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Modeling and Optimization of Carbon Dioxide Removal in Packed Bed Column Reactor

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Abstract **- Global warming due to greenhouse gases has become a serious global issue. Extensive efforts are being made to fighting this phenomenon through carbon capture as carbon dioxide (CO_2) is its major contributor. This study focused on CO_2 capture in packed bed column reactor using Poly-(D) glucosamine under the various process parameters such as temperature, feed flow rate and mass of the adsorbent. Statistical design of experiments was carried out in order to analysis the effect process parameters on the capacity of CO_2 capture in packed bed column. The obtained results show that feed flow rate has the significant affect compared to others. The maximum of 956 mg of CO_2 is captured under the following operating conditions; temperature of 40°C, feed flow rate of 30 ml/min and 0.25 g of the Poly-(D) glucosamine. The ability of Poly-(D) glucosamine to capture the CO_2 in packed bed column is confirmed.**
Keywords: **CO_2 Capture, Packed Bed Column, Poly-(D) Glucosamine, Adsorption, Optimization**

I. INTRODUCTION

Nowadays, fossil fuels are the key conventional energy source and consumption of them will increase constantly, every day [1]. The combustion of very huge amount of fossil fuels releases, carbon dioxide and other greenhouse gases that have a significant impact on global warming and climate change. The global warming and greenhouse effect have become serious global environmental issues [2]. The content of carbon dioxide in the atmosphere has increased from 2.84×10^{-4} before the industrial revolution to 3.56×10^{-4}. Hence, the stability, safety and environment acceptability of CO_2 capture methods have been paid worldwide notice. Therefore, there is critical need to develop a technology, which reduces the carbon dioxide in atmosphere [3].

The technologies include the chemical absorption and adsorption methods, membrane separation and chemical looping combustion, underground storage technology, terrestrial vegetation and marine microalgae fixation were used for CO_2 capture. Among these technologies, adsorption is the most favorable technique because of its advantages such as high adsorption capacity, low cost and easy to operate [4]. Moreover, the key desired characteristics of the adsorbent in adsorption is high density (it allows operation at higher velocity, so smaller adsorber vessels are needed for carrying out preferred level of separation), a wide particle size allocation and high porosity (reduced mass transfer resistances and resulting in enhanced dynamic adsorption capacity. Packed beds reactors are mainly used for CO_2 capture using various adsorbents [5]. The advantage of using a packed bed reactor is the higher conversion per weight of catalyst than other catalytic reactors [6]. The conversion is based on the amount of the solid catalyst rather than the volume of the reactor. Many researchers have reported the impact of parameters (temperature, feed flow rate and mass of the adsorbent) on the performance of packed beds, with different adsorbents and columns. Moreover, optimization of theses parameters will improve the adsorption performance [7-9].

Best of our knowledge, none of studies were reported for the CO_2 capture in packed bed column via statistical methods. Response surface methodology (RSM) coupled with Box-Behnken design (BBD) is a statistical method which used to analyze the influence of effect process parameters in various process [10]. Hence, in this study an attempt has been made to study the individual and interactive effect of process parameters such as temperature, feed flow rate and mass of the adsorbent on CO_2 capture in packed bed column. Also the response surface methodology coupled with numerical optimization was applied to model and optimize the CO_2 capture process in packed bed column. It is believed that, the results obtained from this study will be useful understand the relationship between the process parameters and CO_2 capture, mathematically.

II. MATERIALS AND METHODS

A. Chemicals and Experimental Setup

The entire chemical used in this study is analytical grade and purchased from local suppliers. The experimental set up used in this study was reported in elsewhere (Muofhe *et al.*, 2017) with slight modifications. The performance evaluation of Poly-(D) glucosamine was determined using a gas mixture containing CO_2 (15%) and N_2 (85%).

B. Modeling

Response surface methodology (RSM) coupled with Box-Behnken design (BBD) was used to analyze the influence of effect process parameters on CO_2 capture in packed bed column. Experimental runs were established based on a BBD and the complete design consists of 17 experiments were designed and the obtained data was analyzed by multiple regression analysis [11]. Then, the individual and interactive effects of process variables on CO_2 capture in packed bed column were determined by constructing response surface plots. Finally, optimization of process variables for maximum CO_2 capture was carried out by numerical optimization technique [12]. All the statistical analyses were carried out with Stat ease Design Expert 8.0.7.1.

III. RESULTS AND DISCUSSION

A. Effect of Temperature

Temperature is one of the key process variables for the packed bed column performance on CO_2 capture. To examine effect of temperature on CO_2 capture experiments were carried out in temperature (25– 75°C) and the results are shown in Fig. 1.

From the observations, it is found that, the CO_2 capture is increased rapidly with increasing the temperature upto 60°C. This phenomenon could be explained by that, the increase in temperature increases the adsorption capacity Poly-(D) glucosamine, which improves the CO_2 capture.

Beyond, temperature of 60°C shows the negligible effect on CO_2 capture. Similar observations were obtained for carbon dioxide adsorption hysteresis in ultramicroporous metal-organic frameworks (MOFs) [13].

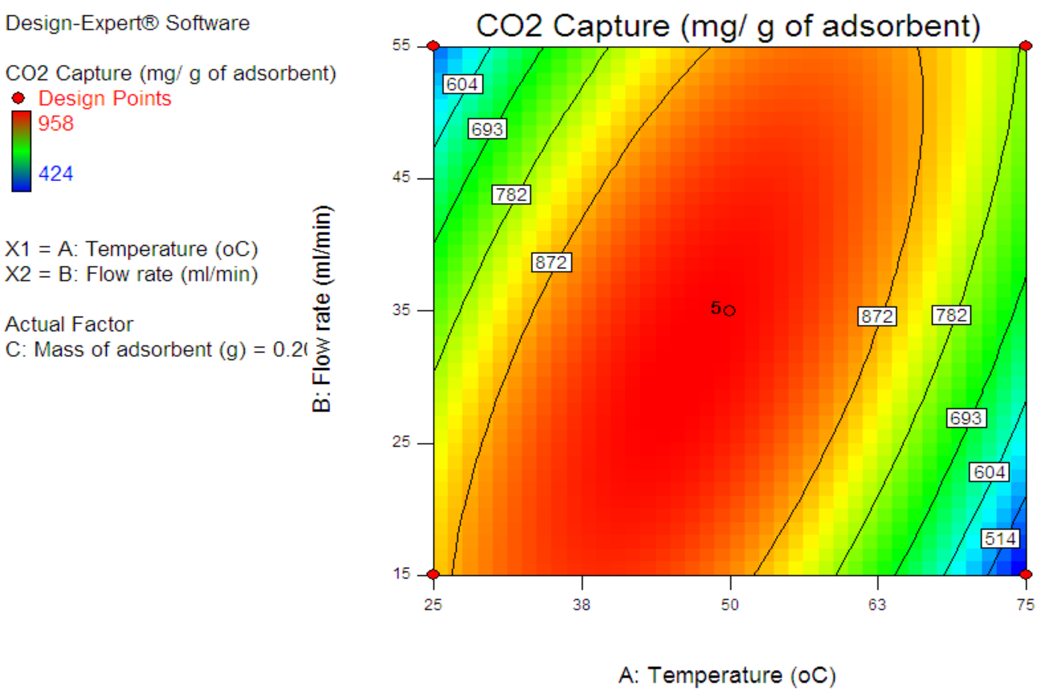

Fig. 1 Response surface plots representing the effect of process variables on CO_2 capture (A and B)

B. Effect of Flow Rate

Flow rate is one of the most important parameter that affects the CO_2 capture in packed bed column, significantly. In order to study the effect of flow rate on CO_2 capture in packed bed column, experiments were carried out in various flow rates (15-55 ml/min) and results are depicted in Fig. 2.

From the results, it is found that CO_2 capture in packed bed column is increased with increasing flow rate upto 45 ml/min. This may be due to the fact that more mixture would be spread on the packing surface, and this leads to an increase in the interfacial area per unit volume and hence CO_2 capture in packed bed column is increased. Thereafter, there is a negligible effect on the CO_2 capture. Similar kind of results was obtained for CO_2 adsorption from ambient air using a supported amine based sorbent in a fixed bed reactor [14].

C. Effect of Mass of Adsorbent

Mass of the adsorbent used in CO_2 capture in packed bed column significantly affects the process performance. Because the surface of adsorbent is the main factor to adsorption and it is directly proportional to mass. Hence, various adsorbent mass (0.1-0.3 g) are employed in order to determine its effect on CO_2 capture in packed bed column.

From the results (Fig. 3), it was observed that, the maximum CO_2 capture in packed bed column is obtained in 0.25g. This can explain by the fact that, reactive sites are directly proportional to mass. Hence, CO_2 capture is increased with increasing mass of adsorbent. The trend obtained this study is close agreement with CO_2 adsorbent developed with high adsorption properties in a coal mine refuge chamber [15].

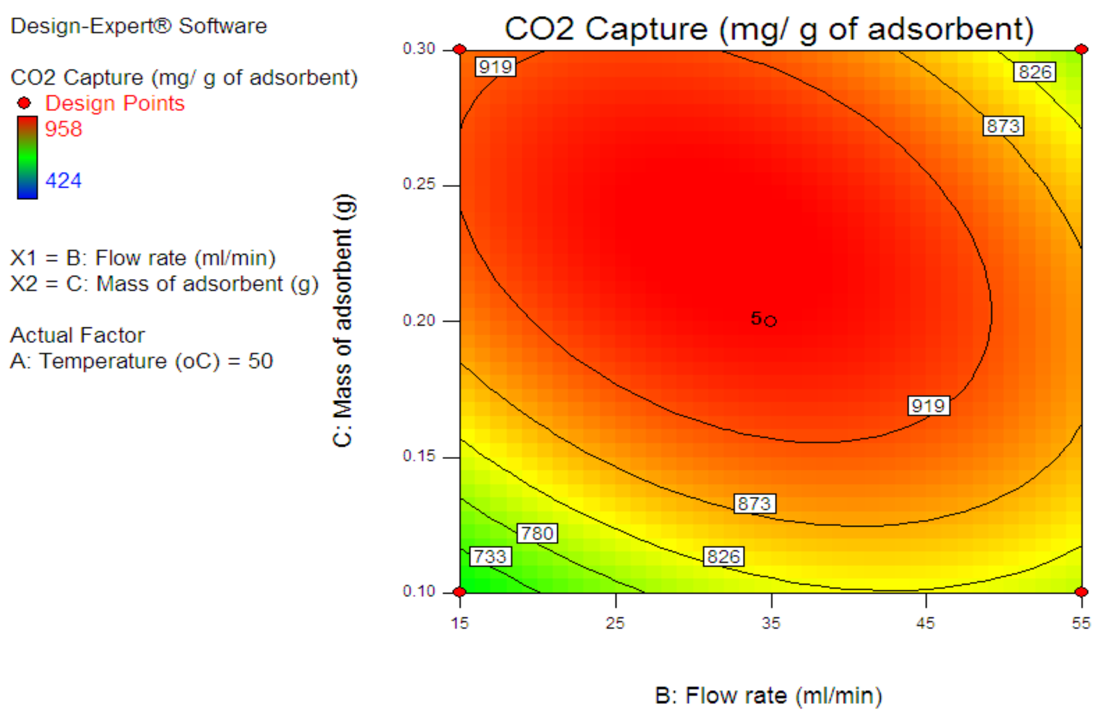

Fig. 2 Response surface plots representing the effect of process variables on CO_2 capture (A and B)

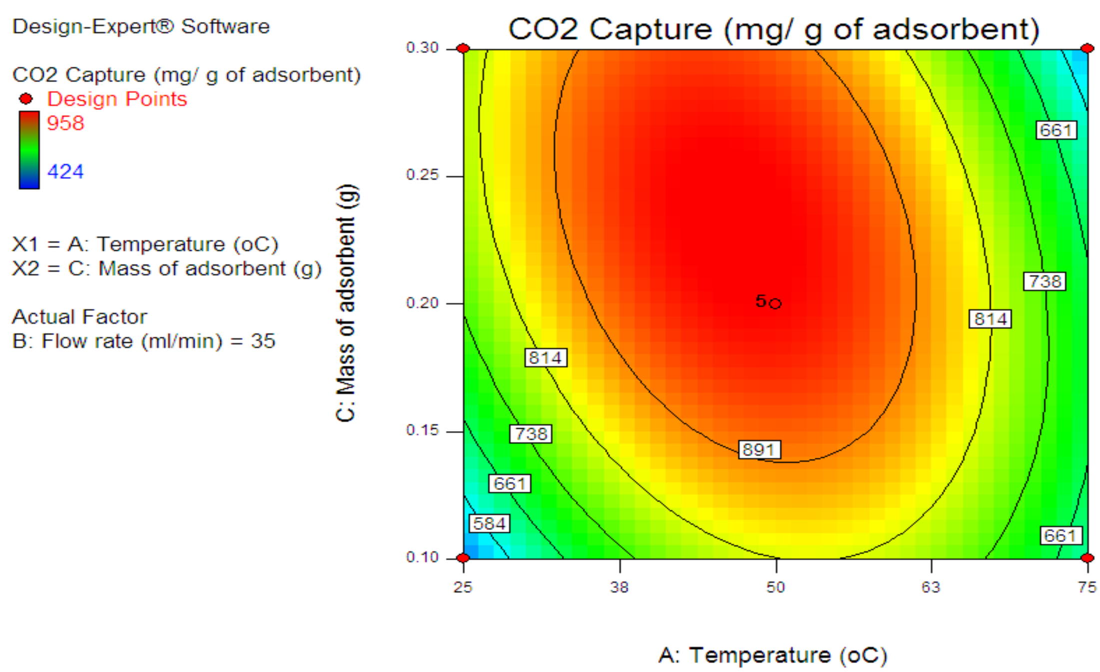

Fig. 3 Response surface plots representing the effect of process variables on CO_2 capture (A and C)

D. Statistical Analysis

CO_2 capture in packed bed column is examined by statistical method using RSM. Three factors three levels Box-Behnken response surface design (BBD) is used in order to estimate and optimize the effect of process variables in packed bed column. A total number of 17 experiments were carried out (Table I) and the response is CO_2 Capture (R_1: mg/g of adsorbent). The response values obtained in BBD are analyzed by multi regression analysis (Table II) in order to select the effective model among various models such as linear, interactive (2FI), quadratic and cubic to explain the CO_2 Capture. From the results, it is found that second order polynomial model is found to be best fit with F value and lower p value. Therefore the second order polynomial model with linear, interactive and quadratic terms is selected to explain the effects of process variables on CO_2 Capture [16]. Final second order polynomial model obtained in terms of coded factors are given below.

$$CO_2 \text{ Capture (mg/g of adsorbent)} = 958-36.25A-4.25B+48.50C+179AB-91.50AC-59.50BC-250.50A^2-71.50B^2-96C^2 \quad (1)$$

TABLE I STATISTICAL DESIGN OF EXPERIMENTS

S. No.	A	B	C	R1
1	50	35	0.2	958
2	50	35	0.2	958
3	50	35	0.2	958
4	75	35	0.1	590
5	75	15	0.2	424
6	25	35	0.3	816
7	50	55	0.3	746
8	75	35	0.3	520
9	50	15	0.1	716
10	50	35	0.2	958
11	25	35	0.1	520
12	50	35	0.2	958
13	50	15	0.3	916
14	25	15	0.2	814
15	25	55	0.2	490
16	75	55	0.2	816
17	50	55	0.1	784

TABLE II SEQUENTIAL MODEL SUM OF SQUARE AND MODEL SUMMARY STATISTICS FOR RESPONSE

Model	Model summary statistics					
	Std.Dev.	R^2	Adjusted R^2	Predicted R^2	Press	Remarks
	CO_2 Capture					
Linear	202.4170	0.0524	-0.1662	-0.6516	928392.1	
2FI	188.8996	0.3652	-0.0157	-0.8817	1057735.5	
Quadratic	32.5247	0.9868	0.9699	0.7892	118480.0000	Suggested
Cubic	0.0000	1.0000	1.0000		+	Aliased
Source	Sum of Squares	Df	Mean Square	F Value	Prob > F	Remarks
Sequential model sum of squares for CO_2 Capture						
Mean	9852668.47	1.00	9852668.47			
Linear	29475.00	3.00	9825.00	0.24	0.8670	
2FI	175814.00	3.00	58604.67	1.64	0.2415	
Quadratic	349425.53	3.00	116475.18	110.10	< 0.0001	Suggested
Cubic	7405.00	3.00	2468.33	63660000.00	< 0.0001	Aliased

Where, A, B and C are temperature, feed flow rate and mass of the adsorbent, respectively. In order to validate the capability of developed second order polynomial model, experimental values are selected randomly from selected process variable ranges and are plotted with model predicted versus actual plots. The data points on this plot lie very close to the diagonal line indicates (Fig. 4) the good adequate agreement between experimental data. Moreover, P (<0.0001) and F (>1) values of response indicates the suitability of developed mathematical models. From these results (Table III), it is concluded that the developed mathematical models can describe the extraction process very robustly.

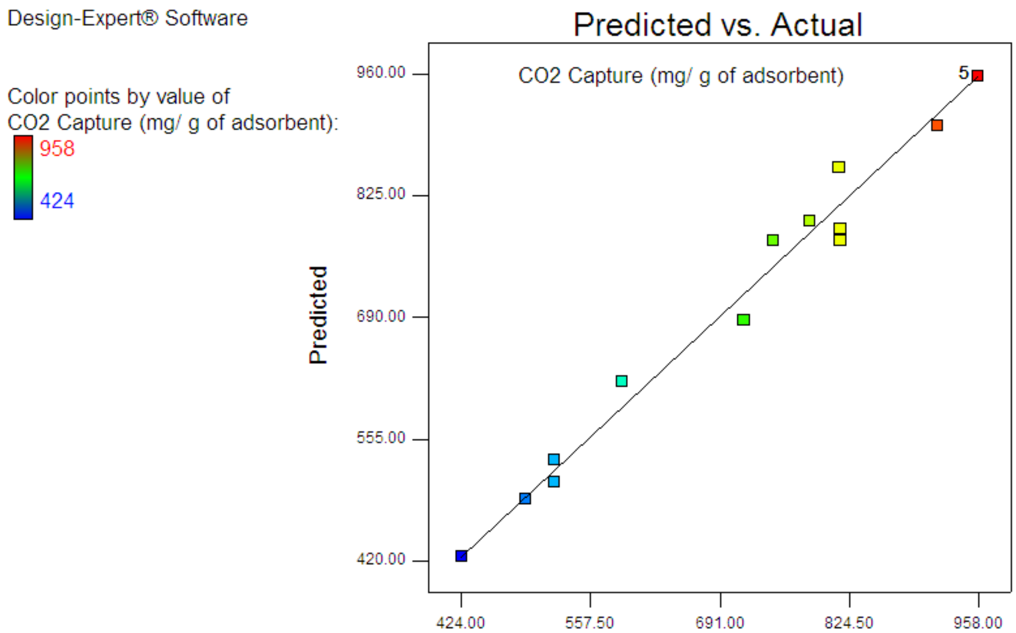

Fig. 4 Perturbation plot for CO_2 capture

TABLE IV ANOVA RESULTS FOR CO_2 CAPTURE

Source	Sum of Squares	df	Mean Square	F Value	p-value Prob > F	Remarks
Model	554715	9	61634.9	58.264	< 0.0001	significant
A-Temperature (^oC)	10512.5	1	10512.5	9.93754	0.0161	
B-Flow rate (ml/min)	144.5	1	144.5	0.1366	0.7226	
C-Mass of adsorbent (g)	18818	1	18818	17.7888	0.0039	
AB	128164	1	128164	121.154	< 0.0001	
AC	33489	1	33489	31.6574	0.0008	
BC	14161	1	14161	13.3865	0.0081	
A2	264212	1	264212	249.761	< 0.0001	
B2	21525.3	1	21525.3	20.348	0.0028	
C2	38804.2	1	38804.2	36.6819	0.0005	
Residual	7405	7	1057.86			
Lack of Fit	7405	3	2468.33			
Pure Error	0	4	0			
Cor Total	562120	16				

E. Optimization and Validation

In order to determine the optimum operating conditions for CO_2 capture in packed bed column, numerical optimization technique is applied. Optimal operating conditions to obtain the maximum electricity from MFC are found to be as follows: temperature of 40^{o}C, feed flow rate of 30 ml/min and 0.25 g of the Poly-(D) glucosamine. Under these optimal conditions, predicted CO_2 capture is found to be 956 mg CO_2 with desirability value of 0.9854. The confirmation experiment is carried out in aforementioned conditions and the result obtained is close agreement with predicted one [17-18].

IV. CONCLUSION

This study focused on CO_2 capture in packed bed column reactor using Poly-(D) glucosamine under the various process parameters such as temperature, feed flow rate and mass of the adsorbent. Individual and interactive effective of process parameters on the CO_2 capture is examined statistically. The developed second order polynomial model is examined ANOVA and actual versus predicted plot. Numerical optimization is used to optimize the process parameters to capture maximum CO_2. The maximum of 956 mg CO_2 is captured under the following operating conditions; temperature of 40^{o}C, feed flow rate of 30 ml/min and 0.25 g of the Poly-(D) glucosamine. Also, under various conditions experiments were performed in order to verify the reliability of statistical analyses and results were confirmed. Hence, CO_2 capture in packed bed column reactor using Poly-(D) glucosamine is a promising method which will helpful to solve the global warming and climate change issues.

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