PAPER • OPEN ACCESS

A Computational Fluid Dynamic Comparative Study on CO_2 Adsorption Performance using Activated Carbon and Zeolite in a Fixed Bed Reactor

View the article online for updates and enhancements.

A Computational Fluid Dynamic Comparative Study on CO₂ Adsorption Performance using Activated Carbon and Zeolite in a Fixed Bed Reactor

N Sylvia[1], R Mutia[2], Malasari[1], R Dewi[1], Y Bindar[3], and Yunardi[4]

[1] Chemical Engineering Department, Malikussaleh University, Lhokseumawe, Indonesia
[2] Postgraduate Program, Chemical Engineering Department, Syiah Kuala University, Banda Aceh, Indonesia
[3] Department of Chemical Engineering, Faculty of Industrial Technology, Bandung Institute of Technology, Bandung, Indonesia
[4] Chemical Engineering Department, Syiah Kuala University, Banda Aceh, Indonesia

Email: yunardi@unsyiah.ac.id

Abstract. The increasing emission of carbon dioxide to the atmosphere from various sources has become an issue of great concern all over the world due to its significant contribution to climate change. Carbon capture and storage are commonly recognized as the major approaches to prevent carbon dioxide from entering the atmosphere. A number of CO_2 removal technologies have been reported, including absorption, adsorption, membrane separation, and microalgal fixation. In this study, a Computational Fluid Dynamics (CFD) study was performed to investigate the performance of two adsorbents, coconut fiber activated carbon and zeolite 13X in removing CO_2 from a continuous gas stream in a fixed bed adsorption column. A CFD code ANSYS R18.2 was used to investigate the influence of flow rate and bed height on the CO_2 removal efficiency and adsorption capacity by varying the inlet feed velocity and bed heights. The results of the simulation showed that the highest CO_2 removal efficiency of 63.13 percent was observed when the gas flowed at a rate of 50 cm^3/minute to the column filled with the activated carbon adsorbent of 10 cm in height. While in the zeolite adsorbent 13X, the highest CO_2 removal efficiency of 57.86 percent was also seen when the gas flowed at a rate of 50 cm^3/minute at the bed height of 10 cm.

1. Introduction

Indonesia is currently facing serious energy problems due to the high dependence on fossil fuels. In fact, the country has a huge potential for renewable resources originated from agricultural wastes for energy generation. It is estimated that the country is capable of producing a potential bioenergy of 50 GW, nevertheless, only less than 2 GW has been utilized up to now. The Indonesian Science Institute has suggested using biogas to reduce the dependence on fuel import. Such consideration was based on its availability, low capital and operational costs, renewable sources and environmentally friendly energy. Either it is produced at industrial or smaller scale, biogas generally consists of CH_4 (50-75%),

CO_2 (25-50%), and another minor number of gases. Its calorific value ranges from 17,900-25,000 kJ/m^3; for a comparison, natural gas (LNG) has a calorific value of 37,300 kJ/m^3 [1]. It is clearly seen from the biogas composition that its main drawback is its high content of CO2 which significantly reduces its calorific values. Therefore, for the purpose of utilizing biogas as the source of energy, removal of CO2 prior to utilization is required.

There are a number of methodologies available for removing CO2 from biogas. Conventional technologies for removing CO2 include water scrubbing, chemical and physical scrubbing, membranes and Pressure swing adsorption [2]. New methodologies have been also introduced for the use of improving the quality of biogas such as CO2 liquefaction and separation, amine absorption [3] and cryogenic distillation [4]. Although such new development technologies provide better performance, its implementation on a small scale and in the developing countries is still not beneficial at the present time. Therefore, adsorption-based technologies would suit the need for implementation in the developing countries due to its low energy required for regeneration, easy to operate, low-pressure drop, and easier to scale down. With regard to the adsorbents, porous inorganic materials such as zeolite 13X, zeolite 4A, bentonite, molecular sieve, and activated carbon have been utilized for this purpose [5, 6, 7, 8,9,10,11,12]. Each adsorbent has its own advantages and disadvantages, however, activated carbon is easy to prepare from different sources of agricultural biomass which is abundance in every part of Indonesia. The same case was also applied to zeolite and bentonite which are abundant in the local region.

CFD has been used to study the flow phenomena involving momentum, heat and mass transfer for the purpose of design and optimization of process equipment. Such a method is a suitable tool to be used when the process performance is dictated by fluid dynamics. In relation to the present study, CFD is utilized to study the adsorption phenomena and adsorbent performance on the removal of CO2 from a mixture of CH4-CO2 [13,14] Two type of adsorbents, activated carbon and zeolite 13X, were employed in the modelling of fixed-bed adsorption column by varying the height of the adsorbent bed and the gas flow rate entering the column. Equilibrium characteristics of the CO2 adsorption process were evaluated by test the data with various isotherm models.

2. Materials and Method

The present study modeled the adsorption column for separating of CO_2 from a gas mixture containing CH_4 and CO2, using coconut fiber activated carbon and zeolite type 13X as adsorbents. Each adsorbent was having the same particle diameter of 0.0029 m, while the bed porosity (ε) was set 0.39 for activated carbon and 0.43 for zeolite 13 X, respectively. Table 1 presented the geometry of the adsorption column used in this study, while the modeling design of the adsorption column is shown in Figure 1 [14]. All stages in the simulation, including pre-processing, processing and post-processing were performed using the Fluent Ansys R18.2. The feed flow rates were varied by 50 cm^3/minute, 100 cm^3/minute 150 cm^3/minute 200 cm^3/minute and 250 cm^3/minute [14] while the bed height was varied with 6 cm, 8 cm, and 10 cm. Observations were taken on the removal efficiency, adsorption capacity and adsorption isothermal.

Table 1 Geometry of the adsorption column

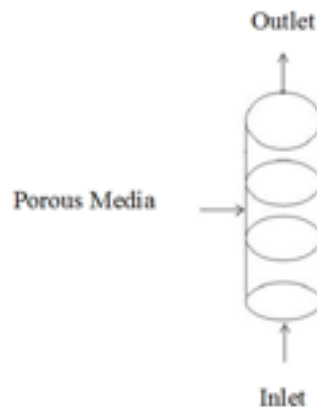| Geometry	Height	Diameter
Adsorbent	50 cm	5 cm
Filter	-	5 cm

Figure 1. Geometry for the adsorption column being studied

3. Results and Discussion

The Computational Fluid Dynamics (CFD) study on the simulation adsorption process of CO_2 removal was done by varying the flow rate and column bed height for each adsorbent being used. Table 2 presented results on CO_2 removal efficiency and adsorption capacity due to a variation of flow rate and adsorbent bed height. The discussion of these results is presented in the next sub-sections.

Table 2. Results on CO_2 removal efficiency and adsorption capacity due to a variation of flow rate and adsorbent bed height

RUN	Flow Rate (cm^3/min)	Bed Height (cm)	CO_2 Removal Efficiency (%)		Adsorption Capacity (mg/gr)	
			Activated Carbon	Zeolite	Activated Carbon	Zeolite
1		6	57,66	50,21	10898,14	6079,64
2	50	8	61,01	53,82	6446,13	3643,53
3		10	63,13	57,86	3614,14	2491,81
4		6	55,60	47,18	21033,27	11431,92
5	100	8	58,93	50,43	12550,55	6880,09
6		10	61,02	55,54	8074,48	4767,34
7		6	53,44	45,12	30333,87	16408,37
8	150	8	57,12	47,06	18314,2	9662,89
9		10	58,18	51,85	11780,52	6747,03
10		6	51,75	41,34	41194,89	19062,49
11	200	8	56,02	44,13	23136,78	11077,18
12		10	56,67	47,25	15814,86	9842,38
13		6	48,49	41,21	46573,06	25672,01
14	250	8	54,97	41,47	27956,2	13048,70
15		10	55,5	43,24	19490,6	11885,53

3.1. The Effect of Bed Height to the CO_2 Removal Efficiency

From Table 2, it can be seen that the highest CO_2 removal efficiency obtained from the use of activated carbon and zeolite adsorbents were 63.13% and 57.86%, respectively, which occurred at a

flow rate of 50 cm^3/minute and with a bed height of 10 cm. Meanwhile, the lowest CO_2 removal efficiency for activated carbon and zeolite adsorbents were 48.49% and 41.21%, respectively, which occurred at a flow rate of 250 cm^3/min and with a bed height of 6 cm. The results indicated that activated carbon was having a higher capability to absorb CO_2 compared to that of zeolite 13X. The CFD results of this study are in line with experimental results obtained by Chue et al [15] and Das et al [16], demonstrated that the pore surface area of activated carbon is much higher than that of zeolite 13X. Consequently, when activated carbon is used as an adsorbent, it can purify more CO_2 from a gas mixture that other adsorbents of lower pore surface area.

Figure 2 illustrated the relationship between flow rate and CO2 removal efficiency at different bed heights for each type of adsorbent. This figure suggested that the CO2 adsorption is much higher in the activated carbon adsorbent and the adsorption rate increases with the increase of the bed height. However, the removal efficiency decreases as the flow rate of the feed to the column increased [17]. In other words, the influence of flow rate on the adsorption capacity is the greater the feed flow rate, the smaller the adsorption rate will be. When the greater CO_2 flow rate entering the column, the less contact time between CO_2 and adsorbent will be, Consequently, the percentage of adsorption will also be smaller. Figures 3 to 5 show the contours of the influence of the flow rate on adsorption rate using zeolite 13X adsorbent, while Figure 6 to 8 shows the contours of the influence of the flow rate on the adsorption rate using activated carbon of coconut fiber adsorbent.
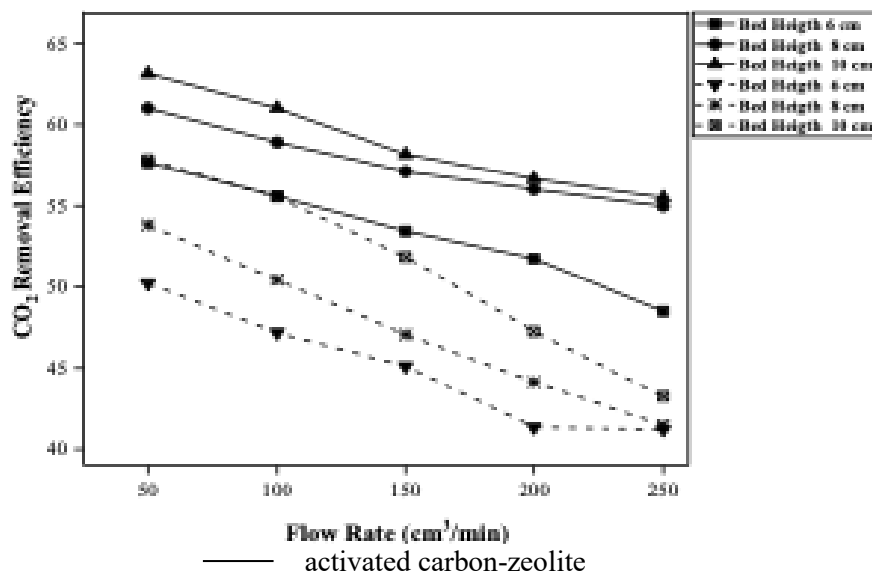

Figure 2. The effect of adsorbent bed height on CO_2 removal efficiency.

From Figure 3 to 8, it can be seen that there is a color difference in terms of velocity in the adsorption column. The redder in color illustrated the higher the flow rate, while the bluer in color indicated the lower the flow rate entering the adsorption column. The results clearly showed that at the higher bed the velocity of the gas in the column decreases, due to the increase of the resistance to the flow allowing more CO2 to be retained on the surface of the adsorbent.
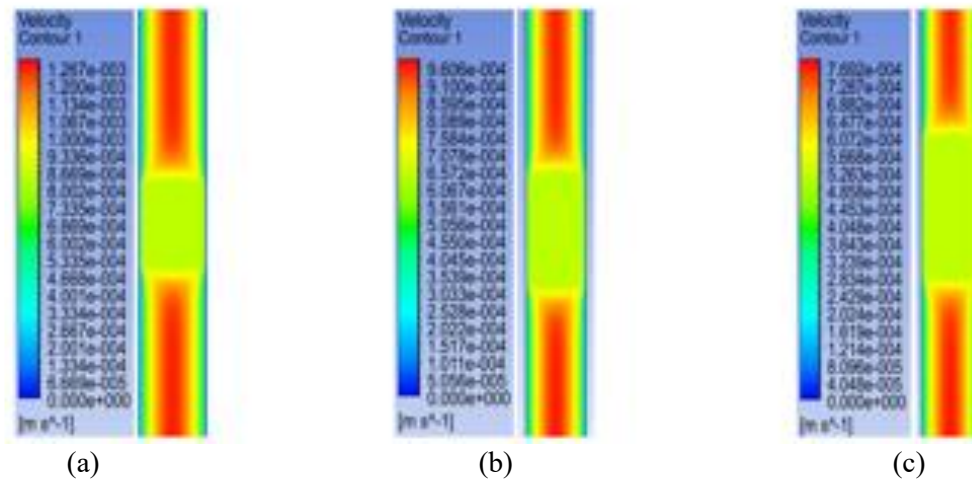
(a)   (b)   (c)

Figure 3. A contour of fluid flow rate at 50 cm^3/minute (a) bed height of 6 cm, (b) bed height of 8 cm, and (c) bed height of 10 cm
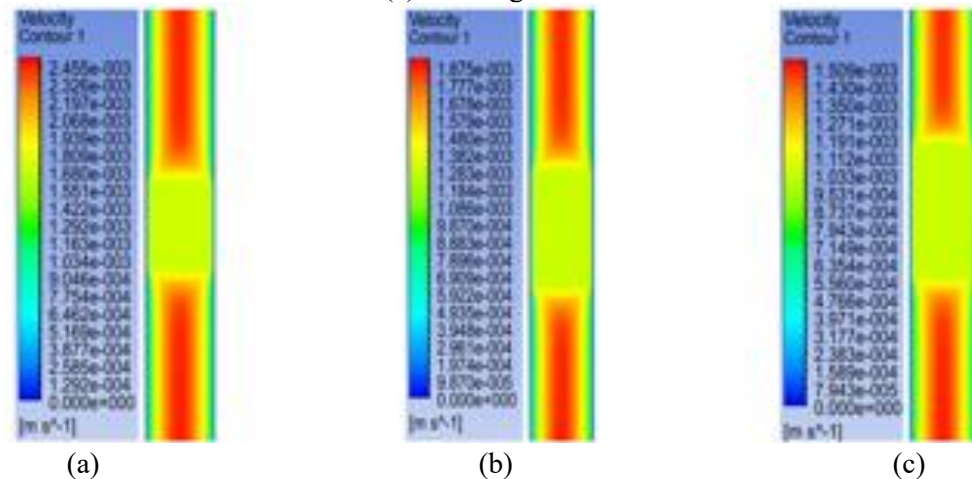

(a)   (b)   (c)

Figure 4. A contour of fluid flow rate of 100 cm^3/min (a) bed height of 6 cm, (b) bed height of 8 cm, and (c) bed height of 10 cm.

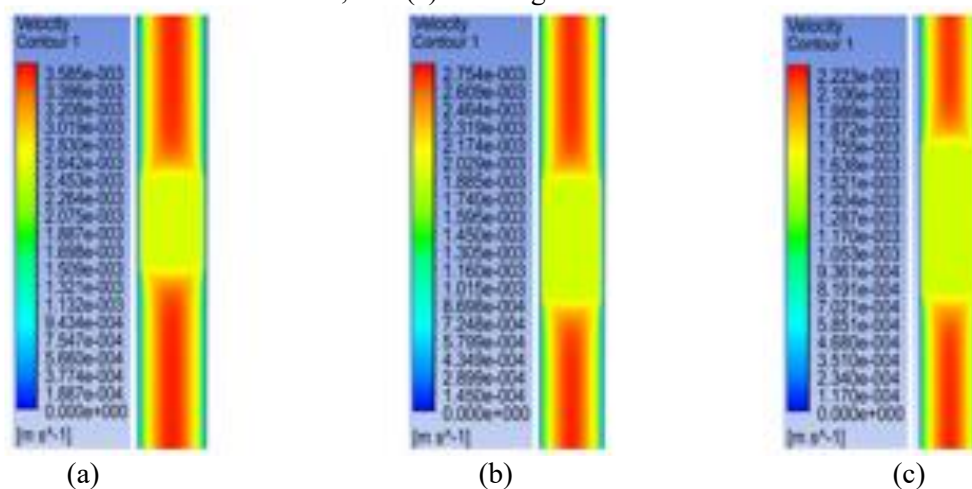(a)   (b)   (c)

Figure 5. A contour of fluid flow rate of 150 cm^3/min (a) bed height of 6 cm, (b) bed height of 8 cm, and (c) bed height of 10 cm
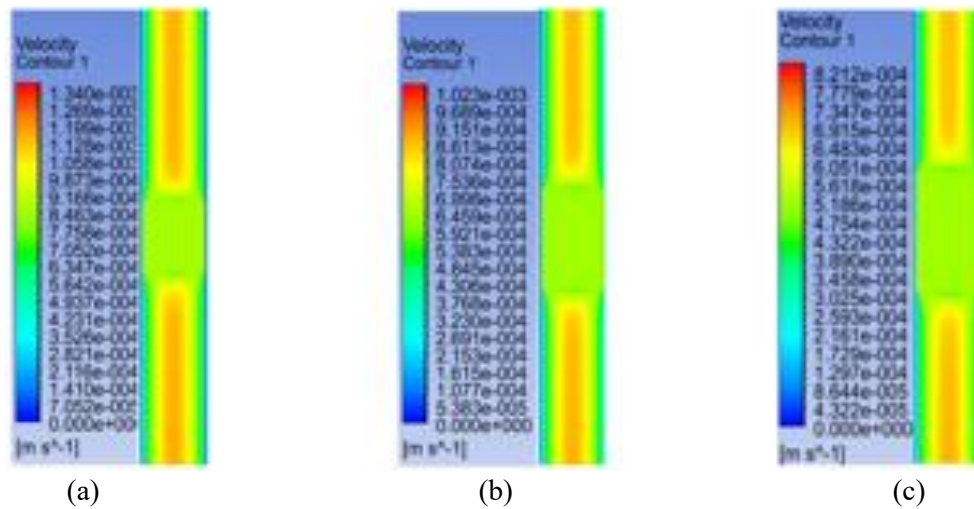
(a)   (b)   (c)

Figure 6. A contour of fluid flow rate of 50 cm3/minute (a) bed height of 6 cm, (b) bed height of 8 cm, and (c) bed height of 10 cm
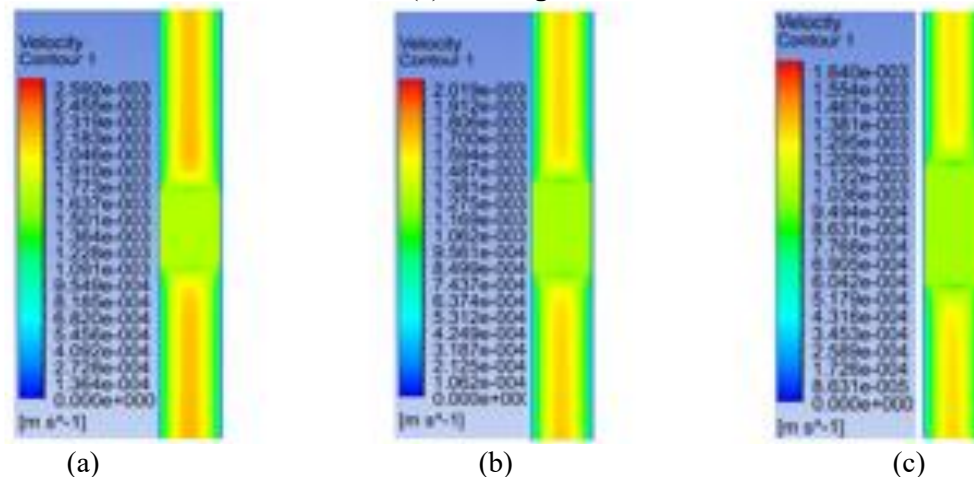

(a)   (b)   (c)

Figure 7. A contour of fluid flow rate of 100 cm^3/min (a) bed height of 6 cm, (b) bed height of 8 cm, and (c) bed height of 10 cm.

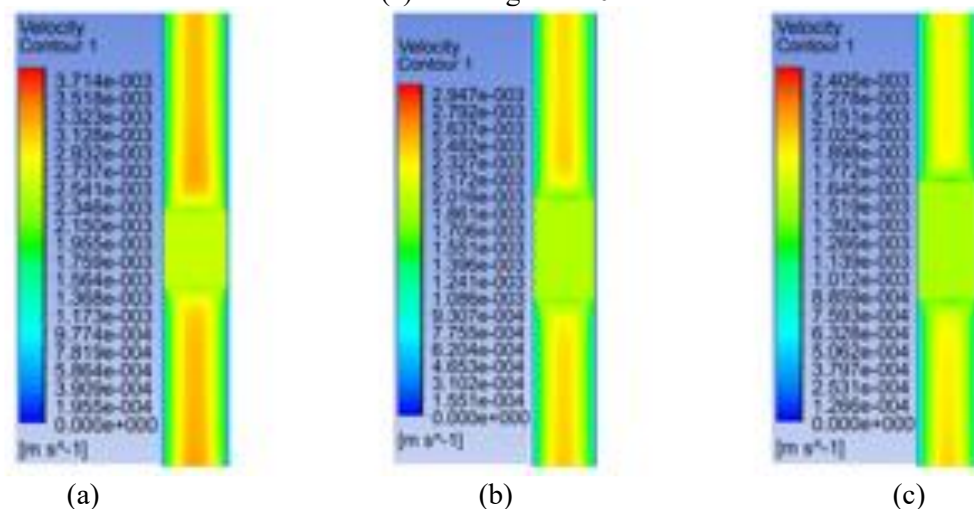(a)   (b)   (c)

Figure 8. A contour of fluid flow rate of 150 cm^3/min (a) bed height of 6 cm, (b) bed height of 8 cm, and (c) bed height of 10 cm

From Figure 3 to 8, it can be seen that there is a color difference in terms of velocity in the adsorption column. The redder in color illustrated the higher the flow rate, while the bluer in color indicated the lower the flow rate entering the adsorption column. The results clearly showed that at the higher bed the velocity of the gas in the column decreases, due to the increase of the resistance to the flow allowing more CO2 to be retained on the surface of the adsorbent.

3.2. The Effect of Flow Rate on Adsorption Capacity

Figure 9 depicted the relationship between flow rate and adsorption capacity in both columns. It is seen that the highest adsorption capacity of 46,573.06 mg/g occurred in the column filled with activated carbon adsorbent made of coconut fiber at a flow rate of 250 cm^3/min and bed height of 6 cm. Meanwhile, the lowest adsorption capacity of 2491.81 mg/g occurred at the column filled with the adsorbent of zeolite 13X at a flow rate of 50 cm^3/minute and bed height of 10 cm. It shows that the activated carbon adsorbent is better when it is used for CO2 purification process compared to that of zeolite 13X. In this case, it can be seen that the greater the flow rate, the higher the adsorption capacity, indicating that the higher the flow rate, the more CO2 molecules will come into contact with the pore surface of the adsorbent so that the adsorption capacity increases [18, 19] as marked by the red color in the lighter part of the porous zone.
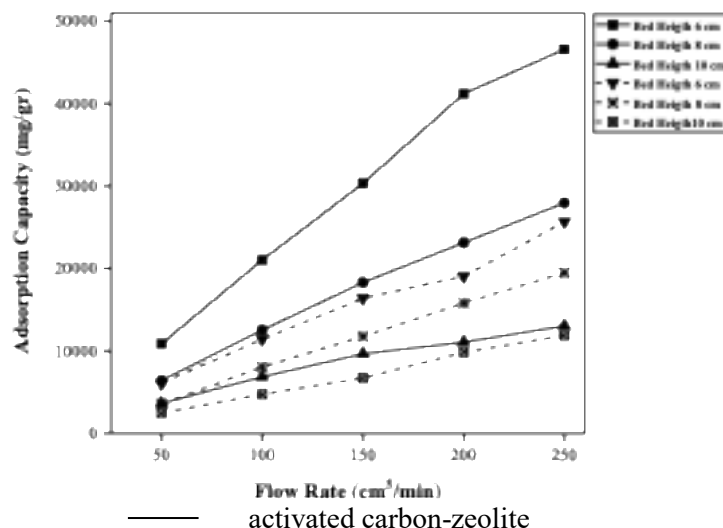

activated carbon-zeolite

Figure 9. The correlation between flow rate and adsorption capacity in both columns

3.3. Isothermal Adsorption

Figures 10 and 11 showed the adsorption isotherm of carbon dioxide with different adsorbents, respectively. The adsorption data were fitted with standard isotherm models, including those of Langmuir and Freundlich. With regard to adsorption isotherm of carbon dioxide in activated carbon, the Langmuir model seems to give a better fit compared to that of Freundlich. the equation and linearization results are also shown in table 3.

The linearity of Freundlich isotherm adsorption is higher than Langmuir isotherm. It shows the process of CO_2 adsorption with an activated carbon of coconut fiber and zeolite 13X adsorbents is in a multilayer process. The adsorption process in activated carbon of coconut fiber occurs because it has CO_2 adsorbing properties through N_2 [20, 21, 22]. Besides, activated carbon has a physical structure with a very hard granular shape making it has the potential to adsorb gas, while the adsorption process in zeolite 13X occurs because the zeolite 13X has a very small and uniform pore size, high Si/Al content, and Na content as a minor element of the zeolite.
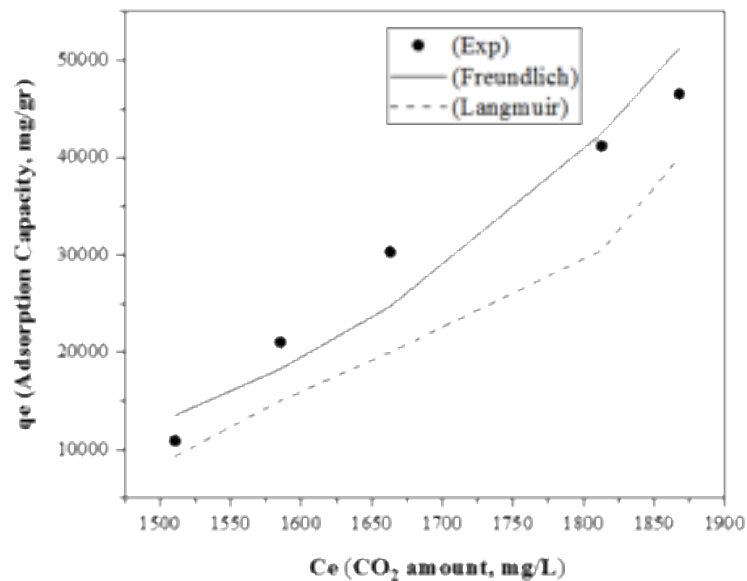
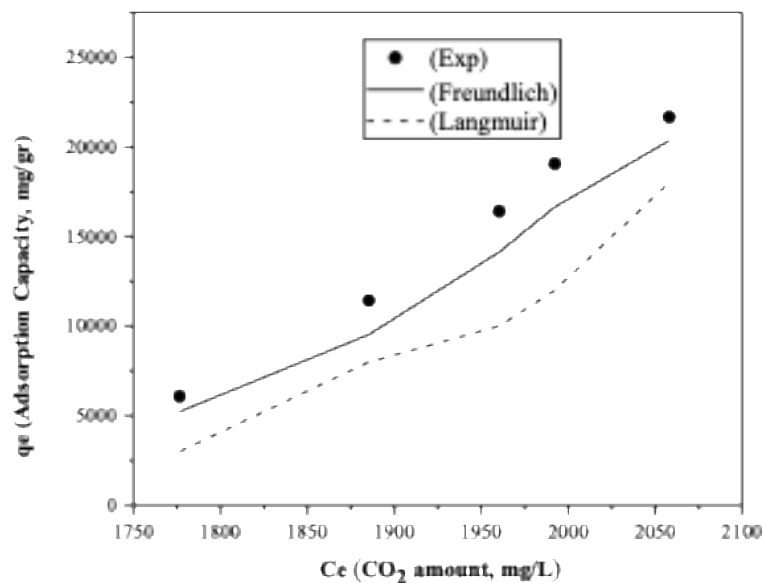**Figure 10**. Adsorption isotherm of carbon dioxide in activated carbon adsorbent

Figure 1. Adsorption isotherm of carbon dioxide in activated carbon-zeolite 13X

Table 3. Parameter isotherm model via linearized technique for pressure 1atm and temperature 25°C

Type		Equation	
		Nonlinier	Linier
Langmuir			
q_e	0.072	$q_e = \dfrac{q_m \times k_L \times Ce}{1 + k_L \times Ce}$	$\dfrac{Ce}{q_e} = \dfrac{1}{q_m \times k_L} + \dfrac{Ce}{q_m}$
k_L	29.73		
R^2	0.89		
Freundlich			
k_f	0.00138	$q_e = k_f \times Ce^{\frac{1}{n}}$	$\text{Log } q_e = \log k_f + \dfrac{1}{n} \log Ce$
n	0.15		
R^2	0.91		

4. Conclusion

The higher CO_2 removal efficiency and CO_2 adsorption capacity were produced by the adsorbent of activated carbon made of coconut fiber than that of zeolite 13X. It shows that the relationship between adsorption rate and capacity are inversely proportional. The process of CO_2 adsorption using activated carbon and zeolite 13X is in multilayer one. Further research is still required to investigate the optimization of operating parameters with the aim at obtaining higher removal efficiency.

References

[1]   Harihastuti N, Purwanto and Istadi 2014 Study of activated carbon and zeolite integrated application on biomethane production based on biogas *J.Ind.Research.* **8** 1 65

[2]   Yousef A M, Eldrainy Y A, El-Maghlany W M, and Attia A 2017 Biogas upgrading process via low-temperature CO liquefaction and separation *J. Nat. Gas. Sci. Eng* **45** 812

[3]   Kim J, Pham D A, and Lim Y I 2016 Gas-liquid multiphase computational fluid dynamic (CFD) of amine absorption column with structured-packing for co_2 capture *Comput. Chem. Eng*. **88** 39

[4]   Bauer F, Hulteberg C, Persson T, Tamm D 2013 Biogas upgrading-review of commercial technologies *SGC's Report* **270** Swedish Gas Technology Centre Malmo Sweden

[5]   Samanta A, Zhao A, Shimizu G K H, Sarkar P and Gupta R 2011 Post combustion co_2 capture using solid sorbents: review *Ind. Eng. Chem. Res*. **51** 1438

[6]   Bezerra D, Oliveira R, Vieiria R, Cavalcante Jr C and Azevedo D S 2011 Adsorption of co_2 on nitrogen-enriched activated carbon and zeolit 13X *Adsorption* **17**

[7]   Song C 2006 Global challenges and strategies for control , conversion and utilization of CO_2 for sustainable development involving energy, catalysis, adsorption and chemical processing *Catalysis Today.* **115** 2

[8]   Zhang Z, Zhang W, Chen X, Xia Q, and Li Z 2010 Separation science and technology adsorption of co_2 on zeolite 13x and activated carbon with higher surface area *Sep. Sci. Technol.* **45** 710

[9]   Duduku K, Awang B, Anisuzzaman S M , Collin J and Teo B K 2014 Carbon dioxide removal by adsorption. *J. Appl. Sci*.**14** 3142

[10]   Reema S , Vinod K S , E. Anil K R2014 Carbon dioxide capture and sequestration by adsorption on activated carbon *Energy Procedia.* **54** 320

[11]   Hauchhum L and Mahanta P 2014 Carbon dioxide adsorption on zeolites and activated carbon by pressure swing adsorption in a fixed bed *I.J.E.E.E.* **5** 4 349

[12]   Siriwardane R V, Shen M S, Fisher E P and Poston J A 2001 Adsorption of CO2 on molecular sieves and activated carbon *Energy & Fuels* 15, 279-284

[13]   Versteeg H K and Malalasekera W 1995 *An Introduction to Computationl Fluid Dynamic (Longman Scientific & Technical)* Longman House, Burnt Mill, Harlow England pp 8

[14]   Ali Q, Zamri M A, Lau K K, Suzana Y 2014 Computational fluid dynamics simulation of CO_2 adsorption on nanoporous activated carbon: effect of feed velocity *J. Appl. Sci.Agri* **9** 18 163

[15]   Chue K, Kim J, Yoo J Y, Cho S H and Yang R 1995 Comparison of activated carbon and zeolite 13x for co_2 recovery from flue gas by pressure swing adsorption *Ind.Eng.Chem.Res* **34** 591

[16]   Das D, Samal D P and Meikap B C 2016 Removal of CO_2 in a multistage fluidized bed reactor by diethanol amine impregnated activated carbon *J. Environ. Sci. Health., Part A*, **51** 9769

[17]   Salmasi M, Fatemi S, Doroudian Rad M, Jadidi F 2013 Study of carbon dioxide and methane equilibrium adsorption on silicoaluminophosphate-34 zeotype and T-type zeolite as adsorbent *Int. J. Environ. Sci. Technol.* **10** 1067

[18]   Tan Y L, Azharul Islam Md, Asif M, Hameed B H 2014 Adsorption of carbon dioxide by sodium hydroxide-modified granular coconut shell activated carbon in a fixed bed *Energy* **30**

1

[19] Novi S, Lukman H, Nur F and Yunardi 2018 Adsorption performance of a fixed-bed column for the removal of Fe (II) in groundwater using activated carbon made from palm kernel shells *IOP Conf. Series: Materials Science and Engineering* 334

[20]   Nor A R, Suzana Y, Azri B 2016 Isotherm and thermodynamic analysis of carbon Dioxide on activated carbon *Procedia Engineering* **148** 630

[21]   Nor A R, Suzana Y and Lam H L 2013 Kinetic Studies on Carbon Dioxide Capture using Activated Carbon *Chemical Engineering Transaction* **35** 361

[22]   Dantas T L P, Luna F M T, Silva Jr J I,   Torres A E B, de Azevedo D C S, Rodrigues A E and Moreira R F P M 2011 Modeling of the fixed-bed adsorption of carbon dioxide and a carbon dioxidenitrogen mixture on zeolite 13x, Braz. J. Chem. Eng. 28 (3): 533-544.