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Kinetics models of hydrogen sulphide adsorption from hydrogel biochar derived from empty fruit bunch (EFB)

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ABSTRACT

Purpose: This research aims to investigate the detailed state of adsorption kinetics modelling and research on the application of hydrogen sulfide adsorption by hydrogel derived from empty fruit bunch (EFB), the determination of the kinetics parameters, and the comparison between models in a selection of the best-fit model.

Design/methodology/approach: The kinetics modelling used are pseudo-first-order and pseudo-second-order models. The correlation coefficient was used to evaluate the suitability of the equation R^2. After obtaining the results, the comparison was made by comparing the R^2 of each model. The pseudo-second-order model has a higher value of correlation coefficient, R^2, making it the most suitable kinetics model for adsorption systems.

Findings: The R^2 for pseudo-first-order on the effect of dry bed height was 0.8814, whereas its effect on powder bed height was 0.9537, and that of the wet bed height was 0.9607. Meanwhile, the R^2 for pseudo-second-order on the effect of dry bed height was 0.89, on the effect of the powder bed height was 0.99, and on the effect of the bed height of wet was 0.99, the highest among kinetic models. Based on the results, the pseudo-second-order model best describes the adsorption of hydrogen sulfide (H_2S) by hydrogel biochar.

Research limitations/implications: The kinetics modelling used are pseudo-first-order, and pseudo-second-order models for hydrogen sulfide adsorption by hydrogel originating from empty fruit bunches (EFB).

Practical implications: Based on the results, the pseudo-second-order model best describes the adsorption of hydrogen sulfide (H_2S) by hydrogel biochar. Kinetic studies are important in understanding the reactions and design of the process.

Originality/value: The authenticity results of this article were found to be 17% similar. The novelty of this paper is the kinetics study of the new adsorbent developed based on EFB to adsorb H_2S.

Keywords: Hydrogen sulphide, Adsorption, Kinetics models, Empty fruit bunch, Hydrogel

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METHODOLOGY OF RESEARCH, ANALYSIS AND MODELLING

1. Introduction

Determining which pollutants exist in the environment and which waste contributes to contaminants on land or in water is challenging. Hydrogen sulphide (H_2S) is the industry's second most toxic gas [1]. The emission of H_2S can cause many diseases that are very dangerous to humans. In addition, H_2S can affect human breathing, in which inhalation and high exposure to highly concentrated H_2S can result in the worst scenario, which is rapid death [2]. Because hydrogen sulfide (H_2S) is non-degradable, it can be classified as hazardous waste. Hazardous waste is any waste or mixture of trash that forms a considerable amount of waste and poses current or future harm to human health or living organisms on land or in water. The aforementioned hazardous waste can be managed based on the identification and classification of the waste while considering the application of risk management to monitor the effect of hazardous waste on human health and the environment [3]. Most industries consider taking a control system to control the use of hydrogen sulfide. All industries adopt control systems, such as adsorption, chemical oxidation, biological treatment, and others, to control hazardous and dangerous chemicals [4]. The adsorption process is a process by which solute molecules attach to the surface of an absorbent. Meanwhile, the adsorption process can be described as a processing step in the chemical engineering context and process, which interacts with surface forces and saturation of molecules on the solid surface, referring to adsorption [5,6]. Two processes in adsorption occur in the process: physical adsorption (physisorption) and chemical adsorption (chemisorption).

The physisorption and chemisorption processes can occur on the adsorbent in parallel; for example, physisorption can occur on inactive sites, while chemisorption occurs on active sites involving free ions present on the adsorbent [7]. In addition, adsorbents prepared from agricultural waste like oil palm waste, rice husk wood waste, and other abundance waste stated a meagre cost and effective material as an adsorbent [8]. Therefore, it is essential to describe adsorption kinetics and compare the adsorption parameters calculated by each model to the observed adsorbent behaviour [4]. The determination of suitable and fitted models is based on optimizing the adsorption mechanism pathways and the effectiveness of the adsorption system [3]. Many researchers have developed a model focusing on hydrogen sulfide, and the most common adsorbent used is activated carbon. Meanwhile, this work focuses on hydrogen sulfide and hydrogel adsorption kinetics. This paper discusses the detailed state of adsorption kinetics modelling and research on the application of hydrogen sulfide adsorption by hydrogel derived from empty fruit bunch (EFB), the determination of the kinetics parameters, and the comparison between models in the selection of the best-fit model.

2. Methodology

2.1. Experimental data

The lab-scale experiment is required to obtain the raw data of the adsorption system. The experimental data is obtained from the work of [9] with two parameters (bed height and adsorption performance); meanwhile, the thickness of the adsorbent and time of hydrogen sulfide concentration is kept constant. As for hydrogel-based adsorbent, empty fruit bunch-based hydrogel biochar composite (EFB-HBC) was used in this research.

2.2. Kinetics modelling

Adsorption kinetics modelling is one of the best systematic methods used to analyse the performance of the adsorption system between the solute and the adsorbent surface [10]. It can provide information on the adsorption rate, performance of the adsorbent, and mass transfer mechanisms [11]. In kinetic adsorption models, it is usually the case when the adsorbate uptake on the adsorbent is chemical. R^2, defined as the correlation coefficient value, is required to obtain suitable kinetic modelling for this adsorption system. R^2 can be estimated using a graph with a straight line, which is obtained from a linearized equation. The adsorption rate can also be determined from the graph after the slope and intercept have been determined.

The equation for linearised of the pseudo-first-order model and pseudo-second-order model is shown in Eq. (1) and Eq. (2) [5]:

$$\ln(q_e - q_t) = \ln(k_1 q_e) - k_1 t \quad (1)$$

where q_e is the adsorption of equilibrium and (mg/g), q_t is the adsorption of equilibrium over time (mg/g), and k_1 is the PSO rate constant (g/mg.min). The value of k_1 is the adsorption rate constant, calculated from the plots of $\ln(q_e-q_t)$.

$$\frac{t}{q_t} = \frac{1}{k_2 q_{e^2}} + \frac{t}{q_t} \quad (2)$$

where k_2 in g/mg.h is the rate constant for pseudo-second-order adsorption.

3. Results and discussion

3.1. Kinetics modelling

Pseudo-first order model

Figure 1, Figure 2, and Figure 3 demonstrate the kinetic modelling on the effect of dry bed height, the effect of the powder bed height, and the effect of wet EFB-HBC, respectively. It can be seen that when the height of the bed was increased, the R^2 value became more beneficial. The higher the bed height, the more particle surface area is provided for the gas-solid reaction [12].

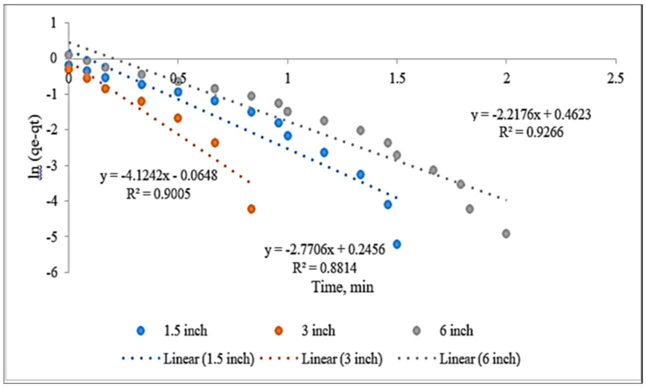

Fig. 1. Kinetic modelling pseudo-first order on the effect of the bed height of EFB-HBC

Based on the results, it can be observed that the higher the dry bed height, the higher the value of R^2, which better fits the model. Similarly, as the powder bed height increased, the value of R^2 from 1.5 inches to 6.0 inches was 0.98, 0.95, and 0.97, whereby the increment of the bed height observed inconsistencies. As for the higher wet bed height, it is observed that the value of R^2 is also inconsistent with the bed height, where it decreases with a higher bed height.

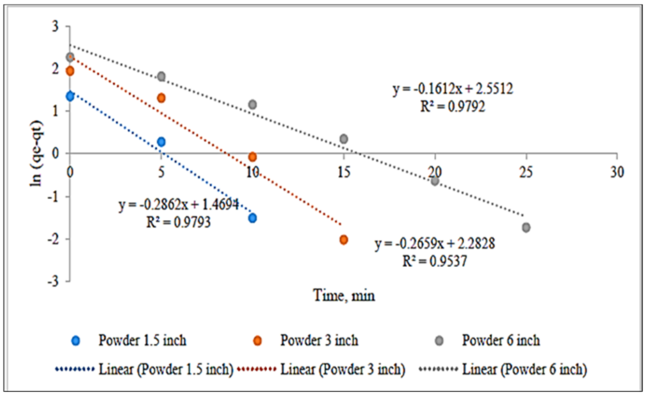

Fig. 2. Kinetic modelling pseudo-first order on the effect of the bed height of powder EFB-HBC

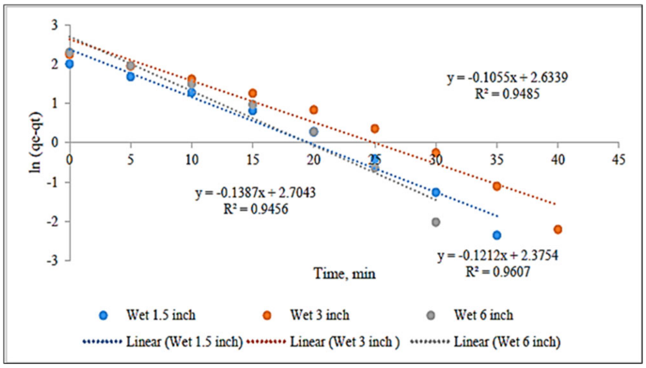

Fig. 3. Kinetic modelling pseudo-first order on the effect of the bed height of wet EFB-HBC

Table 1.
Pseudo-first order model parameters

Type of EFB-HBC	MV in.	Slope	R^2	q_{cal} mg/g	k_1 1/min
Dry EFB-HBC	1.5	-2.77	0.88	1.29	2.77
	3.0	-4.12	0.90	1.07	4.12
	6.0	-2.21	0.93	1.59	2.22
Powder EFB-HBC	1.5	-0.26	0.98	4.34	0.89
	3.0	-0.28	0.95	9.80	0.27
	6.0	-0.16	0.97	12.82	0.16
Wet EFB-HBC	1.5	-0.12	0.96	10.76	0.12
	3.0	-0.10	0.95	13.99	0.11
	6.0	-0.13	0.95	14.94	0.14

From Table 1, it can summarises that the value of R^2 is inconsistent with the bed height. The value of q_{cal} is also inconsistent based on the thickness of the bed height, which means it will affect the model's accuracy and lead to the failure to apply this pseudo-first-order model in the industry for pollutant removal. The results are consistent with the reported work from [2] on the adsorption of hydrogel biochar adsorbents. The pseudo-first-order model is not suitable for the adsorption process in a system, as the value is inconsistent.

Pseudo-second order model

The pseudo-second-order kinetic model depends highly on the rate-determining step based on the assumption of chemisorption [13]. The rate-limiting stage is chemical adsorption, which involves valence forces through sharing or exchanging electrons between adsorbent and adsorbate. If the adsorption process follows pseudo-second-order kinetics by evaluating the equation of each manipulative, differences can be found. The data in this research will be substituted into a pseudo-second-order equation to plot the graph. Figure 4, Figure 5, and Figure 6 below portray the results of pseudo-second-order models based on the effect of bed height.

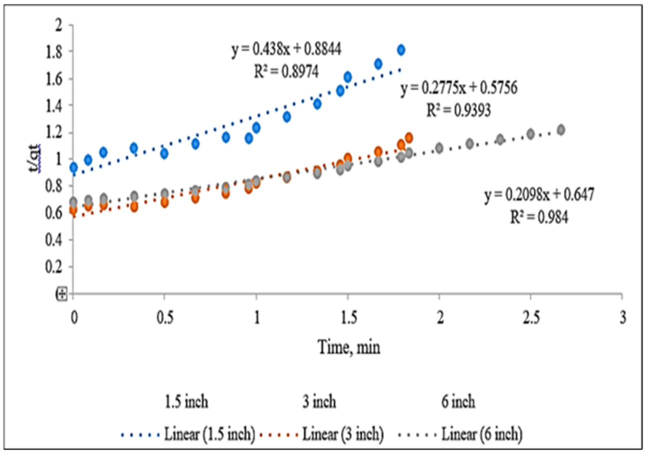

Fig. 4. Kinetic modelling pseudo-second order on the effect of the bed height of EFB-HBC

Table 2 shows data from Figures 4, 5, and 6. The information obtained from the graphs are: manipulative, slope, R^2, q_{cal}, and k_2.

Based on Table 2, k_2 is the rate constant of the pseudo-second-order adsorption model, and q_{cal} is the amount of hydrogen sulfide adsorbed in the meantime. From Table 2 it can summarises that the value of R^2 increases with higher bed height, but it is different for powder and wet EFB-HBC, as it was kept constant through the three sizes of bed height. On the other hand, the value of q_{cal} decreases based on the thickness of the bed height, which means it will affect the accurateness of the model, but q_{cal} can be defined as small values of sensitivity that result in experimental errors.

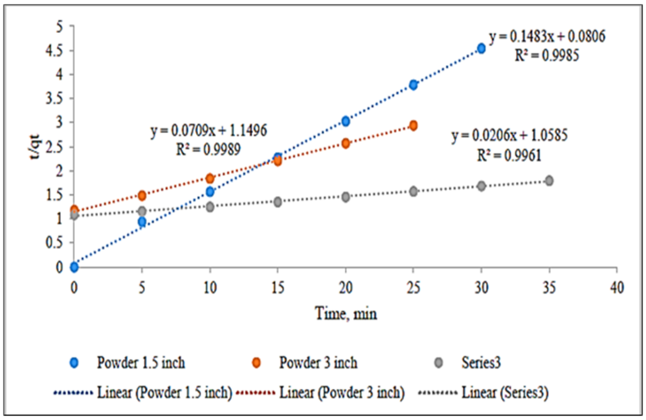

Fig. 5. Kinetic modelling pseudo-second order on the effect of the bed height of powder EFB-HBC

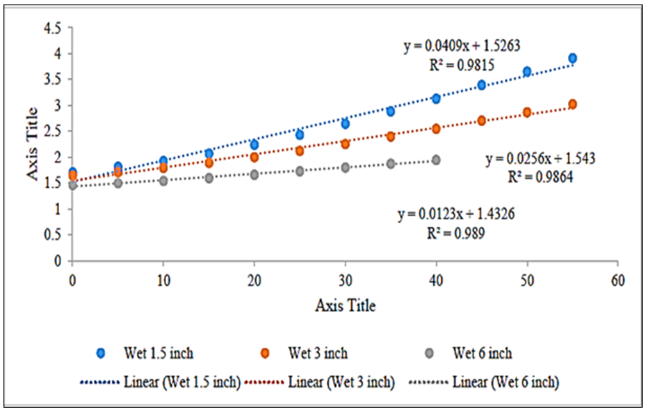

Fig. 6. Kinetic modelling pseudo-second order on the effect of the bed height of wet EFB-HBC

Table 2.
Pseudo-Second Order Model Parameters

Type	MV in.	Slope	R^2	q_{cal} mg/g	k_2 g/mg.min
Dry EFB-HBC	1.5	0.43	0.89	0.22	2.28
	3.0	0.27	0.94	0.13	3.60
	6.0	0.20	0.98	0.07	4.77
Powder EFB-HBC	1.5	0.14	0.99	0.27	6.74
	3.0	0.07	0.99	0.004	14.10
	6.0	0.02	0.99	0.0004	48.54
Wet EFB-HBC	1.5	0.04	0.99	0.01	24.44
	3.0	0.02	0.99	0.0004	39.07
	6.0	0.01	0.99	0.0001	81.30

Thus, q_{cal} is accepted as the value of R^2, which indicates the fitting towards the process. The result is consistent with the reported work from [2] on the adsorption of hydrogel biochar adsorbent, as the pseudo-second-order model is considered suitable for the adsorption process in a system due to its consistent value. Table 2 shows the pseudo-second-order model parameters.

3.2. Application of kinetics modelling to H_2S by hydrogel biochar

Comparison between the time ranges for kinetics modelling

As seen in Figures 1-6, the pseudo-first-order and pseudo-second-order models are compared in the entire time range available based on the bed height. However, limiting the research to the first or last stage of the process does not represent both models. It can result in an underestimating or overestimation of the kinetics parameters provided. Collecting data throughout the full uptake procedure is the easiest technique to obtain an average [3,14]. Therefore, it is better to use a pseudo-second-order model at the 1.5 inches of the bed height in the entire duration range instead of pseudo-first-order range models, as seen in Figure 4. This conclusion can be expanded, and the models can elucidate the whole range of preferred processes, which can then be developed.

Comparison between kinetic parameters

Table 3 below shows the kinetics parameters for the adsorption of H_2S on EFB-HBC. It discusses the apparent kinetics parameters estimated from the pseudo-first-order and pseudo-second-order models.

According to Table 3, the adsorption equilibrium capacity was increased in dry EFB-HBC, followed by powder EFB-HBC, and then wet EFB-HBC. The pseudo adsorption rate constant or the sorption rate and the amount of H_2S, q_{cal} can be calculated based on Figures 1-6, the fitting plots for all adsorption models, Table 3, and the kinetics parameters obtained from the modelling concerning the pseudo-first-order model and pseudo-second-order model. The pseudo-second-order model better describes the kinetics than the pseudo-first-order model. For the pseudo-first-order model based on dry EFB-HBC, the pseudo rate constant for 1.5-inch, 3.0 inch, and 6.0 inch are 2.77/min, 4.12/min, and 2.22/min, respectively, the maximum amount of H_2S adsorbed is on 6 inches at 1.59 mg/g. In this case, different from pseudo-second-order model based on dry EFB-HBC, the pseudo rate constant for 1.5-inch, 3.0-inch, and 6.0-inch are 0.22 g/mg/min, 0.13 g/mg.min, and 0.07 g/mg. min, respectively, and the maximum amount of H_2S adsorbed is for the 6 inches at 4.77 mg/g. Nevertheless, all R^2 values in the pseudo-second-order model were greater than those in the pseudo-first-order model and had reached unity, indicating that the pseudo-second-order model better matched and fitted the kinetics data than the pseudo-first-order kinetic model; this indicates chemisorption behaviour. The adsorption process (i.e., chemisorption) involves the sharing or exchange of electrons between the adsorbent and metal ions, resulting in valence forces [15,16], thus making the pseudo-second-order model suitable for industrial use.

4. Conclusions

The paper aims to investigate the mathematical derivations from the adsorption kinetics model used, which are the pseudo-first-order model and pseudo-second-order model, as well as the physical meaning between the kinetics adsorption models and apply them to the sorption of hydrogen sulfide (H_2S) by hydrogel biochar. The kinetics model was used in this research to optimize the adsorption system of hydrogen sulfide. Thus, the pseudo-first-order model and pseudo-second-order model are studied in this

Table 3.
Kinetics parameters

Type	Parameter						Pseudo-first order kinetic			Pseudo-second order kinetic		
	Co, mg/L	F, L/h	L, inch	M, g	V, L	q_{exp}, mg/g	q_{cal}, mg/g	k_1, min^{-1}	R^2	q_{cal}, mg/g	k_2, g/mg.min	R^2
Dry EFB-HBC	25	60	1.5	12	0.0660	1.66	1.29	2.7706	0.88	2.28	0.2169	0.89
	25	60	3	18	0.1321	3.12	1.07	4.1242	0.90	3.60	0.1337	0.94
	25	60	6	36	0.2642	4.78	1.59	2.2176	0.93	4.77	0.0680	0.98
Powder EFB-HBC	25	60	1.5	18	0.0660	6.61	4.34	0.2862	0.98	6.74	0.2728	0.99
	25	60	3	30	0.1321	13.61	9.80	0.2659	0.95	14.10	0.0043	0.99
	25	60	6	45	0.2642	44.58	12.82	0.1612	0.97	48.54	0.000401	0.99
Wet EFB-HBC	25	60	1.5	21	0.0660	19.16	10.76	0.1212	0.96	24.44	0.01096	0.99
	25	60	3	36	0.1321	31.38	13.99	0.1055	0.95	39.065	0.000425	0.99
	25	60	6	60	0.264294	69.38	14.94	0.1387	0.95	81.30	0.000106	0.99

work based on several kinetics parameters. In this study, based on the highest correlation coefficient value compared in both models, it can conclude that the pseudo-second-order model best describes the adsorption of hydrogen sulfide (H_2S) by hydrogel biochar.

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Additional information

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