Characterization, isotherm and kinetic data for adsorption of Congo red and 2-naphthol on different bamboo hydrochars

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A B S T R A C T

Hydrochars were prepared using bamboo sawdust as raw material through hydrothermal carbonization with the present of acid or alkali in the medium and applied to remove Congo red and 2-naphthol from aqueous solutions. This data article provides information on FTIR and SEM profiles of the bamboo hydrochars, and the equation fitting results of the adsorption isotherms and kinetics for the two organics. The FTIR spectra show the differences of functional groups on the hydrochars with different process conditions. The SEM images show the surface morphology of selected hydrochars. Freundlich equation is slightly better than Langmuir model for the correlation of adsorption isotherms for both Congo red and 2-naphthol. Correlation coefficients from the pseudo-second order equation are greater than those of the pseudo-first order equation for both the organics on selected hydrochars.

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### Specifications Table

| Subject area               | Chemical Engineering |
|----------------------------|----------------------|
| More specific subject area | Adsorption           |
| Type of data               | Table, image, figure |
| How data was acquired      | The adsorption amount of Congo red and 2-naphthol by the hydrochars ($Q_e$) was determined based on the subtraction of the initial and final concentration of the organics. |
| FTIR: Bruker Vertex 70 FT-IR spectrometer |
| SEM: Hitachi S3700 scanning electron microscope |
| Data format                | Analyzed             |
| Experimental factors       | Bomboo hydrochars were grounded evenly for characterization. |
| Experimental features      | The adsorption of Congo red and 2-naphthol on bamboo hydrochars. |
| Data source location       | Zhejiang University of Science and Technology, Hangzhou, China |
| Data accessibility         | Within this article  |
| Related research article   | The associated research article related to this data is [1]. |

### Value of the data

- The data shows detailed FTIR spectra of the bamboo hydrochars and provides detailed surface features of selected hydrochars.
- The isotherm fitting data gives information for modeling the capacity and explaining the mechanism for the adsorption of Congo red and 2-naphthol by the hydrochars.
- The kinetic fitting results will be useful for modeling and predicting the adsorption rate and rate-limiting step of Congo red and 2-naphthol on the hydrochars.

### 1. Data

FTIR spectra of the bamboo hydrochars are shown in Fig. 1. Fig. 2. presents SEM images of selected hydrochars as well as the raw material bamboo sawdust. The parameters from Langmuir and Freundlich isotherm equations together with the correlation coefficients for Congo red and 2-naphthol at 298 K are summarized in Table 1, and those on selected hydrochars at 298, 308, and 318 K are listed in Table 2. Kinetic parameters as well as the correlation coefficients for Congo red and 2-naphthol on selected hydrochars at 298 K are presented in Table 3.

### 2. Experimental design, materials, and methods

#### 2.1. Preparation of the bamboo hydrochars

Bamboo hydrochars were prepared through acid-assisted or two-stage hydrothermal treatment. The feed solutions in acid-assisted hydrothermal treatment for the preparation of hydrochar sample 1–9 are 5 wt% HNO$_3$, 10 wt% HNO$_3$, 15 wt% HNO$_3$, 5 wt% H$_2$SO$_4$, 10 wt% H$_2$SO$_4$, 15 wt% H$_2$SO$_4$, 5 wt% H$_3$PO$_4$, 10 wt% H$_3$PO$_4$, and 15 wt% H$_3$PO$_4$, respectively. The feed solutions in two-stage hydrothermal carbonization process for the production of hydrochar sample 10–12 are 5 wt% NaOH in the first stage, and 5 wt% HNO$_3$, 5 wt% H$_2$SO$_4$, and 5 wt% H$_3$PO$_4$, respectively in the second stage.

In an acid-assisted HTC process, about 6.00 g of wet bamboo sawdust was mixed with 36.0 mL of acid solution in a 100 mL autoclave reactor with an internal Teflon insert, and the concentrations of the acid solution were from 5 to 15 wt%. The reactor was sealed and heated at 200°C for 3 h, then cooled down to room temperature in cold water. The solid product was collected by vacuum
filtration, washed with deionized water until pH of the washed water was around 7.0, and dried at 100 °C for 12 h.

In a two-stage hydrothermal treatment process, 6.00 g of bamboo sawdust was added into 36.0 mL of 5 wt% NaOH solution in a Teflon lined autoclave reactor and the mixture was held at 200 °C for 3 h. The reactor was then cooled down and the solid product was collected, washed and dried. 6 mL of 5 wt% acid solution was mixed with per 1 g of the obtained solid material, the mixture was loaded in a Teflon lined autoclave reactor and hydrochars were prepared through an acid-assisted HTC process described above.

2.2. Characterization of the hydrochars

Fourier transform infrared spectroscopy (FTIR) spectra of all hydrochar samples were recorded by a Bruker Vertex 70 FT-IR spectrometer. Hitachi S3700 scanning electron microscope (SEM) was used to study the surface morphology of the hydrochars.

2.3. Adsorption isotherms

Hydrochars (0.0100 g) were placed in 30 mL of Congo red or 2-naphthol solutions with known initial concentrations \( C_0 \) in capped glass flasks. The flasks were shaken at 170 rpm and set temperatures in a TS-1102TENSUC shaker for 8 h. The suspensions were then filtered, and the equilibrium concentrations \( C_e \) (mg/mL) of Congo red and 2-naphthol in the supernatant were determined using a
UV–vis spectrophotometer at wavelength of 499 nm and 274 nm respectively. Adsorption capacities $Q_e$ (mg/g) were calculated from the difference between equilibrium concentrations and initial ones:

$$Q_e = (C_0 - C_e) \cdot \frac{V}{m}$$

(1)

Where $V$ (mL) is the volume of the suspension and $m$ (g) is the adsorbent dry mass.

The experimental adsorption isotherm data was analyzed using the Langmuir and Freundlich models:

**Langmuir model:**

$$Q_e = \frac{Q_m K_L C_e}{1 + K_L C_e}$$

(2)

**Freundlich model:**

$$Q_e = K_F C_e^{1/n}$$

(3)

Where $Q_m$ (mg/g) is the quantity adsorbed per gram of adsorbent to give a complete monolayer, $K_L$ (mL/mg) is the Langmuir constant related to capacity and rate of adsorption [2]. $K_F ((mg/g)(mL/mg)^{1/n})$ and $1/n$ are the Freundlich constants indicating relative adsorption capacity and favorability of the adsorption, respectively [3].
### Table 1
Langmuir and Freundlich isotherm parameters and correlation coefficients for the adsorption of Congo red and 2-naphthol at 298 K.

| Adsorbate  | Hydrochar sample | Langmuir isotherm | Freundlich isotherm |
|------------|------------------|-------------------|---------------------|
|            |                  | $Q_m$ (mg/g) | $K_L$ (mL/mg) | $R^2$ | $K_F$ (mg/g) | $(mL/mg)^{1/n}$ | $1/n$ | $R^2$ |
| Congo red  | Sample 1         | 43.02            | 6.67           | 0.988 | 47.13      | 0.430            | 0.994 |
|            | Sample 2         | 46.34            | 9.39           | 0.991 | 52.99      | 0.377            | 0.998 |
|            | Sample 3         | 37.80            | 13.45          | 0.975 | 43.60      | 0.313            | 0.991 |
|            | Sample 4         | 20.50            | 12.06          | 0.989 | 22.59      | 0.301            | 0.994 |
|            | Sample 5         | 14.04            | 16.17          | 0.995 | 15.21      | 0.239            | 0.990 |
|            | Sample 6         | 17.88            | 7.91           | 0.942 | 19.50      | 0.384            | 0.966 |
|            | Sample 7         | 37.65            | 6.81           | 0.983 | 41.16      | 0.423            | 0.992 |
|            | Sample 8         | 29.78            | 5.92           | 0.969 | 31.77      | 0.445            | 0.988 |
|            | Sample 9         | 22.23            | 7.63           | 0.953 | 24.15      | 0.389            | 0.976 |
|            | Sample 10        | 220.73           | 4.76           | 0.990 | 228.18     | 0.489            | 0.998 |
|            | Sample 11        | 234.91           | 4.69           | 0.980 | 243.79     | 0.496            | 0.995 |
|            | Sample 12        | 255.61           | 5.47           | 0.994 | 273.50     | 0.470            | 0.999 |
| 2-naphthol | Sample 1         | 51.32            | 3.73           | 0.997 | 51.41      | 0.551            | 0.999 |
|            | Sample 2         | 48.38            | 1.92           | 0.983 | 38.48      | 0.661            | 0.991 |
|            | Sample 3         | 44.68            | 3.12           | 0.994 | 42.50      | 0.582            | 0.997 |
|            | Sample 4         | 54.82            | 4.84           | 0.991 | 58.04      | 0.500            | 0.996 |
|            | Sample 5         | 50.57            | 9.66           | 0.959 | 58.93      | 0.384            | 0.974 |
|            | Sample 6         | 62.02            | 5.29           | 0.991 | 67.65      | 0.492            | 0.997 |
|            | Sample 7         | 67.17            | 3.30           | 0.998 | 66.20      | 0.584            | 0.999 |
|            | Sample 8         | 95.26            | 2.93           | 0.986 | 92.39      | 0.618            | 0.996 |
|            | Sample 9         | 68.44            | 4.48           | 0.988 | 72.78      | 0.527            | 0.999 |
|            | Sample 10        | 322.56           | 1.26           | 0.992 | 213.81     | 0.745            | 0.993 |
|            | Sample 11        | 272.20           | 3.66           | 0.995 | 268.69     | 0.546            | 0.997 |
|            | Sample 12        | 302.78           | 1.89           | 0.977 | 240.95     | 0.670            | 0.981 |

### Table 2
Langmuir and Freundlich isotherm parameters and correlation coefficients for the adsorption of Congo red on Sample 12, and 2-naphthol on Sample 11 at 298 K, 308 K and 318 K.

| Adsorbate  | Hydrochar sample | T (K)   | Langmuir model | Freundlich model |
|------------|------------------|---------|----------------|-----------------|
|            |                  | $Q_m$ (mg/g) | $K_L$ (mL/mg) | $R^2$ | $K_F$ (mg/g) | $(mL/mg)^{1/n}$ | $1/n$ | $R^2$ |
| Congo red  | Sample 12        | 298     | 255.61         | 5.47           | 0.994 | 273.50      | 0.470            | 0.999 |
|            |                  | 308     | 375.50         | 2.89           | 0.983 | 351.06      | 0.597            | 0.995 |
|            |                  | 318     | 635.16         | 1.32           | 0.999 | 445.49      | 0.766            | 0.977 |
| 2-naphthol | Sample 11        | 298     | 272.20         | 3.66           | 0.985 | 268.69      | 0.546            | 0.997 |
|            |                  | 308     | 327.07         | 2.15           | 0.984 | 274.52      | 0.648            | 0.991 |
|            |                  | 318     | 299.60         | 1.96           | 0.985 | 241.44      | 0.663            | 0.993 |

### Table 3
Kinetic parameters for adsorption of Congo red on sample 12 and 2-naphthol on sample 11 at 298 K.

| Adsorbate  | Hydrochar sample | Pseudo-first-order equation | Pseudo-second-order equation |
|------------|------------------|-----------------------------|------------------------------|
|            |                  | $q_e$ (mg/g) | $k_1$ (1/min) | $R^2$ | $q_e$ (mg/g) | $k_2$ (mg/(g.min)) | $R^2$ |
| Congo red  | Sample 12        | 169.59          | 0.564           | 0.959 | 174.42      | 0.0030           | 0.969 |
| 2-naphthol | Sample 11        | 156.50          | 0.614           | 0.938 | 163.62      | 0.0026           | 0.978 |
2.4. Adsorption kinetics

0.0100 g of the selected hydrochars was added into 30 mL of 0.5 mg/mL Congo red or 2-naphthol solution in a capped glass flask. The flasks were shaken at 170 rpm and 298 K, the contact time \( t \) (min) was ranging from 5 to 300 min, and the concentrations of Congo red and 2-naphthol in the suspensions at \( t \) \( C_t \) (mg/mL) were determined after filtration. Adsorption capacities at \( t \), \( Q_t \) (mg/g) were calculated by:

\[
Q_t = (C_0 - C_t)V/m
\]  

(4)

The adsorption kinetic data was analyzed by the pseudo-first order and pseudo-second order models:

Pseudo-first order equation:

\[
Q_t = q_e (1 - e^{-k_1 t})
\]  

(5)

Pseudo-second order equation:

\[
Q_t = \frac{t q_e^2 k_2}{t k_2 q_e + 1}
\]  

(6)

Where \( k_1 \) (1/min) and \( k_2 \) (g/(mg min)) are the pseudo-first-order rate and the pseudo-second-order rate constants, \( q_e \) (mg/g) is the calculated adsorbed quantity at equilibrium.

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Transparency document. Supporting information

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