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Monte Carlo Simulation Hydrogen Sulphide Gad Adsorption By Using Hydrogel Biochar

Nursafika Bahira Juli,[a] Norhayati Talib*, [a] Normadyzah Ahmad, [a] Azil Bahari Alias [a,*]

[a]Faculty Chemical Engineering Univeriti Teknologi Mara (UiTM) Shah Alam, Malaysia

Abstract

Monte Carlo simulation is popular in engineering because it is a flexible simulation. It can reduce the uncertainty of the possibilities, and it can run a large number of cycles that are suitable for studying the kinetics and mechanism of adsorption, leading to better data accuracy than practical results. This simulation is chosen to investigate the phenomena of H_2S gas adsorption in hydrogel biochar. Hydrogel biochar adsorbent is made from highly available biomass sources by using the pyrolysis process. There are two parameters studied: the effect of the flow rate of H_2S gas and adsorbent bed height. This parameter can show the efficiency of the adsorption process. From this research, the kinetic model that suitable for this H_2S gas adsorption is by First- Pseudo Kinetic model based on the correlation coefficient R^2 values generated from the MATLAB program is between 0.7 to 0.9. Thus, physical adsorption is the best way to describe the adsorption in hydrogel biochar in which the uniform energies of adsorption on the surface of biochar and no shifting of adsorbate in the plane of surfaces. It can be concluded that at the optimize condition used Langmuir's isotherm where the maximum amount of adsorption capacity is obtained, and the adsorption process occurs at monolayer of adsorbent with an equivalent adsorption site.

Keywords: Hydrogel Biochar, Hydrogen Sulfide, Adsorption, Monte Carlo Simulation

1. Introduction

Hydrogen sulfide is acid gas that is a toxic, corrosive, colorless, and flammable gas. The emissions of hydrogen sulfide can be risky to human health. It is also produced from oil and gas production, wastewater treatment, combustion of fossil fuels. This gas also can result in corrosion at the piping system. Two methods that are commonly used to remove the H_2S gas are through the adsorption and absorption process. According to Bamdad et al., the monoethanolamine (MEA) and diethylamine (DEA) were solvents that were used to remove the H_2S gas [1]. However, this method is expensive because it is required high energy. The toxic gas is currently removed using the porous solid adsorbent such as carbon based like activated carbon, silica-based, and metal-organic frameworks (MOFs). Activated carbon is needed high cost for activation [2]. Thus, it is required to substitute the biochar.

To improve the adsorption efficiency, the biochar was then modified to hydrogel biochar by adding acrylamide (AAm) as a monomer [3]. The hydrogel biochar is made from the pyrolysis process, which used a raw empty fruit bunch (EFB). The modification of biochar to hydrogel biochar is by polymerization process in which the EFB biochar and the crosslinker are added in the AAm solution. This polymerization type used multipurpose of crosslinking agents blended with the ionic or neutral monomer [4]. The polymerization is thermally initiated by UV/IR radiation or by a redox initiator system. The hydrogel was then washed with distilled water to remove the unreacted monomer, oligomers, initiator, crosslinking agent, the soluble polymer, and other impurities. Phase separation occurs, which formed a heterogeneous hydrogel when the polymerization water quantity is more than the water content in proportion to equilibrium swelling. Solvents used for solution polymerization of hydrogels include ethanol, water, ethanol-water mixture, and benzyl alcohol [4]. This modification can improve the gas separation of H_2S in industry and can increasing the holding up of water. Thus, a good

*Corresponding author e-mail: norhayati0653@uitm.edu.my ; (Norhayati Talib).
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understanding of the thermodynamic transport properties of H_2S adsorption in microporous materials is needed to make this model successful.

Nowadays, molecular simulations have become popular among researchers. Due to the experiment taking a long time and required to predict the outcomes. So, with the aid of molecular simulation such as Monte Carlo (MC), molecular dynamic (MD), and density functional theory (DFT), the understanding of adsorption behavior has increased [5]. These simulations help reduce the experimental effort to predict the properties and carry out experiments that cannot be accomplished in experimental work.

The Monte Carlo simulation is very important because it can run multiple times and run many cycles based on the properties of the subject suitable for study the kinetic ad mechanism of adsorption [6]. It can also handle many random variables with different distribution types and highly nonlinear engineering models [7]. Besides, this simulation can consider a wide range of possibilities and help to reduce uncertainty. Thus, the Monte Carlo simulation investigates the H_2S adsorption in the biochar hydrogel and compares the simulation results with the experimental. The finding will help the researcher predict and assume under all parameters and thus model a range of possible outcomes.

2. Materials and Method

2.1. Simulation

MATLAB (R2018a) software was used to study the kinetics and isotherm model for the experimental data obtained using Monte Carlo Simulation. The experimental data was done in previous work on the effect of different hydrogen sulfide flow rate and bed height on the gas adsorption [8]. The Monte Carlo Simulation was run at N= 100 to N=100000 to compare the solid-gas adsorption in contrast and analyze the effect of hydrogen sulphide flow rate and adsorption using different sizes of adsorbents as shown in Figure 1.

```
%Initialization for Monte carlo simulation
N=100; %number of runs
MCsum=0;
%run the simulation
for i=1:N
    M1=MCsum+rand(1,10); %random number for mass adsorbed for 10 data
    Qt1=MCsum+rand(1,10);
end
```

Fig 1: Monte Carlo simulation command in MATLAB

2.2. Kinetic Model

The kinetics studies provide adsorbent performance in the batch adsorption process, mechanism of sorption, and rate of adsorption. There are three models of the best-fit equation kinetic model: the pseudo-first-order model, pseudo-second-order model, and Elovich Model [9].

2.2.1. Physical adsorption

The pseudo-first-order model (PFO) indicates that the adsorption is inclined towards physisorption, which involves the van der Waals binding force. Qian et al. (2015), state that hydrogen is difficult to store. Thus, the physisorption on sorbent has been implemented because it can employ high surface area sorption material that can effectively adsorb hydrogen [10, 11, 12].

Linear

$$\mathrm{Ln}\,(q_e - q_t) = \ln q_e - k_1 t$$

Equation 1 First- Pseudo Kinetic Model's

Where q_t is adsorption over time (mg/g), q_e is adsorption of equilibrium (mg/g), k_1 is the PFO rate constant (min^{-1})

2.2.2. Chemical adsorption

Likewise, if the adsorption occurring is chemisorption, an adsorption system will fit into the pseudo-second-order model and Elovich kinetics. Vardhan (2014), also stated that removing chemisorbed species from the surface might be possible if the extreme temperature condition is applied when the activation energy for desorption is large. This form of adsorption is noticeable in adsorbents depending on the functional groups.

Linear

$$\frac{t}{q_t} = \frac{1}{k_2 q_e^2} + \frac{1}{q_e} t$$

Equation 2 Second- Pseudo Kinetic Model's

Where qt is adsorption over time (mg/g), qe is adsorption of equilibrium (mg/g), k^2 is the PSO rate constant (g/mg.min), k^2qe^2 or h is the initial PSO desorption rate (mg/g.min), α and β are the Elovich initial adsorption rate (mg/g.min)

2.3. Adsorption isotherm

2.3.1. Langmuir's Model

The Langmuir isotherm model is a semi-empirical isotherm with a kinetic basis and was derived based on the thermodynamic properties and it was applied to gases adsorbed on solid surfaces.

$$\frac{1}{q_e} = \frac{1}{q_{max}K_L} + \frac{C_e}{q_{max}}$$

Equation 4 Langmuir Model's

Where Ce is the equilibrium concentration(mg/L), qe is the amount of gas adsorbed onto adsorbent (mg/g), q_{max} is the maximum amount of gas that can become adsorbent by adsorbent (mg/g), and $K_L$is Langmuir adsorption equilibrium constant (L/mg).

2.3.2. Freundlich's Model

The Freundlich isotherm correlated with a decrease in binding strength with the increasing site occupancy, stronger affinities of adsorbed molecules in front of weaker sites. According to Abdullah et al. (2009), this isotherm is better suited to chemisorption than Langmuir because of its non-uniform surface energy. This model was used to explain heterogeneous surface chemisorption.

$$logq_e = logK_F + \frac{1}{n} logC_e$$

Equation 5 Freundlich Model's

Where Ce is the equilibrium concentration (mg/L),q_e is the amount of gas adsorbed onto adsorbent (mg/g), Freundlich adsorption equilibrium K_F and n related to adsorption capacity and adsorption intensity respectively.

3. Result and Discussion.

3.1. Adsorption Kinetic Model

The adsorption kinetic method describes the rate of solute uptake at the solid interface (hydrogel biochar), reaction pathways, and reaction rate. The kinetic of hydrogel biochar adsorption studied is First-Pseudo, second pseudo, and Elovich kinetics.

3.1.1. First Pseudo Kinetic Model

The First-pseudo kinetic model result from MATLAB simulation is tabulated as Tables 1 and 2. The relationship of Hydrogen flow rate with First-Pseudo kinetic model is shown in Table 1. The amount of H_2S adsorbed is inversely proportional to the H_2S flow rate. Hence, the amount of H_2S adsorbed is decreased as the flow rate increased. The correlation coefficient is around 0.9 to 0.7. The R^2 of this kinetic model is the best to describe the reaction rate of H_2S adsorption in hydrogel biochar as the value is an approach to unity.

Table 1: The adsorption first- pseudo kinetics of different H_2S flow rate.

First- pseudo-order kinetic model				
Flow rate (L/s)	**Equation**	**R^2**	**$Q_{e\ (mg/g)}$**	**k_1 (s^{-1})**
60	Y = 0.013 X – 0.0363	0.7047	0.9198	0.0130
100	Y = 0.041 X- 1.717	0.8815	0.0192	0.0410
200	Y = 0.0384 X - 1.458	0.8211	0.0348	0.0382

The relationship of bed height with First- Pseudo kinetic model is shown in Table 2. The amount of H_2S adsorbed is directly proportional to bed height, with the correlation coefficient is around 0.7 to 0.8. Thus, this kinetic model is also the best to describe the reaction rate of H_2S adsorption in hydrogel biochar.

Table 2: The adsorption first- pseudo kinetics of different bed height.

First- Pseudo Kinetic Model				
Bed height (Inch)	**Equation**	**R^2**	**Q_e**	**k_1**
1.5	Y = 0.0119 X + 0.2037	0.7155	4.909	0.0119
3	Y = 0.0177 X +0.1945	0.723	5.141	0.0177
6	Y = 0.0211 X - 0.1651	0.7318	6.057	0.211

3.1.2. Second Pseudo Kinetic Model

The relationship of Hydrogen flow rate with First-Pseudo kinetic model is shown in Table 3. The amount of Hydrogen sulphide absorbed, Q_e is decreased as the flow rate of H_2S increased, as shown in Table 2. Hence, the amount of H_2S adsorbed is inversely proportional to the H_2S flow rate. The correlation coefficient is too small and approaches zero. Thus, this kinetic model not the best model to describe the reaction of H_2S adsorption in hydrogel biochar.

Table 3: The adsorption second- pseudo kinetics of different H_2S flow rate.

Second- pseudo-order kinetic model				
Flow rate	**Equation**	**R^2**	**Q_e**	**k_2**
60	Y=-1492 X +253.3	0.1796	6.70E-04	8788.25
100	Y = -1272 X+217	0.0409	7.86E-04	7456.15
200	Y= -2770 X 367.7	0.037	3.61E-04	20867.28

The relationship of bed height with First- Pseudo kinetic model is shown in Table 4. Based on Table 4, the amount of Hydrogen sulphide absorbed, Qe is decreased as the flow rate of H_2S increased. Hence, the amount of H_2S adsorbed is inversely proportional to H_2S flow rate. The correlation coefficient is too small and approaches zero. Thus, this kinetic model not the best model to describe the reaction of H_2S adsorption in hydrogel biochar.

Table 4: The adsorption second- pseudo kinetics of different bed height.

Second- pseudo kinetic model				
Bed height (inch)	**Equation**	**R^2**	**Q_e**	**K_2**
1.5	Y = -7259 X + 426.9	0.0622	-1.38E-04	123431.91
3	Y = -2912 X + 196.5	0.0661	-3.43E-04	43153.91
6	Y= -2213 X + 156.6	0.0845	-4.52E-04	31273.11

3.1.3. Elovich Kinetic model

The Elovich kinetic model result from the simulation is tabulated in Tables 5 and 6. The relationship of Hydrogen flow rate with the Elovich kinetic model is shown in Table 5. Based on Table 5, the amount of hydrogel biochar has been absorbed decreases as the flow rate of H_2S increases. Hence, the amount of H_2S adsorbed is inversely proportional to the H_2S flow rate. The correlation coefficient is too low and approaches zero. Besides, the value of α at 200L/s is too high, and it is not suitable to discuss the chemical adsorption of hydrogel biochar. Thus, this kinetic model may not be suitable to describe the rate of reaction of H_2S adsorption in hydrogel biochar.

Table 5: The adsorption Elovich kinetics of different H_2S flow rate.

Elovich kinetic model				
Flow rate	**Equation**	**R^2**	**α**	**β**
60	Y= -0.1077 x +0.6011	0.1723	-2.82E-07	-9.285
100	Y = 0.1092 x+0.1718	0.0479	4.088	9.158
200	Y = 0.0696 x +0.4626	0.0159	308433.089	14.368

While in Table 6 shows the relationship of bed height with the Elovich kinetic model. The correlation coefficient is too small and approaches zero. Thus, this kinetic model not the best model to describe the reaction of H_2S adsorption in hydrogel biochar. Besides, the value of α at 1.5 and 3 inches is a negative value, and it is not suitable to discuss the chemical adsorption of H_2S. Thus, this kinetic model may not describe the rate of reaction of H_2S adsorption in hydrogel biochar.

Table 6: The adsorption Elovich kinetics of different bed height.

Elovich kinetic model				
Bed Height (Inch)	**Equation**	**R^2**	**α**	**β**
1.5	Y = -0.192 X + 1.912	0.04156	-0.117	-5.208
3	Y = -0.0633 X + 1.376	0.0050	-0.0528	-15.797
6	Y = 0.0052 X + 0.7900	6.60E-05	0.0053	192.300

To see the clear comparison of R^2 between the kinetic models, the graph of R^2 vs. H_2S flow rate and R^2 vs. bed height are plotted and shown in Figures 2 and 3, respectively. The correlation coefficient, R^2 is used to identify between experimental data and the model which the relatively high R^2 value indicated a successfully model that describes the kinetics of H_2S gas adsorption.

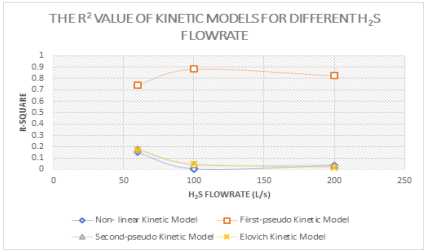

Fig 2: Comparison of R^2 of kinetic model with different hydrogen sulphide flow rate.

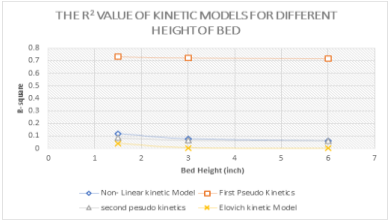

Fig 3: Comparison of R^2 of the kinetic model with different hydrogen sulphide flow rate.

It can be concluded that first-pseudo kinetic model, which described the physical adsorption, is the best model to describe the reaction and mechanism of hydrogen sulphide gas adsorption in hydrogel biochar. The attraction forces existing between adsorbate and adsorbent are Van der Waal's forces, which are very weak. Thus, it can be reversed by heating or by decreasing pressure.

3.2. Adsorption Isotherm

3.2.1. Effect of H_2S Flowrate

The effect of H_2S flow rate on gas adsorption is studied by using Langmuir and Freundlich Isotherm. The experimental data was run using the Monte Carlo simulation. Table 9 shows the data generated from the simulation for both isotherms.

Based on Table 9, the maximum capacity of adsorbent increases as the number of simulations of the run increases. The adsorption process happens mainly because of the static attraction between the carboxyl groups in adsorbents [13]. However, Figure 4 shows at the lower H_2S flow rate, the highest amount of adsorbent capacity. The relationships between maximum adsorbate adsorbed by hydrogel biochar are inversely proportional to hydrogen sulfide flow rate as the cycle is increased. The increasing flow rate makes it take a longer contact time between adsorbate and adsorbent. The relationship between the number of runs is directly proportional to the capacity adsorbent. Figure 4 (a), at 60 L/h of Hydrogen sulphide has the highest maximum capacity in hydrogel biochar.

Table 9 Effect of H_2S flow rate in H_2S adsorption on hydrogel biochar.

N	*F(L/h)*	*Langmuir's*	*R^2*	*Q_m*	*K_L*	*b*	*Freundlich's*	R^2	$\frac{1}{n}$	n	K_f
100	200	Y= 0.1752X +1.0130	0.897	5.708	0.173	5.782	Y= 0.3863 X - 0.0002	0.9120	0.3863	2.6054	1.0132
	100	Y= 0.1543X +0.0540	0.987	6.481	2.859	0.350	Y= 0.1847 X + 0.5271	0.9116	0.1874	5.6174	3.4132
	60	Y= 0.0736X +0.0487	0.969	13.585	1.511	0.662	Y= 0.2203 X + 0.9212	0.5476	0.2203	4.5401	8.3484
1000	200	Y= 0.1712X +1.0620	0.838	5.841	0.161	6.203	Y= 0.3937X + 0.0020	0.8328	0.3937	2.6387	1.0300
	100	Y= 0.1121X +0.0443	0.989	8.921	2.529	0.395	Y= 0.1145X + 0.6910	0.7627	0.1145	9.0271	4.9724
	60	Y= 0.0587X +0.0543	0.942	17.030	1.081	0.925	Y= 0.2168 X + 0.9184	0.7133	0.2168	4.6166	8.3309
10000	200	Y= 0.2549X +0.6405	0.961	3.923	0.398	2.513	Y= 0.3970X + 0.0322	0.9364	0.3970	2.7044	1.1209
	100	Y= 0.1071X +0.0476	0.981	9.337	2.248	0.445	Y= 0.1235X + 0.6670	0.8009	0.1235	8.1759	4.7044
	60	Y= 0.0593X +0.0338	0.967	16.869	1.755	0.570	Y= 0.1899X + 0.9572	0.6829	0.1899	5.2699	9.0702
10000	200	Y= 0.2361X +0.9987	0.924	4.235	0.236	4.230	Y= 0.4142X - 0.0101	0.8655	0.4142	2.4999	1.0991
	100	Y= 0.1230X +0.0815	0.974	8.130	1.509	0.663	Y= 0.1258X + 0.6713	0.8921	0.1258	8.5190	4.7877
	60	Y= 0.0583X +0.0460	0.957	17.156	1.268	0.789	Y= 0.1603X + 1.0209	0.7209	0.1603	6.3674	10.5020

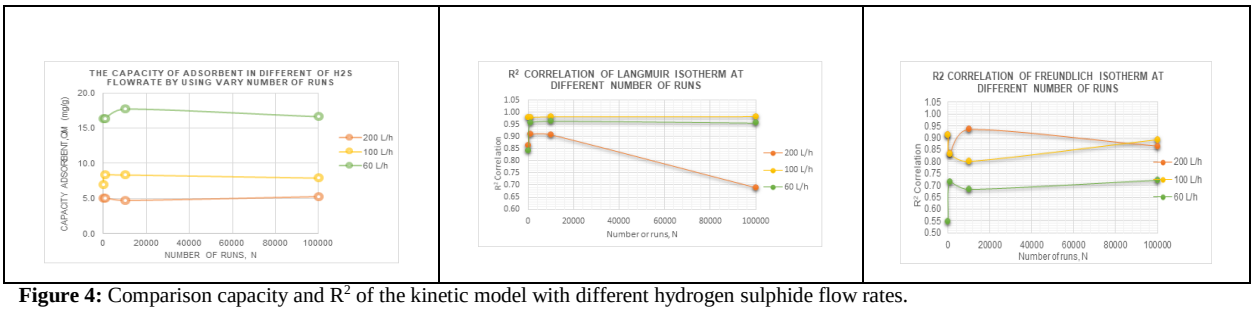

Figure 4: Comparison capacity and R^2 of the kinetic model with different hydrogen sulphide flow rates.

The R^2 correlation is to measure how close the data to the fitted regression line. According to Krause et al. (2005), the range of R^2 lies between 0 to 1 is a good prediction. As mentioned by Shi, Qiantao (2020), the adsorbate concentration will affect the value of the coefficient, and if the value is apart from 1, it indicates that the data is not fit with the model. At the 100 L/h of H_2S, it has the highest value of R^2, and it was closed to 1, followed by 60 L/h and 200 L/h. From the simulation result, the Langmuir model is suitable to use at 100 L/h and 60 L/h. However, at 200 L/h was not suitable for the Langmuir isotherm model because the adsorbate concentration was too high. Hence, the highest flow rate will be used by Freundlich isotherm. By comparing with the experimental result by Azmi (2019), the obtained Value of R^2 shows that adsorption of H_2S on hydrogel biochar Langmuir isotherm model is better graph fitting than the Freundlich isotherm model. This shows that the Freundlich model is not suitable for the adsorption of H_2S on hydrogel biochar. It can be shown in Figure 4, it has the highest value of R^2, and it was closed to 1 at N=10000. Examination of the linear isotherm plots suggested that the Langmuir model yielded a much better fit than the Freundlich model.

The constant in both isotherms related to the adsorption capacity. Based on experimental result, As the flow rate decrease, KL value increase. While in the simulation result, the constant is related to the number of cycles. As the number of simulation cycles increased, the isotherm constant also increased. At a flow rate of 100 L/h of hydrogen sulfide has the highest capacity monolayer of adsorption as it has the highest Value of Langmuir constant. It can conclude at this flow rate of the adsorption on hydrogel biochar was at the monolayer surface. When the gas molecules contact a solid surface, they are attached or bonded by chemical or physical reactions [13]. The isotherm constant of 60 L/h of Hydrogen Sulphide is increased. It has the highest capacity heterogeneous adsorption and Freundlich constant. It can conclude that the adsorption flow rate on hydrogel biochar was at a heterogeneous surface at this flow rate.

The molecular level of hydrogen sulfide adsorption on hydrogel biochar at lowest hydrogen sulfide flow rate applied monolayer adsorption of the adsorbent's outer. There are no lateral interaction and steric hindrance between the adsorbed molecules [14]. According to Papurello et al. (2019), the uniform energies of adsorption on the surface and no adsorbate shifting in the surfaces' plane. The adsorption on hydrogel biochar is on a heterogeneous layer with a reversible adsorption process for the highest flow rate.

The adsorption energy was found from the Linear equation of Langmuir Isotherm, which is b constant. It reveals the adsorption energy through the Arrhenius equation with a different number of runs increase; the adsorption energy also increased while the experimental result stated that the value of b increases as the H_2S gas flow rate decreases. Based on Table 9, the adsorption intensity at 200 L/h of hydrogen sulfide flow rate has the highest adsorption intensity, followed by 60 L/h and 100 L/.

3.2.2. Effect of bed height

The effect of bed height on gas adsorption was also studied using Langmuir and Freundlich Isotherm, which are tabulated in Table 10. There is three-bed height that will be used, which are 1.5, 3.0, and 6.0 inch. The bed height refers to the total amount of hydrogel biochar embedded in the adsorption column.

Based on Table 10, the adsorbent mass and the bed height increase as the hydrogel embed is increased. Hence, it can be said that the bed height is directly proportional to the amount of adsorption capacity, and the residence time taken is longer. The amount of adsorbent capacity is increased as the bed size is increased too. Based on Figure 5, the bed height of 6 inches has the highest amount of adsorbent capacity, followed by 3 inches and 1.5 inches. The adsorption process in hydrogel biochar is taken a long time as more adsorbent in the bed.

Table 10 Effect of bed height in H2S adsorption on hydrogel biochar.

N	*H (inc)*	*Langmuir's*	R^2	*Qm*	*KL*	*b*	*Freundlich's*	R^2	$\frac{1}{n}$	n	K_f
100	1.5	Y=0.0982 X +0.3079	0.8881	10.4632	0.3191	3.2182	Y=0.3852 X +0.9655	0.9304	0.3852	2.6326	9.2558
	3.0	Y= 0.0913 X +0.3211	0.9565	10.9615	0.5538	3.4761	Y= 0.2576X +0.6523	0.8215	0.2756	4.1105	4.6809
	6.0	Y = 0.0545 X+ 0.0352	0.9743	18.3514	1.5543	0.6453	Y = 0.2289 X+ 0.8452	0.7635	0.2289	4.4109	7.0152
1000	1.5	Y= 0.1002X+0.2813	0.9112	9.9807	0.3636	2.8133	Y= 0.5267X+0.5794	0.9665	0.5267	1.8986	3.7966
	3.0	Y=0.0825X +0.0836	0.9678	12.1861	0.9969	1.0114	Y=0.2120X +0.8774	0.8527	0.2120	4.7170	7.5405
	6.0	Y=0.0575 X +0.0456	0.9617	17.6852	1.2828	0.7849	Y=0.1594X +1.1010	0.8204	0.1594	6.2735	12.618
10000	1.5	Y=0.1291X +0.3990	0.9153	7.7459	0.3236	3.0906	Y=0.4515X +0.6265	0.8864	0.4515	2.2148	4.2316
	3.0	Y=0.0832X +0.0869	0.9603	12.0149	0.9577	1.0442	Y=0.2473X +0.7382	0.8323	0.2473	4.0437	5.4727
	6.0	Y=0.0649X+0.0574	0.9468	15.4178	1.1308	0.8844	Y=0.2658X +0.7834	0.8015	0.2658	3.7622	6.0730
10000	1.5	y=0.1024x+ 0.3751	0.8786	9.7656	0.2730	3.6631	Y=0.4140X+0.8935	0.9671	0..4140	2.4155	7.8253
	3.0	y=0.0765x+0.0742	0.9646	13.0753	1.0309	0.9701	Y=0.3491X+0.5780	0.8997	0.3941	2.8645	3.7844
	6.0	Y=0.0719x+0.0479	0.9696	13.9082	1.5026	0.6655	Y=0.2234X+0.8173	0.7307	0.2234	4.4763	6.5660

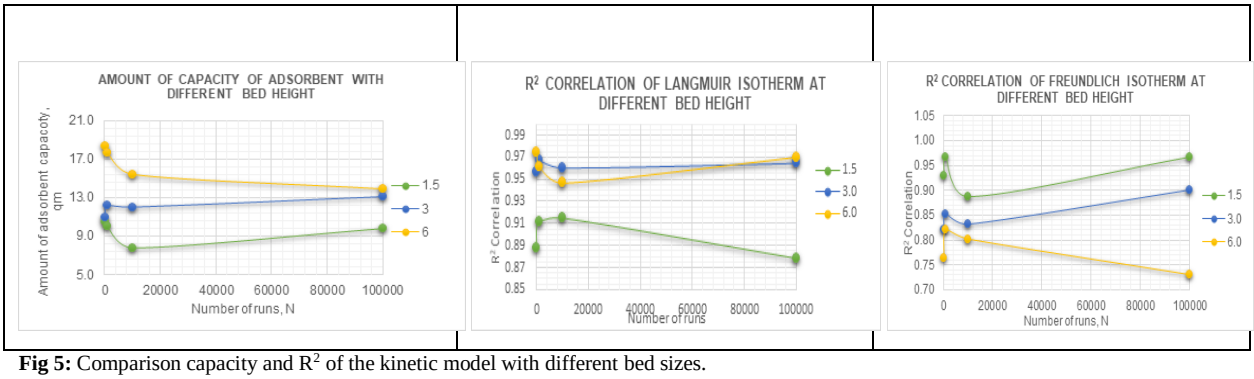

Fig 5: Comparison capacity and R^2 of the kinetic model with different bed sizes.

The trend of R^2 correlation can be shown for each isotherm and bed height in Figure 5 and Table 10. The R^2 correlation from the simulation shows how the separation of gas adsorption in hydrogel biochar occurred. According to the experiment conducted, the Value of R^2 increase as bed height increase. Based on Table 10, the Value of R^2 increased as the bed height increased for Langmuir isotherm, while for Freundlich isotherm, it shows the opposite way. It also reveals that the increased number of cycles tend to make the R2 correlation for bed height of 1.5 inches was the lowest. The range of R^2 correlation is from 0.8 to 0.9. In contrast, the bed height of 1.5 inches has the highest R^2 correlation value above 0.9. A good prediction of R^2 is close to 1.0, according to Alias. (2018), the increase in the thickness of adsorbent tends to decrease the correlation coefficient, R^2. Thus, it can be concluded that the bed height of 1.5 inches was fit to the Freundlich isotherm.

The molecular level of hydrogel biochar on bed height is shown a different trend. Malins et al. (2015), stated that it prefers heterogeneous adsorption as the bed height increased. The short bed height consists of a small amount of adsorbent. Thus, the new chemical bond, which is the strongest bond, is generated at the adsorbent surfaces. The adsorbate (H_2S) will be trapped on the hydrogel biochar surface using a small amount of adsorption energy.

The isotherm constant is related to the adsorption capacity. The increasing number of cycles increased the isotherm constant, whereas, in the experimental, the Value of K_L increases with bed height. The simulation result is accepted as the adsorption constant also increase as bed height increase. It is also shown that a bed height of 1.5 inches has the highest Value of both Langmuir and Freundlich. This can be concluded that the adsorption capacity of this bed is higher than 3.0 and 6.0 inches.

The value of b is the Langmuir constant relates to the adsorption energy. Alias (2018) stated that the Value of b increases when the thickness of the adsorbent increases. This statement was only fit when the simulation was run with N≤10000. For N> 10000, it has the opposite statement from Alias (2018). It can be said that the simulation of adsorption in hydrogel biochar only can run up to N=1000, and the adsorption energy is increased as the bed size increase. There will be more vacant sites provided as the number of adsorbent increases Freundlich constant, 1/n is known as adsorption intensity.

According to Alias et al. (2018), the Freundlich isotherm slope shows strength in the adsorption process. From Table 10, the values of the slope are within the range of 0 to 1. Thus, all bed sizes can run a normal adsorption process against many simulation cycles. Figure 5 shows that the highest adsorption intensity is at a bed height of 1.5 inches, followed by 3 inches and 6 inches. Thus, it can be concluded that the adsorption intensity is increased as the pore volume of the adsorbent increased.

4. Conclusions

Monte Carlo simulation was used to investigate the H_2S adsorption in the biochar hydrogel by using the MATLAB software. It can be concluded that

First-Pseudo Kinetic model is the best model to describe the reaction and mechanism of adsorption in hydrogel biochar. The adsorption isotherm study for Langmuir and Freundlich was conducted. The adsorption in hydrogel biochar required a small amount of energy and can save the adsorption process's cost. For the optimum bed, height required higher adsorption energy. The adsorption process occurs at the monolayer of the adsorbent with an equivalent adsorption site. Which does not have lateral interaction and steric hindrance between the adsorbed molecules.

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