

**Risk evaluation of biochars produced from Cd-contaminated rice straw and optimization of its production for Cd removal**

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### **Details of biochar characterization**

The pH of the biochars was determined based on the works of Alam et al. (2018 a and b) and von Gunten et al. (2017). Briefly, a certain amount (0.1 g) of biochar was mixed with 10 mL of deionized water and shaken at 250 rpm for 24 h. After centrifugation, the pH of the supernatant was measured. The Brunauer–Emmett–Teller (BET) surface area of the biochar was determined by a Tristar II 3020 (Micromeritics) instrument. The C, H, O, N contents of biochar were tested using a CE-440 Elemental Analyzer (Perkin Elmer).

The fundamental vibrations and associated rotational-vibrational structure of the biochars were tested using a VERTEX 70v Fourier-transform infrared spectroscopy (FT-IR) spectrometer (BRUKER) between wavenumbers 4000 to 600  $\text{cm}^{-1}$ . The crystalline phases in the biochar were examined using a D8 ADVANCE X-ray diffractometer (XRD) (Bruker). To do so, dry samples were mounted on a flat holder and examined with a Cu K $\alpha$  source operating at 40 kV and 40 mA, emitting radiation at a wavelength of 1.5406 Å. The scanning regions were between 2 $\theta$  values of 10-60° at a step rate of 0.1 s/step and a resolution of 0.01°/step. The surface morphology of the biochars (coated with Pt) was tested using a SU8010 Ultra-High Resolution (1.0 nm) Scanning Electron Microscope (SEM) (Hitachi, Japan).

### **Details of the cadmium removal tests and data fitting**

Batch adsorption tests were carried out to reveal the characteristics of cadmium (Cd) adsorption on the rice straw biochars. In order to assess the adsorption kinetics, a certain amount of biochar (0.1 g) was added to 20 mL solution of 1 mM  $\text{Cd}(\text{NO}_3)_2$  in 50-mL polyethylene tubes. The mixtures were shaken at 250 rpm for 5 min, 10 min, 20 min, 30 min, 1 h, 2 h, 3 h, 6 h, 12 h, 18 h, 24 h, or 48 h in a temperature-controlled shaker (SHA-CA, Kexi Instrument CO., Ltd.). After the designated shaking time, a mixture was filtered through a 0.45  $\mu\text{m}$  membrane. The Cd concentration in the collected filtrate was measured by inductively coupled plasma/optical emission spectrometry (ICP-OES) (Perkin-Elmer, Optima 8300) after dilution (if necessary) and

acidification. For all sorption studies, the initial pH values of the solutions were not controlled.

In order to construct a sorption isotherm for each biochar, 0.1 g of biochar was added to 20 mL solutions containing different Cd concentrations (0.1, 0.2, 0.3, 0.5, 1, 2, 3, or 5 mM) (equivalent to 11.2, 22.5, 33.7, 56.2, 112, 225, 337, or 562 mg/L). The mixture was shaken at 200 rpm for 24 h to reach equilibrium before filtration and ICP-OES testing as described above.

Pseudo first order, pseudo second order model, and intraparticle diffusion model are three of the most commonly used kinetics models to reveal the time-dependence of adsorption (Cui et al., 2016; Inyang et al., 2011), and were used to simulate the kinetics data:

$$q_t = q_e(1 - e^{-k_1 t}) \quad (1)$$

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

$$q_t = k_i t^{0.5} + C \quad (3)$$

where  $k_1$  ( $\text{h}^{-1}$ ) is the rate constant of pseudo first order adsorption,  $k_2$  ( $\text{g/mg h}$ ) is the pseudo second order rate constant, and  $k_i$  ( $\text{mg/g h}^{-0.5}$ ) is the coefficient of intraparticle diffusion. In equation (2),  $q_e$  ( $\text{mg/g}$ ) is the equilibrium adsorption capacity, and  $q_t$  ( $\text{mg/g}$ ) in each equation is the adsorbed Cd at time  $t$ .

Langmuir and Freundlich models are two of the most commonly used isotherm models and were used to describe the equilibrium sorption data (Foo and Hameed, 2010):

$$q_e = \frac{Q_{\max} b C_e}{1 + b C_e} \quad (4)$$

$$q_e = K_f C_e^{1/n} \quad (5)$$

where  $Q_{\max}$  ( $\text{mg/g}$ ) is the maximum monolayer adsorption capacity,  $b$  is the Langmuir isotherm constant ( $\text{L/mg}$ ),  $K_f$  ( $\text{mg/g}$ ) is the Freundlich isotherm constant,  $n$  represents the adsorption intensity,  $q_e$  is the adsorbed Cd ( $\text{mg/g}$ ) at equilibrium and  $C_e$  ( $\text{mg/L}$ ) is

the equilibrium Cd concentration in solution.

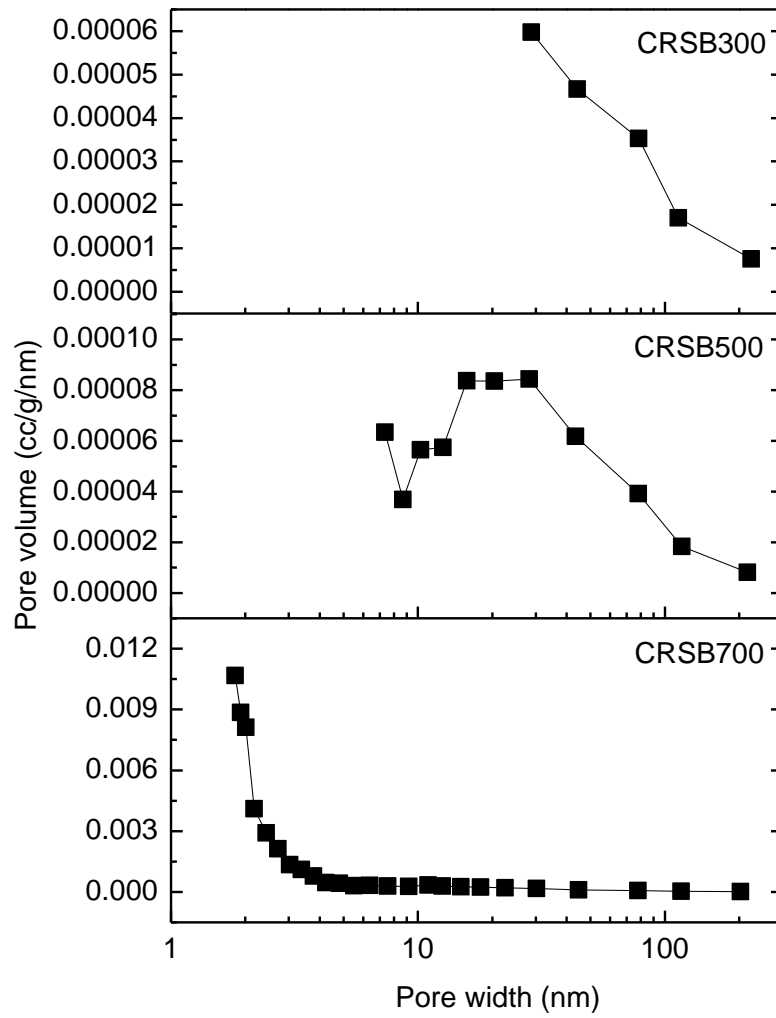


Figure S1 BJH pore size distribution of the biochars

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