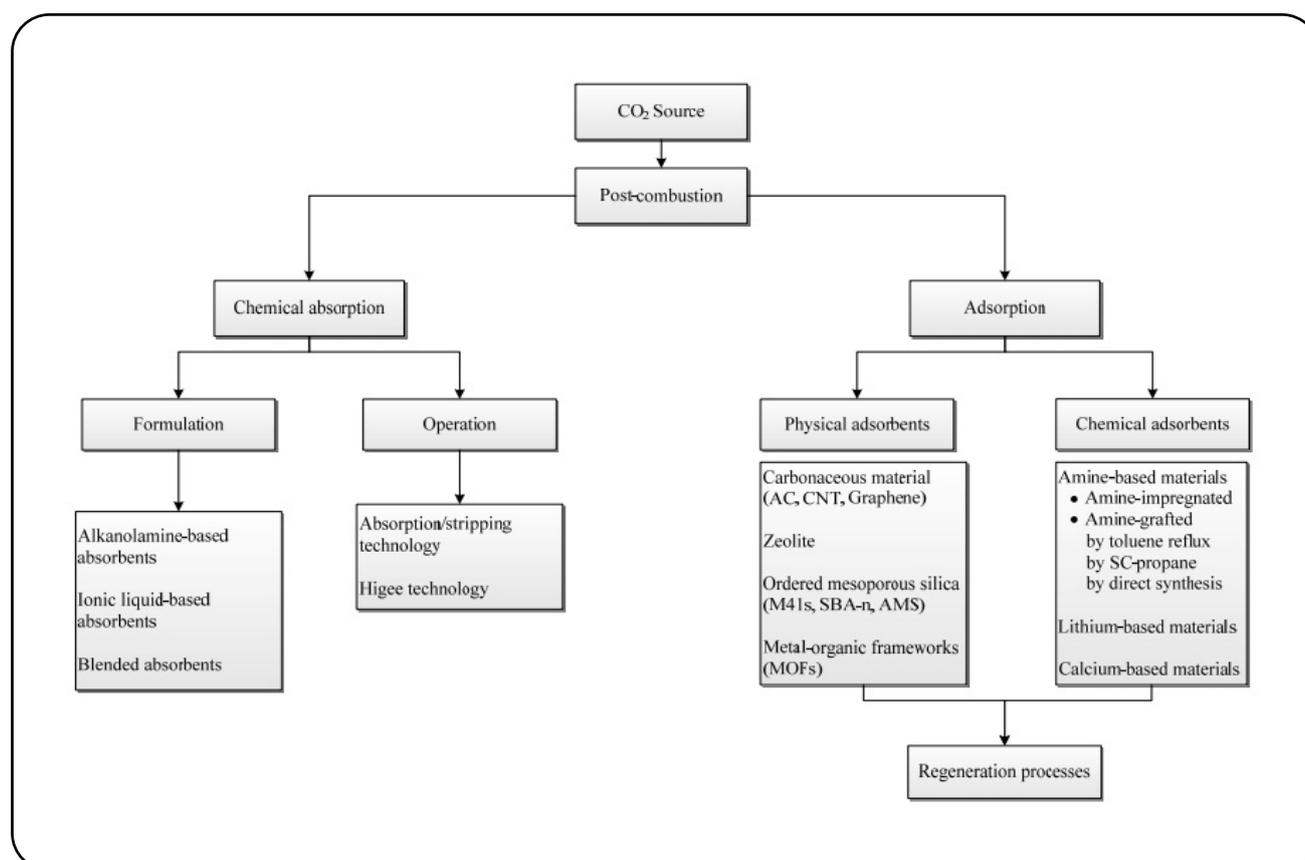
CO₂ gas was delivered by Sabalan Gas Co. (Tehran, Iran) with purity of 99.9%. All other reagents were analytical grade from Merck (Darmstadt, Germany). Deionized (DI) water (resistivity=18MΩ, Milli-Q system, Millipore Inc.) was used for rinsing and arranging all aqueous solutions. The X-ray powder diffraction (XRD) analyses were also done on a Rigaku D/max 2500 V instrument with a graphite monochromator and a Cu target. The XRD was used for characterization of adsorbent composition. The Fourier Transform InfraRed (FT-IR) evaluations were also achieved by a Bruck Equinox 55 IR spectrophotometer through the KBr pellet technique.

Setup procedure

Fig. 2 offers the set up used in this exploration. As exposed in this figure, a batch reactor was employed to explore the influence of the dominant operating parameters on CO₂ adsorption. The reactor has a cylindrical bed. It was filled with KOH sorbent particles. KOH samples, which is in powdered form had been organized and put in a 155 ml cell in a batch reactor in order to assess the CO₂ adsorption capacity. A perforated plate was mounted at the bottom of the reactor bed to allow the gas to flow through the bed. Each sample is in a several weight. Before starting the experiments, we should check and set some parameters. Originally, the pressure gage and heater was set at wanted set points by regulator valve and thermostat separately. After that, in order to the CO₂ gas

Table 1: Reported chemicals for modification of carbonaceous material-based adsorbents and their general effects.

Chemicals	Effects	Ref.
NH ₃ heat treatment	Surface area development and the introduction of alkaline nitrogen groups increase CO ₂ adsorption	[3]
Monoethanolamine	Surface area decreases, but the introduction of alkaline nitrogen groups increases CO ₂ adsorption	[3]
Amines	Amine impregnation increases the basicity, nitrogen content and microporous volume of the activated carbon. CO ₂ capture does not vary linearly with surface area. The CO ₂ adsorption capacities are resulted from the reaction with amine groups. Amine impregnation exhibited different results for different carbonaceous materials.	[4]
KOH	One of the best activating reagents for increasing CO ₂ adsorption etches the soft components of carbonaceous material and increases the number of pores and surface area	[5]
H ₃ PO ₄	Surface area and number of mesopores (2 nm<diameater<50 nm) increase while the size of CO ₂ is 209 pm due to which CO ₂ adsorption increases slightly	[5]
ZnCl ₂	ZnCl ₂ increases surface area and mesoporosity where mesopores are not compatible with CO ₂ size. Thus, CO ₂ adsorption increases very slightly	[5]
NaOH	Surface area decreases as compared to virgin AC, but CO ₂ adsorption increases due to the oxygen-containing functional groups and the formation of basic surface sites for CO ₂ chemisorption	[6]
Metal Oxide	Relatively, CO ₂ adsorption capacity is small for carbonaceous material impregnated with metal oxide. The reason is the large molecular size of metal oxide that blocks the pores	[7]

**Fig. 1: Various types of adsorbents.**

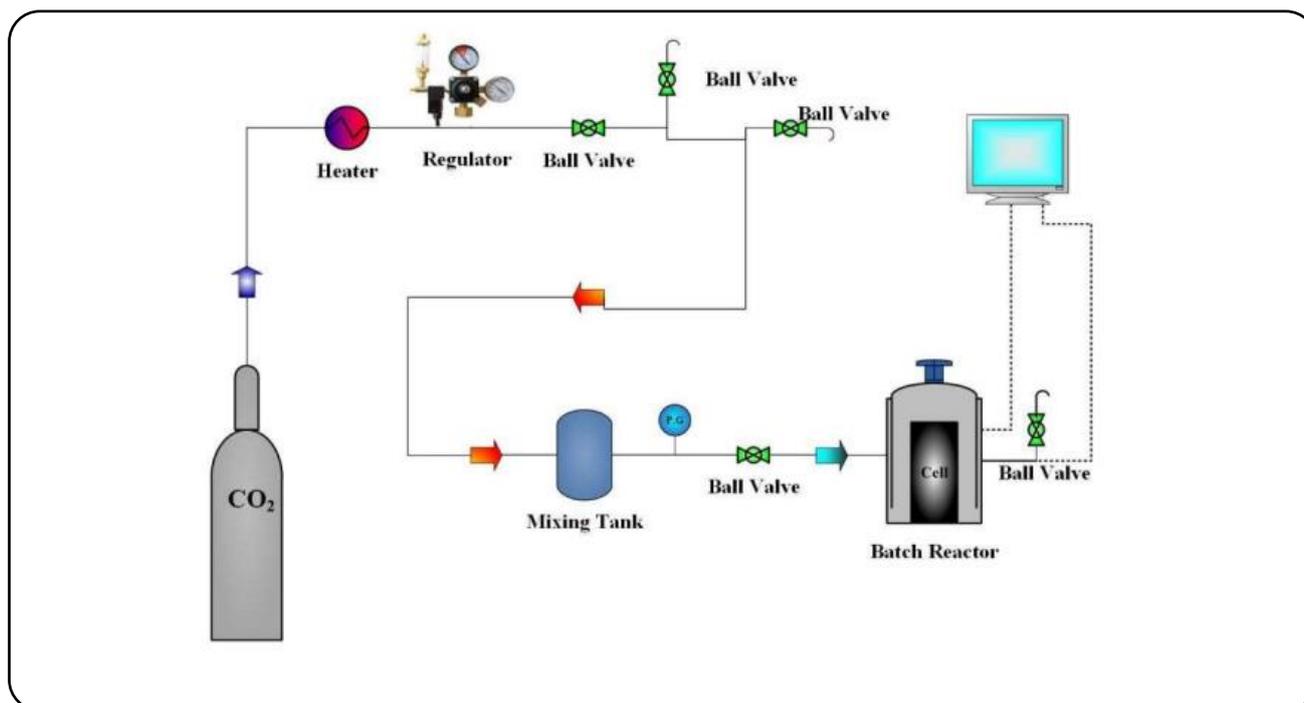


Fig. 2: Adsorption experimental set up.

stream flowing in a tube, the valve of a cylinder was opened. As presented in the Fig. 2, CO₂ gas is entering rotameter at the top, after passing through regulator and mixing tank in order to switch flow rate of gas. Finally, the experiment was started by pushing start key. All of the data was stored in a separate excel files for an hour in reference computer which temperature was at °C, pressure at bar, time at second and date. The CO₂ adsorption rate as the alteration between initial and final of CO₂ pressure by the gas sensor was determined.

CO₂ adsorption capacity assessment

The adsorption percentage of adsorbent was considered consuming Eq. (1). Where, P_i , is initial pressure, P_f is final pressure in the reactor. The adsorption capacity of adsorbent was calculated through the following equation Eq. (2). Where, P_e is equilibrium pressure, V is the volume of the reactor, M_{CO_2} is molecular weight of CO₂, T is temperature, m is adsorbent weight and R is world gas constant. The correlation coefficient (R^2) was also used to determine the best-fitting models to the experimental data. Where, q_{cal} is CO₂ adsorption capacity obtained using kinetics and isotherm models; q_{exp} is experimental adsorption capacity of CO₂ [30].

$$\text{Adsorption (\%)} = \frac{P_i - P_f}{P_i} \times 100 \quad (1)$$

$$q_e = \frac{(P_i - P_e) \cdot V \cdot M_{CO_2}}{z \cdot R \cdot T \cdot m} \times 1000 \quad (2)$$

RESULTS AND DISCUSSION

Response surface methodology analysis procedure

In the current case, the three independent variables effects, containing temperature, pressure and KOH loading on the CO₂ adsorption capacity were examined using central composite design. These variables, along with their respective regions of interest, were chosen based on the literature and preliminary investigations [30]. Table 2 presents the range and levels of the independent numerical variables in terms of actual and coded values. The chief operating parameters such as temperature, pressure and KOH loading of various samples have an influence on the CO₂ adsorption capacity. In this study, these effects have been experimentally examined using RSM method. The suitable circumstances for CO₂ capture using dry KOH have been deliberated. RSM method was applied to project the experiments and to explore the experimental data. Table 3 shows the experimental runs recommended by RSM technique.

Table 2: Independent numerical variables and their levels (actual and coded).

Independent numerical variables	Unit	Symbol	Coded variable levels -2 -1 0 1 2
Temperature	°C	X ₁	25, 35, 45, 55, 65
Pressure	bar	X ₂	2, 4, 6, 8, 10
Adsorbent	gr	X ₃	0.5, 1, 1.5, 2, 2.5

Table 3: ANOVA results for RSM-CCD model of q_e response.

Analysis of variance (q _e)					
Source	Sum of Squares	df	Mean Square	F-Value	p-value Prob > F
Model	69799.16	3	23266.39	13.69	0.0001
A-temperature	27408.95	1	27408.95	16.13	0.0010
B-pressure	23372.14	1	23372.14	13.75	0.0019
C-adsorbent	19018.06	1	19018.06	11.19	0.0041
Residual	27192.62	16	1699.54	-	-
Lack of fit	16558.86	11	1505.35	0.71	0.7067
Pure Error	9691.79	19	-	-	-

A-temperature, B-pressure, and C-adsorbent affect the response variable significantly; this consequence has been taken from the information given in the p-value column of Table 3. As shown in Table 3, the model P-value is lower than 0.001, which displays that the model terms are highly significant. P-values less than 0.05 and 0.001 indicate that the model terms are significant and highly significant in the model, respectively. While P-values greater than 0.1 indicates that the model terms are not significant [18]. In order to industrialize alkali metal-based sorbent, the effects of the operation conditions on CO₂ capture performance should be determined in details (Table 4). There are 8 factorial points, 6 axial points and 6 replicates at the center points, indicated by a total of 20 experiments, as calculated from $N=2^n+2n+n=20$.

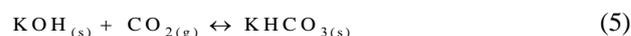
In addition, as can be perceived in Fig. 3, the experimental values for responses were in decent agreement with the amounts predicted by the RSM model. In Fig. 3 the predicted values acquired was more close to the experimental values due to have high R². Fig.4 and Fig. 5 explain the dimensional response surfaces which show the effects of the significant variables (X₁, X₂, X₃).

Adsorbents morphological and structural characteristics

Fig. 6 shows the XRD spectra before the CO₂ capturing process for KOH. It can be observed that XRD patterns of

KOH have the same characteristic peaks for its standard spectra. Before the CO₂ capture runs, KOH samples should be passed XRD test to make sure that they have an appropriate crystallization. Fig. 6 proves an XRD pattern of our samples. It can be seen that there are two important peaks at around 32°, 35°, and some small peaks from 40° to 50°. As compared with the individual commercial materials KOH, it is offering decent agreement.

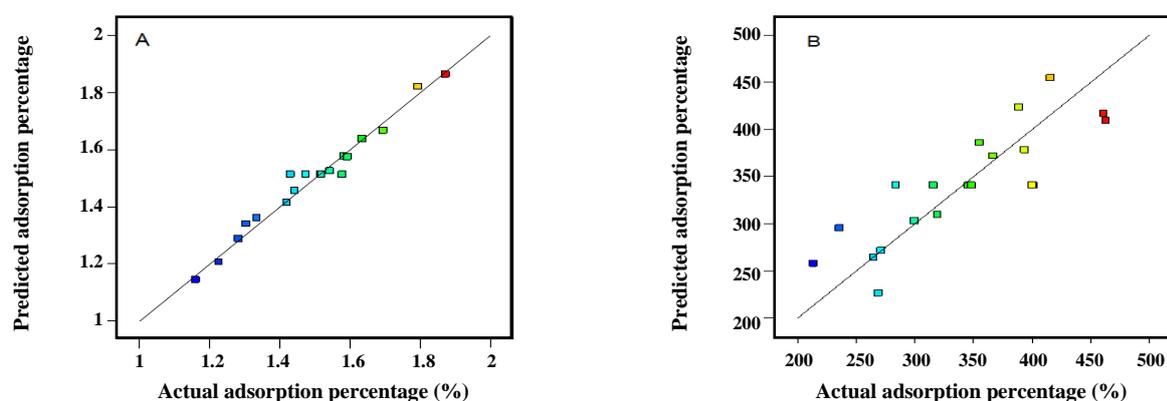
KOH which is in powdered form had been prepared. FT-IR spectrometer was employed to carry out FT-IR (fourier transform infrared) spectroscopy analysis. FT-IR was achieved to recognize the surface functional groups on the KOH. The spectra of the KOH samples were offered in Fig. 7. There are two curves for FTIR in this work one for KOH and another for K₂CO₃ (Eq. 4 and Eq. 5).



The spectra noticed between 4000 and 400 cm⁻¹. In Fig. 7, 1460 cm⁻¹ spectrum are clear for carbonate group in the K₂CO₃ curve and also in KOH when its turn to potassium carbonate. The H₂O release came later than the CO₂ adsorbed on the surface of KOH, and the variation of steam release characteristics with time in terms of the rate and amount was also varied from that in the CO₂ adsorption.

Table 4: The effects of the operation conditions on CO₂ capture performance.

		Factor 1	Factor 2	Factor 3	Response
Std	Run	A: Temp	B: Pressure	C: Absorber	mg/g
15	1	45	6	1.5	284.039
13	2	45	6	0.5	462.964
2	3	55	4	1.0	393.592
8	4	55	8	2.0	355.281
7	5	35	8	2.0	299.777
17	6	45	6	1.5	345.945
5	7	35	4	2.0	269.015
11	8	45	2	1.5	265.006
6	9	55	4	2.0	319.405
14	10	45	6	2.5	271.441
3	11	35	8	1.0	367.006
4	12	55	8	1.0	415.643
12	13	45	10	1.5	460.825
20	14	45	6	1.5	315.802
10	15	65	6	1.5	388.620
1	16	35	4	1.0	235.815
18	17	45	6	1.5	348.325
16	18	45	6	1.5	400.943
19	19	45	6	1.5	400.030
9	20	25	6	1.5	213.661

Fig. 3: Predicted vs. experimental values of CO₂ (A) adsorption percentage, and (B) adsorption capacity.

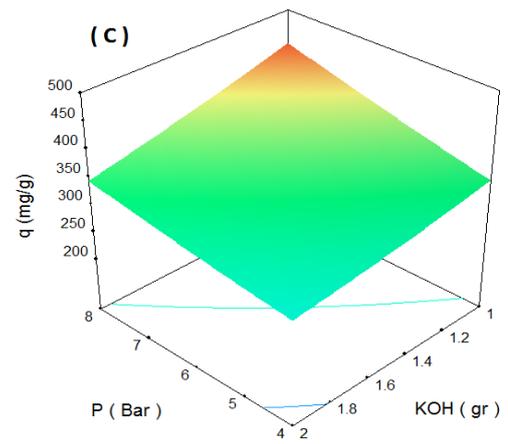
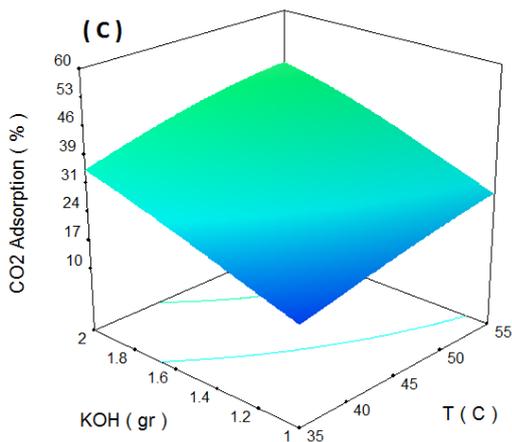
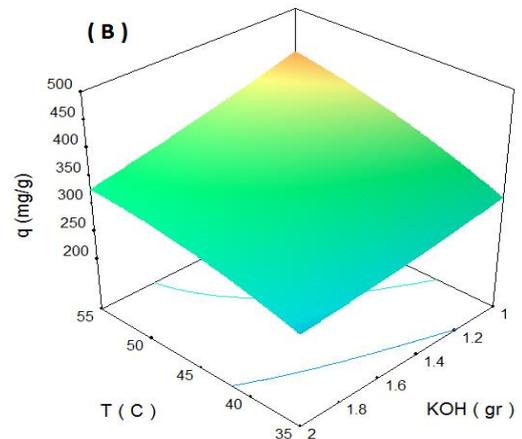
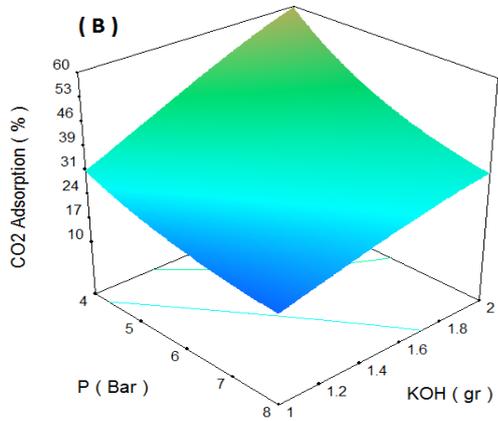
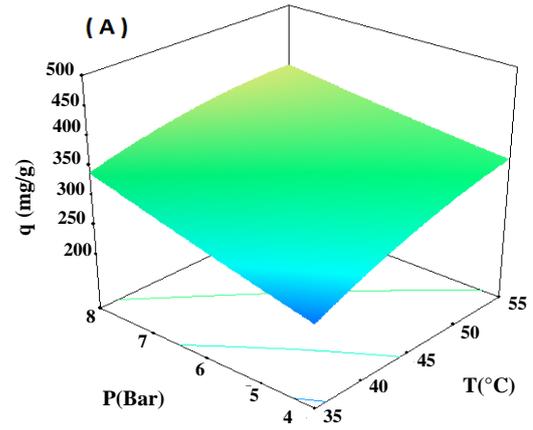
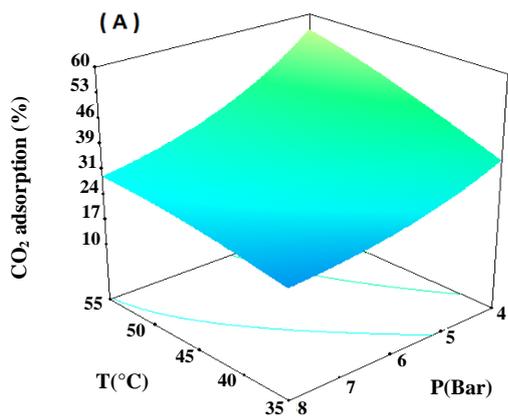


Fig. 4: Response surface plot of CO₂ adsorption percentage of KOH (effect of temperature, pressure, Absorber).

Fig. 5: Response surface plot of CO₂ adsorption capacity of KOH (effect of temperature, pressure, Absorber).

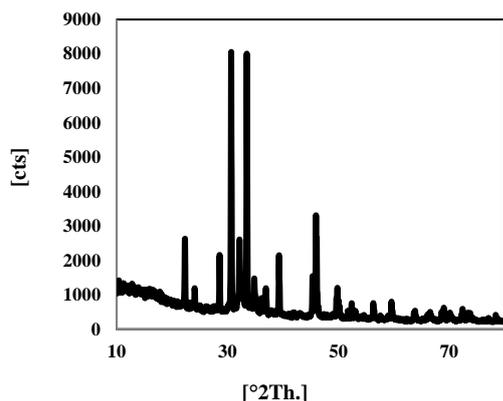


Fig. 6: XRD spectra before the CO₂ capturing process for KOH.

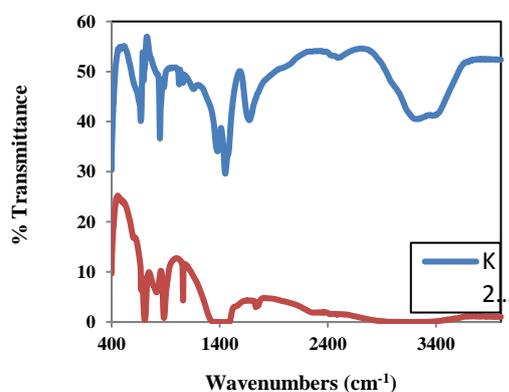


Fig. 7: FT-IR two curves for KOH and K₂CO₃.

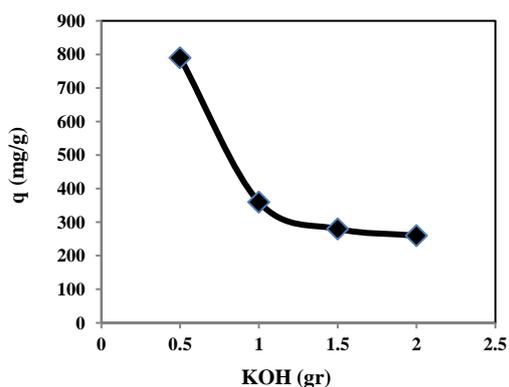


Fig. 8: Effect of adsorbent on CO₂ adsorption capacity.

These exhibit that their action between KOH and CO₂ did not occur directly by following Eq. 4. The delayed release of H₂O should imply that the formed H₂O in CO₂ adsorption was stored in the sorbent. An intermediate carbonate could present in their action procedure so that the reaction of CO₂ with KOH did not form K₂CO₃ and H₂O directly [31-32].

Adsorbent amount effect

KOH loading leads to a growth in CO₂ removal rate due to a direct growth in the reactant amount (i.e., KOH) in the reaction system along with an increase in gas–solid contact surface (Fig. 8). Furthermore, the KOH particle size effect has been reflected using fine KOH with the average size of 500 to 700 μm diameter and coarse KOH with the average diameter of 1250 μm. Diameter of the fine KOH particles was half of the coarse particles. The reduction of particle diameter caused to increase the gas–solid contact surface causing in a faster equilibrium achievement. In current temperature, the vital time to reach equilibrium for fine particles is about half of the time essential for the coarse particles.

Temperature effect

Fig. 9 displays that the optimal temperature for CO₂ removal is 45°C. To describe the perceived trend in Fig. 9, it can be noted that an increase in temperature leads to an increase in carbonation reactions (i.e., forward reactions in Eqs. (4) and (5)). However, above 45°C, the price of reaction become unfavorable, subsequently, the optimal temperature for the present CO₂ removal system is 45°C.

Pressure effect

Several examinations were attained at the CO₂ different pressure under the optimized conditions. In this set of experiments, temperature and KOH loading are the same. According to air sampling, in these investigations, air with CO₂ pressure can simulate Tehran ambient air. In current case, air with higher CO₂ pressure can simulate air in highway tunnels. It is exciting to note that these consequences imply the final CO₂ pressure is controlled by the chemical equilibrium of carbonation reactions (Fig. 10).

Kinetic modeling

The kinetic analysis establishes an adsorption uptake rate and defines the residence time for the adsorption

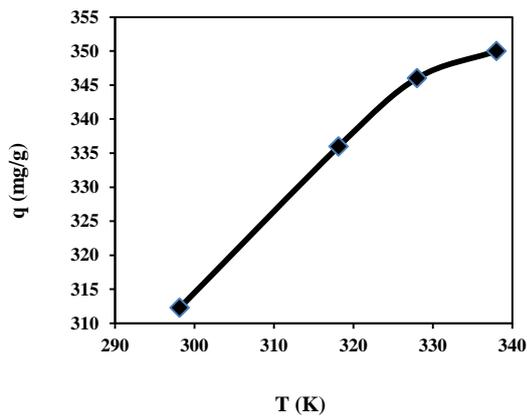


Fig. 9: Effect of temperature on CO₂ adsorption capacity.

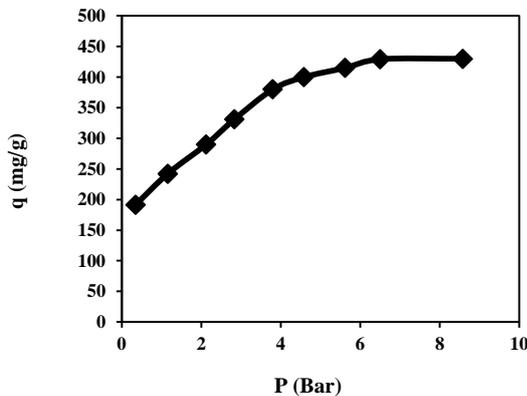


Fig. 10: Effect of pressure on CO₂ adsorption capacity.

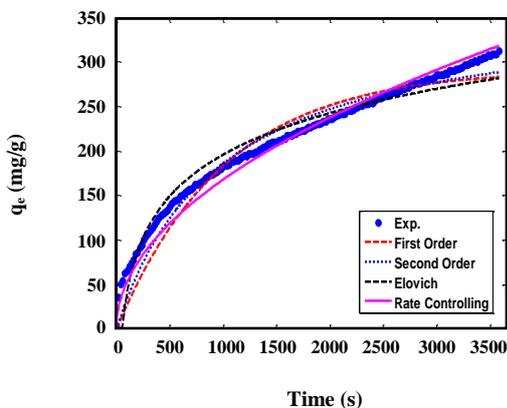


Fig. 11: Experimental and modelled kinetics adsorption for KOH.

process to be completed [20]. It is also a baseline form measuring the adsorption dynamics and its presentation in the real application, such as in fixed-bed system. Accordingly, numerous models were attained in current work. In this case, the R^2 values attained were large at all the temperature deliberated, and the experimental values agree with the calculated values acquired from the linear plots. Based on R^2 values (Table. 5, Fig. 11), first order kinetic model as simple model with novel information was designated.

Isotherm modeling

Adsorption isotherms are employed to define the surface properties and affinity of the adsorbent. Correspondingly, the performance of an adsorbent can be considered by adsorption isotherm data, which can be achieved by a series of experimental examinations. Modeling the adsorption isotherm data is a demanding way for predicting and comparing the adsorption performance, which is critical to improve the adsorption mechanism pathways, for expression of the adsorbents capacities, and effective design of the adsorption organizations. The equilibrium sorption isotherm is essential for the design of sorption systems. The equilibrium relationships between sorbent and sorbate are defined by sorption isotherms, the ratio between the amount adsorbed and that remaining in the reactant at a fixed temperature at equilibrium. In the present case, for exploring the sorption isotherm, 3 normally employed adsorption models; isotherms were exploited to assess the feasibility of adsorbate–adsorbent interaction (Table 6, Fig. 12) [15]. The predicted isotherm constants for the CO₂ adsorption and the corresponding R^2 value from the nonlinear regression process are exposed in Table 6. Based on Table 6, the Langmuir constant, k_L and Freundlich constant, k_F that relates to the adsorption affinity decreases at high temperature, consequently, imply a chemisorption performance. The reduction in CO₂ adsorption was acceptable at raised temperatures. The exothermic behavior of the CO₂ adsorption is in parallel with the q_m value that tends to reduce with growth in the adsorption temperature. Moreover, the favorability of the adsorption procedure can be specified by a separation factor, R_L . In addition, favorability of the CO₂ adsorption can be continued by the Freundlich constant [15]. On the basis of R^2 value, the Freundlich model gives the best fit towards the experimental data over the entire temperature range.

Table 5: Kinetic parameters of KOH.

Kinetic model	Parameter	25 °C	45 °C	65 °C
First order $q_t = q_e (1 - e^{-k_f t})$	q_e	291.539	357.449	379.767
	k_f	0.001	0.001	0.001
	R^2	0.9786	0.9882	0.9931
Second order $q_t = (q_e^2 k_s t) / [1 + q_e k_s t]$	q_e	366.757	484.296	513.502
	k_s	2.8e-6	1.2e-6	1.4e-6
	R^2	0.9858	0.9901	0.9878
Elovich $q_t = (1/\beta \ln(\alpha\beta)) + (1/\beta \cdot \ln t)$	α	2.7e-4	0.00016	0.0001
	β	67.226	80.439	99.275
	R^2	0.9782	0.9639	0.9729
Rate Controlling $q_t = k_{id} t^{0.5}$	k_{id}	5.315	5.736	6.598
	R^2	0.9980	0.9987	0.9675

Table 6: Isotherm models parameters for CO₂ adsorption using KOH.

Model	Parameter	Value	R^2
Langmuir $q_e = (q_m k_L P_e) / (1 + k_L P_e)$	q_m	468.593	0.9513
	k_L	1.104	
Freundlich $q_e = k_f P_e^{1/n}$	n	3.530	0.9825
	k_f	248.105	
DubininRadushkevich $q_e = q_m e^{-\alpha P_e^2}$	q_m	388.766	0.8272
	E	2.491	

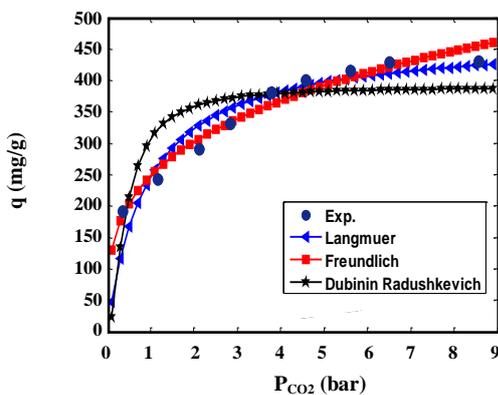


Fig. 12: Experimental equilibrium data and isotherm models.

Thermodynamic modeling

In engineering practice entropy and Gibbs free energy factors should be deliberate in order to define what process will occur spontaneously. The thermodynamic parameters

of the CO₂ adsorption process in terms of the Gibbs free energy change (ΔG°), variation in enthalpy of reaction (ΔH°), and change in entropy of adsorbate and adsorbent interaction (ΔS°) can be calculated from Van Hoff's formulation, as given in equations 6 to 8 [30, 33].

$$\ln K_d = (\Delta S^\circ / R) - (\Delta H^\circ / RT) \quad (6)$$

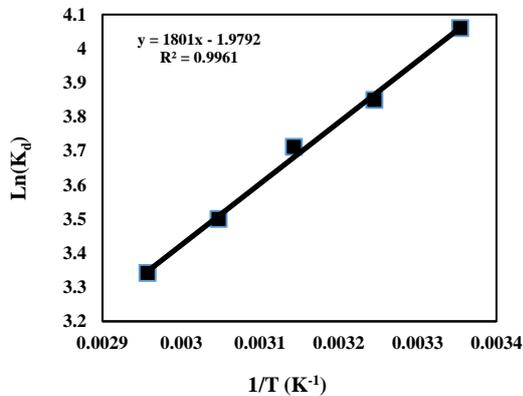
$$K_d = (P_i - P_e) \times (V / W) \quad (7)$$

$$\Delta G^\circ = \Delta H^\circ - T\Delta S^\circ \quad (8)$$

The thermodynamic parameters values are offered in Table 7. Based on the experimental findings, the negative value in ΔH° shows an exothermic nature of the CO₂ adsorption procedure, whereas negative ΔS° value proposes high orderliness of the adsorbate molecules upon adsorption. The negative ΔS° can be interpreted by the behavior of the CO₂ adsorption process, which is from randomized to an ordered form on the surface of the adsorbent. Fig. 13

Table 7: Thermodynamic parameters of CO₂ adsorption.

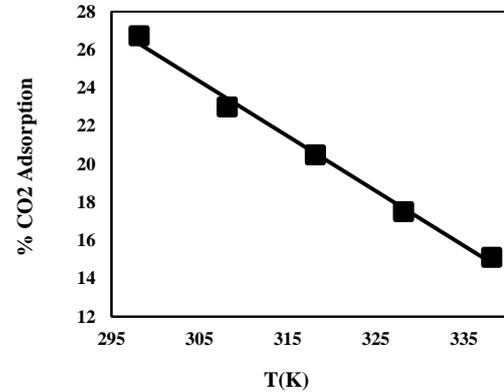
P _{CO₂}	ΔH° (kJ/mol)	ΔS° (kJ/mole K)	ΔG° (kJ mol ⁻¹)				
			25 °C	35 °C	45 °C	55 °C	65 °C
4.00	-14.975	-0.017	-10.068	-9.903	-9.739	-9.574	-9.409

Fig. 13: Plot of $\ln K_a$ vs. $1/T$ for the adsorption of CO₂.

exhibits that the distribution coefficient (K_d) values improved with the rise in temperature depicting the exothermic nature of the adsorption. Furthermore, as offered in Table 6, the ΔG° for all the temperatures is negative and increase in the value of ΔG° with an enhance in temperature displays that the reaction is easier at low temperature. Also, the CO₂ adsorption percentage of the adsorbent reduces growth in temperature (Fig. 14).

CONCLUSIONS

In this research, CO₂ capture by carbonation of KOH has been experimentally investigated. The effects of various operating parameters including KOH loading, temperature, and pressure on the CO₂ removal rate were wisely examined using RSM method. FT-IR and XRD techniques were used to study the consider KOH sorbent. Numerous isotherm models including Freundlich, Langmuir, and Dubinin Radushkevich are exploited to fit the experimental adsorption data. According to the analysis, Freundlich isotherm model is found to give the finest fit to the experimental data over the whole temperature range due to the highest of regression coefficient (R^2) and closeness to unity, consequently, implies a perfect fit to the experimental data. Furthermore, the kinetic analysis establishes an adsorption uptake rate and regulates the residence time for the adsorption

Fig. 14: Variation of CO₂ adsorption percentage with temperature.

procedure. As a conclusion, high surface area of KOH adsorbent makes this adsorbent a new promising material for CO₂ capture and for other relevant requests.

Nomenclature

K_L	Langmuir constant, bar ⁻¹
k_F	Freundlich constant, cm ³ /g.bar ^{1/n}
k_T	Temkin constant, cm ³ /g.bar
k_f	Rate constant of pseudo-first order adsorption, min ⁻¹
k_s	Rate constant of the pseudo-second order kinetics, g/mg.min
k_2	Reaction rate constant of Ritchie second order equation, min ⁻¹
k_{id}	Intraparticle diffusion rate constant, mg/g.min
M_{CO_2}	Molar mass of carbon dioxide, g/mol
M	Mass of adsorbent, g
N	Total number of experiments required
N	Number of variables
n_H	Hill cooperatively coefficient of the binding interaction
P_i	Initial pressure, bar
P_e	Equilibrium pressure, bar
q_e	Equilibrium adsorption capacity, mg/g, cm ³ /g
q_e^-	Average of q_e , mg/g
q_m	Maximum CO ₂ adsorption capacity, cm ³ /g
q_s	Hill isotherm maximum uptake saturation, mg/L
q_t	Amount of adsorbed CO ₂ at time t

R	Universal gas constant, 8.314 J/mol.K
R ²	Correlation coefficient
R _L	Dimensionless constant
T	Temperature of the reactor, K
t	Reaction time, min
V	Volume of the reactor occupied by the CO ₂ gas, mL
W	Grams of adsorbent, g

Greek Letters

A	Initial adsorption rate, mg/g.min
B	Desorption constant, g/mg
λ	D-R constant, mol ² /J ²
ω	Polanyi potential (equivalent to RT ln(1/1+P))
ΔH°	Enthalpy change, kJ/mol
ΔS°	Entropy change, kJ/mol.K
ΔG°	Gibbs free energy change, kJ/mol

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