



Data Article

Isotherm data for adsorption of amoxicillin, ampicillin, and doripenem onto bentonite



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ABSTRACT

The dataset reported in this article describes the adsorption isotherms of amoxicillin, ampicillin, and doripenem onto bentonite. Batch adsorption experiments were carried out on single antibiotic solutions with various dosage of bentonite across temperatures from 30 to 50 °C. The adsorbent loading dataset was later obtained by measuring the concentration of antibiotic solution at adsorption equilibrium via UV-Vis spectrophotometer. The dataset was also fitted using various isotherm models including Freundlich, Langmuir, Toth, Hill, and Dubinin-Radushkevich models to further analyze the adsorption behavior. On top of that, orthogonal regression was applied to avoid fitting biasness, whereby the fitting results revealed the highest adsorption capacities of 82.259 mg g⁻¹ for amoxicillin, 78.851 mg g⁻¹ for ampicillin, and 93.278 mg

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g^{-1} for doripenem using Langmuir model, which gave an accurate representation of the adsorption isotherm dataset that was consistent with the results of Toth and Hill model.

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Specifications Table

Subject	Chemical Engineering
Specific subject area	Adsorption
Type of data	Figures, Tables
How the data were acquired	Single batch adsorption of amoxicillin, ampicillin, and doripenem were performed using bentonite as adsorbent. Equilibrium concentrations of antibiotic solutions were obtained by UV-Vis spectrophotometer to generate the adsorption isotherm dataset. Fitted values of isotherm parameters were obtained using orthogonal regression method on MATLAB.
Data format	Raw, Analyzed, Filtered
Description of data collection	Raw bentonite sourced from Ponorogo, East Java, Indonesia was dried, ground, and treated using hydrogen peroxide at Widya Mandala Surabaya Catholic University (WMCU). The adsorption experiments were performed and isotherm dataset were obtained at WMCU. The numerical fitting procedure was designed and run using MATLAB with implementation of orthogonal regression method at Swinburne University of Technology Sarawak Campus (SUTS) to obtain the values of adsorption isotherm parameters for accurate prediction of adsorption equilibria performances.
Data source location	Widya Mandala Surabaya Catholic University, Surabaya, Indonesia
Data accessibility	Repository name: Mendeley data Data identification number: doi: 10.17632/nzdb7gftph.2 Direct URL to data: https://data.mendeley.com/datasets/nzdb7gftph/2
Related research article	J.Y.J. Yeo, D.S. Khaerudini, F.E. Soetaredjo, G.L. Waworuntu, S. Ismadji, A. Putranto, J. Sunarso, Experimental and modelling study of adsorption isotherms of amoxicillin, ampicillin and doripenem on bentonite-chitosan composite, S. Afr. J. Chem. Eng. 43 (2023) 38–45.

Value of the Data

- This dataset showcases the potential of bentonite as an eco-friendly and cost-effective adsorbent for the removal of antibiotics from contaminated water.
- This dataset can be utilized by Chemical/Environmental Engineers to develop and optimize the wastewater treatment systems utilizing adsorption for the antibiotic removal.
- This dataset can be used as a benchmark to compare the adsorption equilibria performances against other natural, synthetic, or clay-based adsorbents.
- The fitted isotherm curves using this dataset gives a reasonably accurate prediction of the adsorption equilibria performances of antibiotics onto bentonite.
- The adsorption isotherm parameters derived from this dataset *via* numerical fitting provides further insights into the adsorption behaviors to facilitate efficient material/process engineering.

1. Objective

Improper discharge of antibiotic-contaminated wastewater has resulted into the global antibiotic pollution and accelerated the development of antibiotic resistance. As more multidrug-resistant bacteria were developed, antibiotics are becoming more ineffective in curing certain bacterial infections and ultimately giving rise to the antibiotic crisis [1]. Commonly-used antibiotics such as amoxicillin and ampicillin were already resisted by many bacteria species due to their longer exposure to the environment, whereas the last-resort antibiotics like doripenem are also at the same risk of losing its effectiveness in the long run [2–4]. Adsorptive removal procedure using bentonite presents a cost-effective method for antibiotic pollution, and further evaluation onto the adsorption performance is required to incorporate and optimize the adsorption systems in practical scale. In this dataset, the adsorption isotherm of amoxicillin, ampicillin, and doripenem on bentonite was investigated to obtain further insights onto the adsorption behavior. This dataset can also be used as baseline comparison against the modified bentonite in present studies such as the work by Yeo *et al.* [5] to develop better adsorbent materials.

2. Data Description

The experimental and fitted adsorption isotherm datasets were shared on Mendeley data [6], which describe the adsorbent loading of antibiotics onto bentonite at various equilibrium concentrations of antibiotic solutions. Figs. 1–3 depict the experimental and fitted adsorption isotherms of amoxicillin, ampicillin, and doripenem onto bentonite, respectively, at 30 °C, 40 °C, and 50 °C. The fitting results are summarized in Table 1, which consists of the adsorption capacities, equilibrium constants, as well as the evaluation metrics of the orthogonal regression (smaller value indicates better accuracy of the model) of all isotherm models at the three temperatures.

The notations are defined as follows: K_F and n_F are Freundlich equilibrium constant ($(\text{mg g}^{-1})(\text{mg L}^{-1})^{-1/n}$) and degree of surface heterogeneity, respectively; q_L and K_L are Langmuir

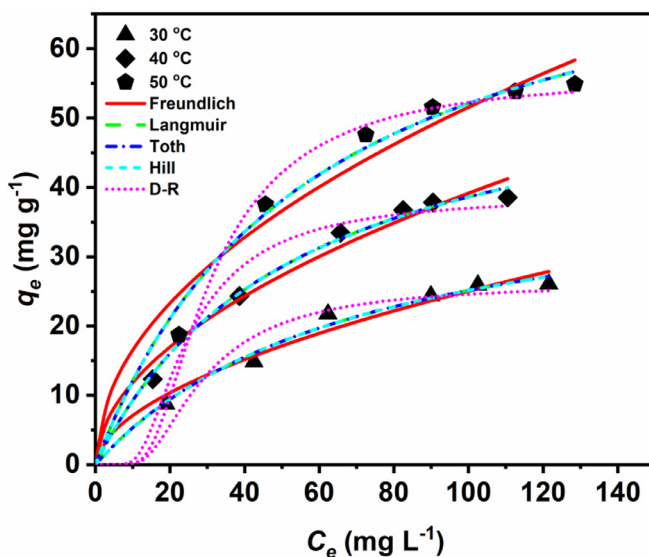


Fig. 1. Experimental and fitted adsorption isotherms of amoxicillin onto bentonite; Dubinin-Radushkevich is abbreviated as D-R.

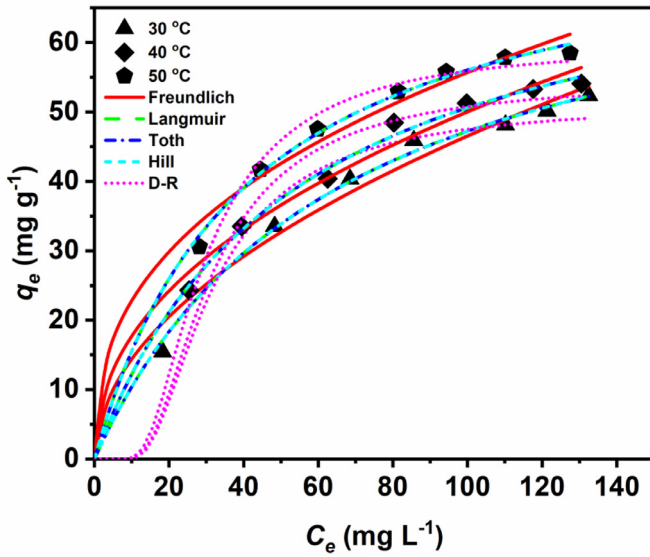


Fig. 2. Experimental and fitted adsorption isotherms of ampicillin onto bentonite.

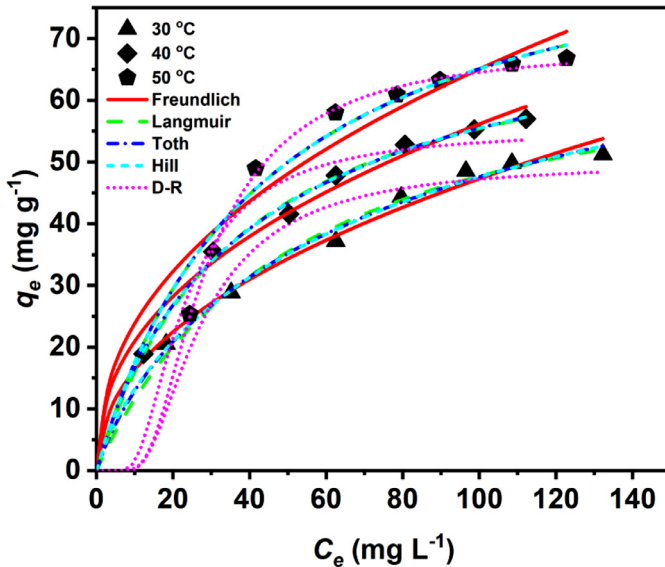


Fig. 3. Experimental and fitted adsorption isotherms of doripenem onto bentonite.

maximum monolayer adsorption capacity (mg g^{-1}) and Langmuir equilibrium constant (L mg^{-1}), respectively; q_T , K_T , and t are Toth maximum sub-monolayer adsorption capacity (mg g^{-1}), Toth equilibrium constant (L mg^{-1}), and degree of surface heterogeneity, respectively; q_H , K_H , and n_H are Hill saturation adsorption capacity (mg g^{-1}), Hill equilibrium constant ($(\text{mg L}^{-1})^{n_H}$), and cooperativity of binding interactions, respectively; q_{DR} and E_S are Dubinin-Radushkevich maximum adsorption capacity (mg g^{-1}) and mean sorption energy (kJ mol^{-1}), respectively; E_{OR} is evaluation metrics of the orthogonal regression.

Table 1

List of fitted adsorption isotherm parameters of single antibiotic adsorption by bentonite at 30 to 50 °C at adsorbent dose of 0.5 to 5 g, contact time of 6 hrs (with continuous stirring), and initial pH and antibiotic concentration of 6 and 250 mg L⁻¹, respectively.

Antibiotic	Amoxicillin			Ampicillin			Doripenem		
	30 °C	40 °C	50 °C	30 °C	40 °C	50 °C	30 °C	40 °C	50 °C
Freundlich									
K_F	2.012	3.577	5.308	4.458	6.278	9.365	5.637	7.846	8.766
n_F	1.827	1.924	2.026	1.963	2.219	2.583	2.165	2.340	2.298
E_{OR}	12.040	17.513	62.015	30.086	22.359	24.836	15.412	21.604	132.662
Langmuir									
q_L	42.996	59.598	82.259	77.908	77.603	78.851	72.769	76.220	93.278
K_L	0.014	0.018	0.017	0.015	0.019	0.025	0.019	0.027	0.023
E_{OR}	5.828	4.078	21.268	5.591	7.232	4.650	10.827	5.627	57.853
Toth									
q_T	42.996	59.598	82.241	77.908	77.603	78.851	97.542	82.351	93.278
K_T	0.014	0.018	0.017	0.015	0.019	0.025	0.021	0.028	0.023
$t (\leq 1)$	1.000	1.000	1.000	1.000	1.000	1.000	0.665	0.866	1.000
E_{OR}	5.828	4.078	21.268	5.591	7.232	4.650	9.725	5.375	57.853
Hill									
q_H	42.996	59.598	82.259	77.907	77.603	78.851	89.106	80.113	93.299
K_H	70.943	54.278	57.902	64.978	53.359	40.706	37.576	32.686	43.338
n_H	1.000	1.000	1.000	1.000	1.000	1.000	0.817	0.934	1.000
E_{OR}	5.828	4.078	21.268	5.591	7.232	4.650	9.442	5.401	57.853
Dubinini-Radushkevich									
q_{DR}	26.218	38.793	56.188	51.218	54.614	59.703	49.968	55.256	68.688
E_S	0.070	0.084	0.070	0.065	0.068	0.074	0.074	0.093	0.076
E_{OR}	24.490	32.110	13.609	62.724	41.044	15.576	88.897	87.228	3.654

3. Experimental Design, Materials, and Methods

3.1. Materials

Raw bentonite was sourced from Ponorogo at East Java, Indonesia, whereas the chemicals such as hydrogen peroxide (H₂O₂), amoxicillin, ampicillin, and doripenem were obtained from Merck and used directly without further treatment. The same preparation method was adopted from the present work by Yeo *et al.* [5], where the raw bentonite was subjected to 30% H₂O₂ solution to eliminate the organic impurities after being dried and ground into 100-200 mesh size. After the H₂O₂ treatment, the bentonite was then subjected to washing and heating to remove the residual H₂O₂ and moisture and stored for later use.

3.2. Adsorption experiment

The antibiotic adsorption experiments were performed across three different temperatures at 30, 40, and 50 °C in batch mode. For each experiment, solutions of each antibiotic were prepared at 200 mL with initial concentration of 250 mg L⁻¹ and pH of 6, which was subjected to purified bentonite with varying weight of 0.5 to 5 g. The mixture of antibiotic and bentonite solution was then stirred continuously at 200 rpm for about 6 hours to ensure the adsorption reached equilibrium. After that, the spent bentonite was separated from the mixture *via* centrifugation, whereas the equilibrium concentration of the antibiotic in the remaining solution was analyzed using a UV-Vis spectrophotometer (SHIMADZU UV/VIS-1700 PharmaSpec) at a maximum wavelength of 628 nm for amoxicillin (using dimethyl sulfoxide-acetonitrile (DMSO-AcN) mixture (50 % v/v)), 461 nm for ampicillin (using sodium 1,2-naphthoquinone-4-sulfonic), and 448 nm for doripenem (using 1,2 naphthoquinone 4-sulphonic acid sodium salt (NQS) reagent in an alkaline medium). All experiments were performed in triplicates to obtain the average values of equi-

librium concentration, the value of which will be used to calculate the adsorbent loading at equilibrium using Eq. (1).

$$q_e = \frac{(C_0 - C_e)}{m} V \quad (1)$$

where q_e is the adsorbent loading at equilibrium, which is the mass of antibiotic adsorbed per mass of bentonite or (mg g^{-1}), C_0 , C_e , m , and V are the initial and equilibrium concentrations of antibiotic solution (mg L^{-1}), mass of bentonite (g), and volume of the antibiotic solution (L), respectively.

3.3. Adsorption isotherm fitting

Multiple adsorption isotherm models were employed in fitting the equilibrium data, and the best fitted model was then used to infer adsorption behavior of these antibiotics on bentonite. This includes the well-known Freundlich (Eq. (2)) and Langmuir model (Eq. (3)), which were used to identify the formation of multilayer or monolayer adsorption on a heterogeneous or homogeneous surface, respectively [7,8].

$$q_e = K_F C_e^{1/n_F} \quad (2)$$

where K_F and n_F are the equilibrium constant of Freundlich ($(\text{mg g}^{-1})(\text{mg L}^{-1})^{-1/n}$) and dimensionless number that characterizes the heterogeneity of adsorbent surface, respectively.

$$q_e = q_L \frac{K_L C_e}{1 + K_L C_e} \quad (3)$$

where q_L and K_L are the Langmuir maximum monolayer adsorption capacity (mg g^{-1}) and Langmuir equilibrium constant (L mg^{-1}), respectively.

Besides, a modified Langmuir model such as Toth model was also used to describe a sub-monolayer adsorption on a heterogeneous surface [9], which is given in Eq. (4).

$$q_e = q_T \frac{K_T C_e}{(1 + (K_T C_e)^t)^{\frac{1}{t}}} \quad (4)$$

where q_T , K_T , and t are the Toth maximum sub-monolayer adsorption capacity (mg g^{-1}), Toth equilibrium constant (L mg^{-1}), and degree of surface heterogeneity, respectively. Heterogeneous surface is indicated when $t < 1$, otherwise homogeneous and monolayer adsorption is implied when $t = 1$ as Langmuir model is recovered.

Hills model was also applied to investigate the cooperativity in the binding of same adsorbate molecules on the adsorbent surface [10], which is given in Eq. (5).

$$q_e = q_H \frac{C_e^{n_H}}{K_H + C_e^{n_H}} \quad (5)$$

where q_H and K_H , are the Hill saturation adsorption capacity (mg g^{-1}) and Hill equilibrium constant ($(\text{mg L}^{-1})^{n_H}$), respectively, while n_H characterises the cooperativity of binding interaction as positive at $n_H > 1$ or negative at $n_H < 1$ [11]. For noncooperative case where $n_H = 1$, Langmuir model is recovered with K_H being the inverse of K_L .

Lastly, Dubinin-Radushkevich model was utilized to identify whether the adsorption obeys micropore filling mechanism [12], which is given in Eq. (6).

$$q_e = q_{DR} \exp \left[-K_{DR} \left[RT \ln \left(1 + \frac{1}{C_e} \right) \right]^2 \right] \quad (6)$$

$$E_S = \frac{1}{\sqrt{2K_{DR}}} \quad (7)$$

where q_{DR} , K_{DR} , R , T , and E_s are Dubinin-Radushkevich maximum adsorption capacity (mg g^{-1}), a constant related to mean sorption energy given in Eq. (7) ($\text{mol}^2 \text{kJ}^{-2}$), gas constant ($\text{kJ mol}^{-1} \text{K}^{-1}$), system temperature (K), and mean sorption energy (kJ mol^{-1}), respectively. The magnitude of E_s characterises the adsorption mechanism as physical at $E_s < 8 \text{ kJ mol}^{-1}$, ion-exchange at $8 < E_s < 16 \text{ kJ mol}^{-1}$ or chemical at $E_s > 16 \text{ kJ mol}^{-1}$.

All the isotherm models above were used in their original form without linearization. On top of that, orthogonal regression was applied to reduce biasness in the fitting as it considers the observation errors in the input variable (C_e), which was obtained manually when the system approached at [13]. The objective function of orthogonal regression is given in Eq. (8) as follows:

$$E_{OR} = \min \sum_{i=1}^n \Delta C_{e,i}^2 + \Delta q_{e,i}^2 \quad (8)$$

where E_{OR} is the evaluation metric of orthogonal regression; ΔC_e and Δq_e are the deviations of their experimental and calculated values, such that the sum of their squares is the squared orthogonal distances between the fitted line and the experimental points. In this context, the model that gives the smallest E_{OR} would therefore be the most accurate model for predicting the adsorption isotherm. Such computations were performed on MATLAB using the functions developed elsewhere [5], which is presented below.

AdsFitting.m – contains the fitting procedures to perform least square method and orthogonal regression method (also known as total least square method)

```
function [errLS,paraLS,errTLS,paraTLS] = AdsFitting(fun,p,lb,ub,xdata,ydata,T)

para0 = zeros(1,p); % initial guess

% Least square method
[paraLS,fval,exitflag,output] = fmincon(@leastsqr,para0,[],[],[],[],lb,ub,[]);
function SSE = leastsqr(paraLS)
    ycal = fun(xdata,T,paraLS);
    res = ycal - ydata;
    SSE = res*res';
    errLS = SSE; % sum of squared errors
end

% Total least square method
[paraTLS,fval,exitflag,outputT] = fmincon(@totalleastssqr,para0,[],[],[],[],lb,ub,[]);
function SSOD = totalleastssqr(paraTLS)
    coord(:,1) = xdata;
    coord(:,2) = ydata;
    SSOD = 0;
    no_points = 10000;
    xx = linspace(0,max(xdata),no_points);
    ycal = fun(xx,T,paraTLS);
    points(:,1) = xx;
    points(:,2) = ycal;
    for m = 1:size(coord,1)
        [~,min_dist] = dsearchn(points,coord(m,:));
        SSOD = SSOD + (min_dist).^2;
    end
    errTLS = SSOD; % sum of squared orthogonal distances
end
end
```

3.4. FreundlichAds.m – contains Freundlich isotherm model

```
function ym = FreundlichAds(xm,~,a)
% Notations:
% ym = adsorbate adsorbed per adsorbent, mg/g
% xm = equilibrium concentration of adsorbate, mg/L
% a(1) = Freundlich constant, (mg/g)((L/mg)^n)
% a(2) = degree of surface heterogeneity

ym = a(1).*(xm.^(1./a(2)));
```

3.5. LangmuirAds.m – contains Langmuir isotherm model

```
function ym = LangmuirAds(xm,~,a)
% Notations:
% ym = adsorbate adsorbed per adsorbent, mg/g
% xm = equilibrium concentration of adsorbate, mg/L
% a(1) = maximum monolayer adsorption capacity, mg/g
% a(2) = Langmuir equilibrium constant, L/mg

ym = a(1).*(xm.*a(2))./(1+xm.*a(2));
```

3.6. TothAds.m – contains Toth isotherm model

```
function ym = TothAds(xm,~,a)
% Notations:
% ym = adsorbate adsorbed per adsorbent, mg/g
% xm = equilibrium concentration of adsorbate, mg/L
% a(1) = Toth adsorption capacity, mg/g
% a(2) = Toth constant, L/mg
% a(3) = degree of surface heterogeneity

aa = a(2).*xm;
bb = (a(2).*xm).^a(3);
cc = 1./a(3);

ym = a(1).*aa./((1+bb).^cc);
```


3.7. HillAds.m – contains Hills isotherm model

```
function ym = HillAds(xm,~,a)
% Notations:
% ym = adsorbate adsorbed per adsorbent, mg/g
% xm = equilibrium concentration of adsorbate, mg/L
% a(1) = Hill saturation adsorption capacity, mg/g
% a(2) = Hill equilibrium constant, (mg/L)^n
% a(3) = dimensionless number characterising binding interactions

ym = a(1).*(xm.^a(3))./(a(2)+xm.^a(3));
```

3.8. DRAds.m – contains Dubinin-Radushkevich isotherm model

```
function ym = DRAds(xm,T,a)
% Notations:
% ym = adsorbate adsorbed per adsorbent, mg/g
% xm = equilibrium concentration of adsorbate, mg/L
% a(1) = DR maximum adsorption capacity, mg/g
% a(2) = constant related to sorption energy, mol2/kJ2
% R = gas constant, kJ/mol.K
% T = temperature, K

R = 8.314/1000;
ee = R.*T.*log(1+(1./xm));
ym = a(1).*exp(-a(2).*(ee.^2));
```

CallAdsFitting.m – custom script to perform data fitting by calling all the functions above; the user is required to change the variables *T* and *expdata* manually to fit different dataset.

```

clear; clc

%% Experimental Data
% T = temperature, K
% m_T = adsorbent dosage at T(C), g
% C0 = initial concentration of adsorbate, mg/L
% Ce_T = equilibrium concentration of adsorbate at T(C), mg/L
% Vol = volume of solution, L
% qe_T = adsorbate adsorbed per adsorbent at T(C), mg/g
% expdata = matrix of m_T and Ce_T

T = 303.15;
expdata = [18.2    20.51
35.2    28.84
62.5    37.15
79.6    44.32
96.5    48.52
108.5   49.78
132.3   51.21];
Ce = expdata(:,1)';
qe = expdata(:,2)';
x = linspace(0,max(Ce),50); x=x';

%% Langmuir Adsorption Isotherm
% Notations:
% para_L = [q_max,K_L]
% q_max = Langmuir maximum monolayer adsorption capacity, mg/g
% K_L = Langmuir constant, L/mg

[errLS_L,paraLS_L,errTLS_L,paraTLS_L] = AdsFitting(@LangmuirAds,2,[0 0],[1000
1000],Ce,qe,T);
yLS_L = LangmuirAds(x,T,paraLS_L);
yTLS_L = LangmuirAds(x,T,paraTLS_L);

%% Freundlich Adsorption Isotherm
% Notations:
% para_F = [K_F,n_F]
% K_F = Freundlich constant, (mg/g)((mg/L)^(1/n))
% n = degree of surface heterogeneity

[errLS_F,paraLS_F,errTLS_F,paraTLS_F] = AdsFitting(@FreundlichAds,2,[0 1],[1000
1000],Ce,qe,T);
yLS_F = FreundlichAds(x,T,paraLS_F);
yTLS_F = FreundlichAds(x,T,paraTLS_F);

%% Toth Adsorption Isotherm
% Notations:
% para_T = [q_max,K_T,t]
% q_max = Toth maximum adsorption capacity, mg/g
% K_T = Toth equilibrium constant, L/mg
% t = degree of surface heterogeneity

[errLS_T,paraLS_T,errTLS_T,paraTLS_T] = AdsFitting(@TothAds,3,[0 0 0],[1000 1000
1],Ce,qe,T);
yLS_T = TothAds(x,T,paraLS_T);
yTLS_T = TothAds(x,T,paraTLS_T);

%% Hill Adsorption Isotherm
% Notations:
% para_H = [q_H,K_H,n_H]
% q_H = Hill saturation adsorption capacity, mg/g
% K_H = Hill equilibrium constant, (mg/L)^n
% n_H = dimensionless number characterising binding interactions
[errLS_H,paraLS_H,errTLS_H,paraTLS_H] = AdsFitting(@HillAds,3,[0 0 0],[1000 1000
1],Ce,qe,T);
yLS_H = HillAds(x,T,paraLS_H);
yTLS_H = HillAds(x,T,paraTLS_H);

%% Dubinin-Radushkevich Isotherm
% Notations:
% para_DR = [q_DR,K_DR]
% q_DR = DR maximum adsorption capacity, mg/g
% K_DR = constant related to sorption energy, mol^2/kJ^2

[errLS_DR,paraLS_DR,errTLS_DR,paraTLS_DR] = AdsFitting(@DRAds,2,[0 0],[1000
1000],Ce,qe,T);
yLS_DR = DRAds(x,T,paraLS_DR);
yTLS_DR = DRAds(x,T,paraTLS_DR);

```

Ethics Statements

Not applicable.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data Availability

Isotherm data for adsorption of amoxicillin, ampicillin, and doripenem onto bentonite ([Original data](#)) (Mendeley Data).

CRedit Author Statement

Jason Yi Juang Yeo: Conceptualization, Formal analysis, Methodology, Software, Writing – original draft; **Deni Shidqi Khaerudini:** Data curation, Investigation, Methodology; **Felycia Edi Soetaredjo:** Data curation, Investigation, Methodology; **Gladly L. Waworuntu:** Data curation, Investigation, Methodology; **Suryadi Ismadji:** Project administration, Supervision, Funding acquisition; **Jaka Sunarso:** Resources, Supervision, Conceptualization, Project administration, Writing – review & editing; **Shaomin Liu:** Supervision, Funding acquisition.

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This work did not involve any animal or human subject in its experimentation process.

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