Mathematical modelling and simulation on the adsorption of Hydrogen Sulfide (H$_2$S) gas

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Abstract. Hydrogen sulfide, H$_2$S, a pollutant in biofuel gas, i.e., biohydrogen and biomethane, is produced at concentrations ranging from 100 ppm to 10,000 ppm and is recommended to be removed at the early stage of gas purification because it is known as a problematic compound. In this study, adsorption technologies show a promising technique to remove H$_2$S from biofuel gas, which mainly depends on the operating parameters and adsorbent ability. In this study, the development of the models is important to investigate the fundamentals of H$_2$S adsorption mechanism. The fitted mathematics model was performed by considering several assumptions made for fixed-bed adsorption, leading to the determination of the breakthrough curve by solving a set of partial differential equations (PDEs). The operating parameters were as follows: varied inlet concentration at 1000 ppm to 10,000 ppm, flow rate at 0.2 L/min to 0.6 L/min, length bed used at 10 cm to 30 cm, and pressure at 1.5 atm to 5 atm. The adsorption performance was also studied by using commercial activated carbon such as palm kernel shell (PKS-AC), coconut shell activated carbon (coconut shell-AC), and zeolite ZSM-5. To support the effectiveness of the mathematical models, the adsorption test was performed by loading the adsorbent into the fixed-bed adsorption column at an overall diameter of 6 cm and height of 30 cm. The system operated under room temperature, H$_2$S inlet concentration of 1000 ppm, and varying flow rate as in the modelling for PKS-AC. As a result, in the modelling study, the inlet concentration effect was highest in adsorption capacity, breakthrough time, and exhaustion time. However, the increase of flow rate and length bed used only affected the breakthrough and exhaustion times but not adsorption capacity. The total pressure used did not affect adsorption performance. Coconut shell-AC shows longer exhaustion time compared with other adsorbents due to the less frequent changes of adsorbent. In the experimental study, the 1000 ppm inlet concentration shows the highest flow rate effect on the adsorption performance, which, at 0.2 L/min, took almost 23 h to achieve 30 ppm compared with 0.6 L/min, which only took 13 min to exhaust the same outlet concentration. Hence, the adsorption system with the right choice of operational parameters, adsorbent, and fitted mathematical models can optimize the adsorption efficiency, adsorption capacity, breakthrough time, and exhaustion time.
1. Introduction

Biogas is a gas mixture that is formed by various types of microorganisms through the degradation of organic matter under anaerobic conditions. Anaerobic digestion, a well-known process of renewable energy production, is the breakdown and conversion of biomass to biogas by microorganisms. The biogas product is composed of major and minor components. Previous studies found that the major products are Methane (60% to 70%) and Carbon Dioxide (30% to 40%) \[^1,2,3,4\] , whereas the minor products consist of Hydrogen Sulfide (H\_2S), Ammonia (NH\_3), Hydrogen (H\_2), Nitrogen (N\_2), Carbon Monoxide (CO), saturated or halogenated carbohydrates, Oxygen (O\_2), and water (H\_2O). The average composition of biogas products as stated in Table 1 is from POME, dairy manure, and waste water treatments. \[^2,3,5,6\].

### Table 1. Components and composition of biogas production \[^4\].

| Components | Composition |
|------------|-------------|
| CO\_2     | 30–40       |
| CH\_4     | 60–70       |
| H\_2S     | 0.15–0.3    |
| NH\_3     | <1          |
| N\_2      | 0–2         |
| CO        | <0.6        |
| O\_2      | 0–1         |
| H\_2O     | 5–10        |

The purification of biogas also attracted considerable attention from many countries in terms of generating renewable energy. As an example, the purification of biogas up to 99.99% of H\_2S is needed for the fuel cell system known as polymer electrolyte membrane fuel cell (PEMFC). PEMFC requires below 1 ppm H\_2S concentration and is an excellent fuel supply for the generation of energy or electricity.

H\_2S are problematic compounds that act as a strong poison for fuel cells, reform catalysts, and also affect the mechanical wear of equipment and the operation \[^7\]. H\_2S combustion can also lead to sulfur dioxide emissions, which have harmful environmental effects. Moreover, biogas-produced H\_2S leads to the inefficiency of biogas production as it corrodes equipment even at low concentrations. Therefore, early removal of H\_2S is recommended in the biogas purification process to upgrade the raw biogas quality, avoid any cost increment, and provide better environment. However, to remove H\_2S gas, an acceptable concentration level in the range of 0 ppm to 5 ppm for boiler feed water or industrial process needs to be met \[^8,9,10,11\].

Besides, the removal of H\_2S can be achieved by several technologies, namely, biological, absorption, adsorption, and membrane technologies. To maximize the H\_2S removal efficiency, the appropriate method should be chosen. In this study, adsorption technology via microporous material (activated carbon) was chosen as the more appropriate and economic method compared with other technologies.

The adsorption technique was reviewed for further study through the performance of mathematical models, as experimental study consumes longer time and higher cost. The mathematical models were performed as necessary to establish the optimization of the design and operation conditions. The ideal model should be convenient, be able to give an exact estimation of the breakthrough behaviour, and evaluate the adsorption effect of each variable. Generally, the modelling of dynamic adsorption consists of macroscopic mass conservation, uptake rate, and isotherm equations. As the mathematical model developed, the performance of fixed-bed adsorption modelling was further studied.

In this modelling, the prediction of the breakthrough method can be used for the determination of fixed-bed adsorption and measuring the full breakthrough curve and equilibrium adsorbed-phase concentrations by using the material balance. This knowledge is important to design and optimize industrial units of adsorbers \[^12,13\]. This method is an early prediction for the evaluation of the adsorption efficiency and adsorption capacity of adsorbents. The adsorption rate also can be determined via time and concentration of H\_2S \[^14\].
Some researchers investigated adsorption performance via several types of adsorbents, operating parameters, and simulation methods. A study by Choo et al. (2013) used impregnated coconut shell activated carbon (coconut shell-AC) in scrubbing units to remove H$_2$S gas. However, this study had simulated mixing three gases. A study by Lau et al. (2013) investigated the optimization study by using statistical analysis. The adsorbent used was palm shell activated carbon. Melo et al. (2006) discussed the performance of different types of adsorbents (Zinnox and Zeolite) to remove H$_2$S from natural gas.

Based on the information discussed above, the researchers focus on the prediction of breakthrough data, obtained from general rate models by solving the partial differential equation (PDEs) to optimize the parametric performance via the efficiency, adsorption capacity, effect of pressure, and types of adsorbent used toward H$_2$S removal. The experimental method was tested using H$_2$S / N$_2$ gas and a single adsorber column at the same operating parameters used in modelling. Hence, the data of experimental and modelling results were validated.

2. Adsorption principles
Adsorption is a phenomenon of attracting, retaining, and accumulating any substance which results in the higher concentration of molecular species on the surface of another substance as compared with that in the bulk. The solid surface that is exposed toward the gas or liquid will concentrate on the surface. The adsorption process, also known as one of the methods for the removal of undesirable compounds in gas or liquid, penetrates into the pores of the adsorbent and not into the lattice itself [17]. Theoretically, the substance that adsorbed on the surface is called the adsorbate, whereas the substance that is used to absorb is called the adsorbent.

Adsorption has two types: physical (physisorption) and chemical adsorption (chemisorption). Physical adsorption is a phenomenon of van der Waals attraction between adsorbate and adsorbent. This attraction is well known as weak and reversible since the molecules (adsorbate) are free to move on the surface. This process requires low temperature. Chemisorption requires an attraction between adsorbent and adsorbate through chemical bond at higher temperature.

However, adsorption is suitable for non-combustible gas as it possesses valuable recovery of pollutants and contains very dilute concentrations of pollutant [18]. The adsorption process is important for dehumidifying gas, removing odours or pollutants from the stream, or recovering valuable solvent vapours from the stream.

In the wastewater treatment industry, adsorption via activated carbon is widely used because of the low solubility of contaminant in the waste, as the contaminant has greater affinity for carbon than for the waste or a combination of both. Basic principles of carbon adsorption required mass transfer and adsorption of a molecule from a liquid or gas into solid surface. Hence, commercial microporous material (activated carbon) is produced as extremely porous carbon particles with large surface area, capable of holding adsorbate molecules.

Microporous materials have been tested for applications in gas separation because of their high surface area, micropore volume, and suitable pore size distribution [19]. The variety of microporous materials has also been studied and developed for physical adsorption of gas mixtures [20, 21, 22]. Moreover, the availability of microporous materials is easily obtained as it has been produced in the industrial scale, together with the wide availability of carbon sources. The use of microporous materials is cost-efficient technology, particularly in separation systems, such as pressure swing adsorption (PSA). PSA is commonly accepted to be the most attractive, efficient, and affordable separation method because of its simple control, low operating and capital investment costs, and higher energy efficiency [22, 23, 24].

The fixed-bed adsorption models were investigated with several models that were derived from different assumptions suitable only for limited situations. The models that are widely used are general rate models; linear driving force; wave propagation theory; constant pattern theory; Clark, Thomas, Bohart-Adams, and bed-depth service time Yoon-Nelson, Wang, Zhang, and Cheng models; Wolborska; and the modified dose-response model [25, 26, 27, 28, 29]. Moreover, the ideal model should predict
the breakthrough curve, including the breakthrough time, exhaustion time, breakthrough concentration, and exhaustion concentration, as mentioned in figure 1 below:

Figure 1. Breakthrough curve.

Where
- \( t_b \) = Breakthrough time
- \( t_x \) = Exhaustion time
- \( C_b \) = Breakthrough concentration
- \( C_x \) = Exhaustion concentration
- \( C_0 \) = Inlet concentration
- \( M_s \) = Adsorption zone from the break point to exhaustion

3. Mathematical model
The mathematical models focused on the calculation of modelling for the fixed-bed adsorption. The breakthrough curve prediction can be determined via solving a set of partial differential equations.

3.1. Fixed-bed adsorption models
As fixed-bed adsorber is commonly used in PSA, the adsorber undergoes four stages, which are pressurization, adsorption, depressurization, and purge. Moreover, the following main assumptions are made for performing the mathematical models: i) ideal gas behavior; ii) axially dispersed plug flow; iii) uniform cross-sectional void fraction; iv) mass and heat transfer are negligible; v) isothermal adsorption; vi) thermal equilibrium occurs between gas and particles; and vii) two component gas, which are adsorb gas (H2S) and carrier gas (N2) [31, 32, 33].

According to the aforementioned assumptions, the mathematical model equations for general rate models with length, \( L = \partial Z \) may be written as follows. The figure 2 shows the schematic of adsorption column [34].

Figure 2. Schematic of adsorption

Then, the general component material balance is given as follows [35, 36]:

\[-D_l \frac{\partial^2 C}{\partial Z^2} + \frac{\partial}{\partial Z} (\nu C) + \frac{\partial C}{\partial t} + \left(1-\frac{\epsilon}{\epsilon_c}\right) \frac{\partial q}{\partial t} = 0\]  \hspace{1cm} (1)
Where
C = Outlet concentration
ε = Bed void fraction
v = Interstitial molar velocity
Z = Spatial coordinate
D = Effective axial dispersion coefficient
t = Time variable
q = Adsorption capacity

For the determination of the adsorption capacity, the initial and boundary conditions were considered as important parts. By integrating Equation (2) into Equation (3), adsorbed mass \(M_{ads}\) and adsorption capacity, \(q \text{ (mg/g)}\), can be revealed. This equation is used in the adsorption and desorption (purge) stage. Hence, the initial and boundary conditions are stated below [16, 37]:

Initial condition,
\[ c(t,z) = 0 \text{ for } t = 0 \] (2)

Boundary condition,
\[ C(t,z) = C \text{ for } z = 0 \] (3)
\[ \frac{\partial C}{\partial z} = 0 \text{ for } z = L \] (4)
\[ \frac{\partial q}{\partial t} = k_d(C - C^*) \] (5)
\[ M_{ads} = QC \int_0^t (1 - \frac{C}{C_0}) \, dt \] (6)
\[ q = \frac{C_0 - C}{M} V \] (7)

Where \(C_0\) and \(C\) are the initial and outlet concentrations (mg/L); \(M\) is the adsorbent dosage (g); \(Q\) is the flow rate and \(V\) is the volume of the column [34]. Then, the pressurized–depressurized stages need to obey the ideal gas law \((PV = nRT)\), and the general material balance is performed as Equation 8 below [33]:

\[ \frac{\partial v}{\partial z} = \frac{1}{p} \frac{\partial p}{\partial t} - E_g \frac{\partial q}{\partial t} \] (8)

Where,
\[ E_g = \frac{R_g T_f}{P} \left( 1 - \frac{\epsilon}{\epsilon} \right) \] (9)

Where \(P\) is total pressure; \(R_g\) is the gas law constant; \(T_f\) is temperature of system; \(\epsilon\) is porosity; and \(E_g\) is concentration gas in systems.

4. Results and discussions
These results are based on the optimization of inlet concentration, flow rate, pressure, length of bed used, and difference of adsorbent through theoretical study. The inlet concentrations varied from 1000 ppm to 10,000 ppm, whereas the gas flow rate and pressure were between 0.1 and 1.0 L/min and 1.5 and 5.0 atm. The \(H_2S\) inlet concentration, flow rate, pressure, and length of bed used were discussed based on palm kernel shell activated carbon (PKS-AC), whereas the performance of adsorbent was discussed based on zeolites ZSM-5, coconut shell, and palm kernel shell. The specification of adsorber column from the actual laboratory scale and the data of pore volume and Brunauer–Emmett–Teller (BET) surface area were determined via characterization test. The breakthrough time was predicted as
the first outlet concentration came out. Moreover, this study was extended to the experimental study at flow rate (0.2 L/min to 0.6 L/min), constant inlet concentration (1000 ppm) and room temperature. The constant parameters used are stated in tables 2 and table 3 [38]

Table 2. Specification of adsorber unit.

| Parameter                  | Value |
|----------------------------|-------|
| Length of adsorber (M)     | 0.30  |
| Diameter of adsorber (M)   | 0.06  |

Table 3. Adsorbent properties.

| Parameters                  | Zeolite ZSM-5 | Coconut shell-AC | PKS-AC |
|----------------------------|---------------|------------------|--------|
| Bulk density, kg/m³         | 680           | 500              | 295    |
| Pore volume, cm³            | 0.001         | 0.413            | 0.007  |
| BET Surface area, m²/g      | 0.064         | 863.043          | 6.156  |

4.1. Effect of the inlet concentration

The optimization data were investigated using PKS-AC. By solving a set of partial differential equations, a breakthrough curve was performed to determine the adsorption capacity, adsorption efficiency, and H₂S adsorbed. In this case, the gas flow rate at 0.2 L/min and the H₂S adsorbed were analyzed at different inlet concentrations, and the result is shown in figure 3 below:

![Figure 3. The H₂S adsorbed at different concentrations.](image)

As observed between the different inlet concentrations, the higher the inlet concentration, the faster the exhaustion of the adsorbent bed. The expected results are stated in table 4, referring to the phenomenon that the binding site was occupied rapidly and the column was saturated faster compared with the lower inlet concentration [39]. The adsorption capacity was also expected to increase because of the increasing inlet concentration:

Table 4. Effect of H₂S inlet concentration on H₂S adsorption.

| Inlet concentration, ppm | Breakthrough time, min | Exhaustion time, min | Adsorption capacity, mg H₂S/g |
|--------------------------|------------------------|----------------------|-------------------------------|
| 1000                     | 1255                   | 12,515               | 3.393                         |
| 3000                     | 420                    | 4175                 | 10.22                         |
The increase of the \( \text{H}_2\text{S} \) inlet concentration will increase the \( \text{H}_2\text{S} \) loading, leading to the higher adsorption capacity [14]. Besides, the transition zone in the fixed bed lengthens at lower inlet \( \text{H}_2\text{S} \) concentrations because of the lower apparent reaction rate between \( \text{H}_2\text{S} \) and the adsorbent [40]. Furthermore, as the \( \text{H}_2\text{S} \) concentration decreases, a longer bed or more active sites, is needed to consume a given amount of \( \text{H}_2\text{S} \) within the same period.

The inlet concentration increased from 1000 ppm to 10,000 ppm, and the results show that the increments of inlet concentration affected the \( \text{H}_2\text{S} \) adsorption. The curve pattern is S-shaped. Similar trends were also already proven by several researchers regarding the adsorption study, such as in the removal of \( \text{H}_2\text{S} \) from methane in packed bed, removal of \( \text{Cu}^{(ii)} \) cations from waste water in fixed bed column, \( \text{H}_2\text{S} \) removal with an iron oxide based CG-4 adsorbent in a fixed-bed reactor, biosorption of \( \text{Cr}^{(VI)} \) by the thermally activated weed Salvina cucullata, biosorption of acid blue 15 using fresh water Azolla filiculoides, adsorption of \( \text{Pb}^{(II)} \) cations onto activated tea waste, and immobilized Pinus sylvestris sawdust [41, 42, 43, 44, 45].

4.2. **Effect of the gas flow rate**

In the following cases, the gas flow rate is shown to play an important role in achieving breakthrough and exhaustion times. The increase of inlet gas flow rate is expected to be faster to meet the breakthrough time. At the inlet concentration of 1000 ppm, the inlet gas flow rate varies at 0.2, 0.4, 0.6, 0.8, and 1.0 L/min.

![Figure 4. The H\(_2\)S adsorbed at different concentrations.](image)

| Flow rate, L/min | Breakthrough time, min | Exhaustion time, min | Adsorption capacity, mg H\(_2\)S/g |
|------------------|------------------------|----------------------|----------------------------------|
| 0.2              | 1255                   | 12,515               | 3.393                            |
| 0.4              | 630                    | 6260                 | 3.393                            |
| 0.6              | 420                    | 4175                 | 3.407                            |

The lower gas flow rate is shown to possess a longer period to saturate and exhaust. The results showed a slight change in adsorption capacity, as shown in **Table 5**.
In the study by Natalie (2012), the model predicted that with increasing volumetric flow rate, breakthrough occurs earlier and adsorption capacity remains the same. As the model is not very sensitive to changes in superficial velocity/flow rate, this indicates that the adsorption of H$_2$S is not limited by kinetics. Practically, the adsorption capacity usually depends on the initial concentration, which provides the necessary driving force to overcome the mass transfer resistances between the aqueous and solid phases. The sorbate interaction increases in terms of vacant sorption site and surface functional group of sorbents when the initial concentration increases [46].

The H$_2$S is expected to be adsorbed more by increasing the gas flow rate. The fixed-bed column was expected to saturate quickly, as shown in Fig. 4. This results in a higher gas flow rate effect for the mass transfer zone to achieve the exit column faster [47, 48]. Moreover, by increasing the volumetric flow rate, breakthrough occurs earlier, whereas adsorption capacity remains the same. As the rate of introduction of contaminants increases, the active sites are blocked off quicker. These results are similar to the study by Natalie (2012) on the effect of flow rate to the adsorption of H$_2$S by activated carbon.

4.3. Effect of different types of adsorbent

Three types of adsorbent are used in this research, zeolite, coconut shell-AC, and PKS-AC. All of the adsorbents have different properties, which may lead to different expected results on adsorption efficiency and capacity.

By solving the partial differential equation via varying the bulk density of zeolite, coconut shell-AC, and PKS-AC, the breakthrough curve behaved as shown in figure 6 by using the constant parameters stated in table 3.

![Figure 5. The H$_2$S adsorbed at different adsorbents.](image)

At 1000 ppm and 0.2 L/min of H$_2$S gas, the PKS-AC had shorter exhaustion time, which is 12,515 min, compared with zeolite ZSM-5 (28,840 min) and coconut shell-AC (21,210 min). However, increasing either inlet concentration or gas flow rate also affects the period of exhaustion. Hence, breakthrough time, exhaustion time, and adsorption capacity are summarized in table 6.

| Adsorbent types | Breakthrough time, min | Exhaustion time, min | Adsorption capacity, mg H$_2$S/g |
|-----------------|------------------------|----------------------|---------------------------------|
| 0.8             | 315                    | 3130                 | 3.42                            |
| 1.0             | 255                    | 2505                 | 3.393                           |

Table 6. Effect of adsorbent types on H$_2$S adsorption.
| Material      | Bulk Density (g/cm³) | Porosity (%) | Adsorption Capacity (mg/g) |
|---------------|----------------------|--------------|----------------------------|
| Zeolite       | 2885                 | 28,840       | 1.473                      |
| Coconut shell-AC | 2125               | 21,210       | 2.0                        |
| PKS-AC        | 1255                 | 12,515       | 3.393                      |

The bulk densities are related to the bed porosity. The adsorption capacity of the column is expected to decrease as porosity increases. This behaviour is expected as less activated carbon is present in more porous beds [49]. Moreover, for higher surface area materials, the higher the concentrations, the higher the adsorption capacity was. As stated by Mangun et al. (1997), the small pores have a higher surface area, which has a higher potential overlap to bind the adsorbate molecule more tightly. The data from BET surface area proved that the larger surface area affected the capability of activated carbon to capture H₂S gas. Therefore, coconut shell-AC is more desirable compared with others because it required a longer period for completing the adsorption process.

4.4. **Effect of pressure**
A study on the effect of pressure in the adsorption via total operating pressure uses Equations (8) and (9). Figure 6 shows the breakthrough curve for various total pressures at constant inlet concentration. The total pressure used are 1.5, 2, 3, 4, 5 atm, at an inlet concentration of 1000 ppm. The breakthrough curves show no obvious change when the total pressure was changed.

![Figure 6](image)

**Figure 6.** The H₂S adsorbed at different pressure.

As shown in figure 6, no changes in total pressure were detected. The total pressure in the range of 1.5 atm to 5 atm shows adsorption capacity at 3.13 mg/g. This result shows a similar trend with a previous study by Wang (2008), wherein the total pressure change in the gas phase does not affect the breakthrough curve characteristics when the other operating conditions are kept constant. This phenomenon is based on a previous study by Garcia-Labiano (2004), which applied the grain model to predict the direct sulfidation of half-calcined CaCO₃-MgO by H₂S. They found that the pre-exponential factor of the Arrhenius-type reaction rate constant decreases when total pressure is higher but the activation energy does not change with total pressure.

4.5. **Effect of bed length**
The breakthrough curve of the different bed lengths applied in the range of 10 cm to 30 cm was related to the mass of adsorbent and height of the bed used. The H₂S inlet concentration (1000 ppm) and flow rate (0.2 L/min) are kept constant (as shown in figure 7).
Figure 7. The H$_2$S adsorbed at different bed length.

By decreasing the bed length, the breakthrough time was shortened and vice versa. This phenomenon is due to the lesser amount of activated carbon used in the adsorber column with shorter bed length. The lesser carbon used refers to the lower active site of palm kernel shell to capture the H$_2$S gas. The use of a 30-cm bed length resulted in a longer breakthrough time (1255 min) compared with 10 cm (420 min). Hence, more carbon and greater bed length are required for effective removal [49]. Table 7 shows the relationship between different bed volumes and breakthrough time, exhaustion time, and adsorption capacity at 0.9 of H$_2$S adsorbed.

Table 7. Effect of different bed lengths on H$_2$S adsorption.

| Length used, cm | Breakthrough time, min | Exhaustion time, min | Adsorption capacity, mg H$_2$S/g |
|----------------|------------------------|----------------------|----------------------------------|
| 10             | 420                    | 4525                 | 3.407                            |
| 20             | 835                    | 6980                 | 3.407                            |
| 30             | 1255                   | 6985                 | 3.393                            |

However, in the context of H$_2$S removal capacity, the longer the bed length, the more exhaustion time needed. As stated by Andrea (2010), as in the previous study, the decreasing removal capacity is due to a decrease in the contact time and vice versa, which is related to the adsorption reaction time. A previous study shows similar trends in the removal of H$_2$S gas through anaerobic digestion by-product activated carbon and carbonaceous activated adsorbent [39, 49]. However, the adsorption capacity is constant even if the bed length varied. This happens because of the greater dependence of adsorption capacity on the different concentrations compared with the bed length used.

4.6. Experimental results

The experiment was set up at flow rates of 0.2 L/min to 0.6 L/min, inlet concentration at 1000 ppm, and operation at room temperature. A total of 250 g of PKS-AC was loaded into a 0.848 L adsorber column. The column specification is the same as that used in the modelling study. The outlet concentration was fixed at 30 ppm and is considered the limit for the exhaustion of H$_2$S gas.
As shown in Figure 8, the 0.2 L/min flow rate had longer breakthrough and exhaustion times compared to 0.4 and 0.6 L/min. The adsorption capacity is the same due to the different flow rates.

Table 8. Effect of gas flow rate on H₂S adsorption.

| Flow rate, L/min | Breakthrough time, min | Exhaustion time, min | Adsorption capacity, mg H₂S/g |
|------------------|------------------------|-----------------------|-------------------------------|
| 0.2              | 363                    | 1450                  | 3.291                         |
| 0.4              | 30                     | 650                   | 3.291                         |
| 0.6              | 8                      | 13                    | 3.291                         |

However, the modelling and experimental results show a slight difference on the adsorption capacity, which are 3.4 mg H₂S/g and 3.291 mg H₂S/g, respectively. Basing on these results, the researchers recommended the application of different types of adsorbents, concentrations, and flow rates to capture H₂S particles and purify biogas. By fixing the outlet gas at 30 ppm, the adsorption time can be estimated and controlled via a modelling study, which calculated the exhaustion time. This study also revealed the expected time to stop the adsorption process and change the adsorbents. Hence, the use of H₂S gas and adsorbent can be controlled in experimental studies.

5. Conclusions
The mathematical models are used to predict the breakthrough curve, adsorption capacity, and saturation time earlier, which may be further validated by the experimental study. The theoretical study shows that by using different types of adsorbent. By increasing the inlet concentration, the adsorption capacity, breakthrough time, and exhaustion time were affected. The highest flow rate and bed length used only affected the breakthrough and exhaustion times, but not adsorption capacity. However, varying the total pressure does not affect the adsorption performance. Hence, coconut shell-AC is concluded to be the best adsorbent to use. Moreover, the optimum operating parameters such as flow rate (0.2-0.4 L/min) and 30 cm of length bed used were best to operate the adsorption process at the optimum exhaustion time. These due to the less frequent changes of adsorbent.

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