Sorption of Carbendazim to Activated Carbons Derived from Rape Straw and its Mechanism

Tao Wang [a,b], Zhen Zhang [a], Huixue Zhang [a], Xiaoxiao Zhong [a], Yonghong Liu [a*], Shuijiao Liao [a], Xiali Yue [a], Guangsheng Zhou [c]

[a] College of Science, Huazhong Agricultural University, Wuhan, 430070, China

[b] Institute of Hydrobiology, Chinese Academy of Sciences, Wuhan, 430072, China

[c] College of Plant Science and Technology, Huazhong Agricultural University, Wuhan, 430070, China

* Corresponding author: Tele/Fax No: 0086 15827001139

E-mail: liuyh913@mail.hzau.edu.cn

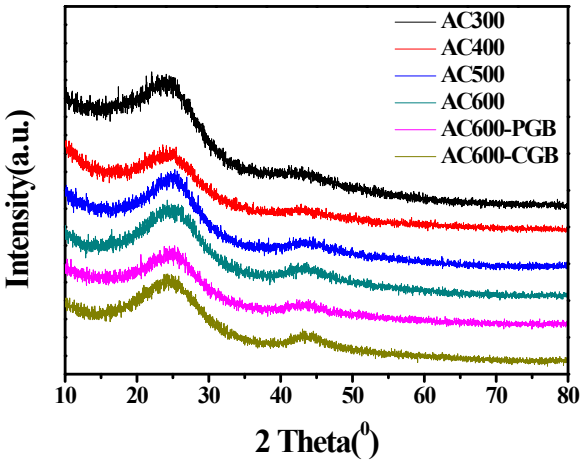

Fig. S1. XRD profiles of the samples

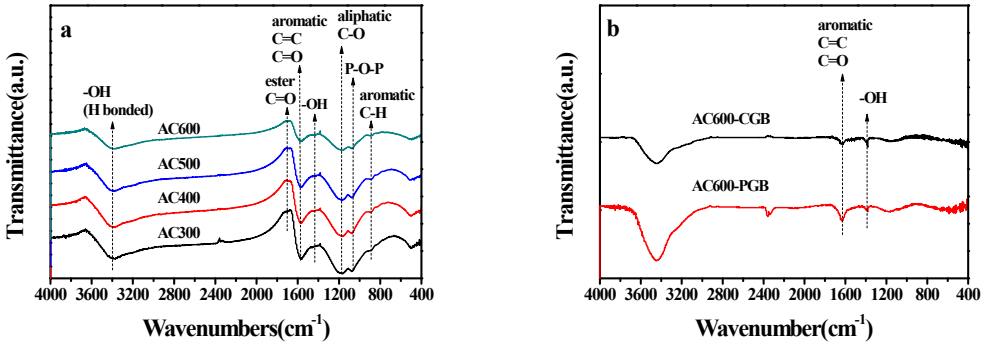

Fig. S2. FTIR spectra of the samples

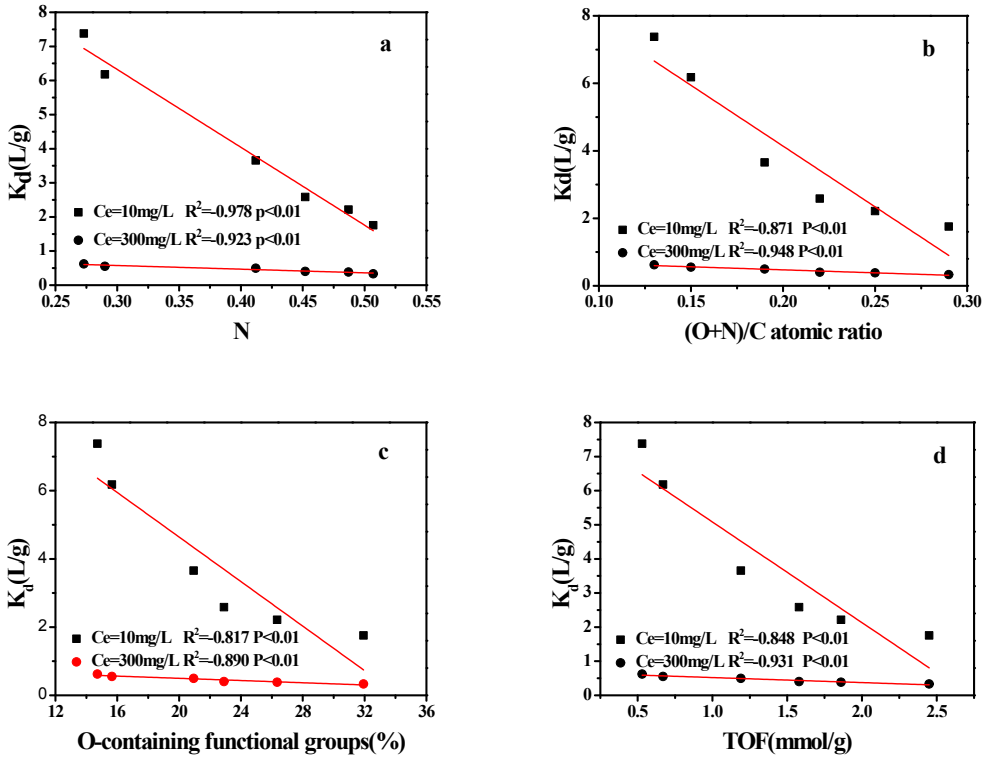

Fig. S3. Correlations between sorption coefficient (K_d) at different CBD concentrations and (a) nonlinearity, (b) polarity index (O+N)/C, (c) the relative contents of the O-containing functional groups determined by C1s XPS spectra, (d) the total O-containing functional groups by Boehm's titration. The correlations were analyzed by Pearson test(two-tailed) using SPSS 18.0.

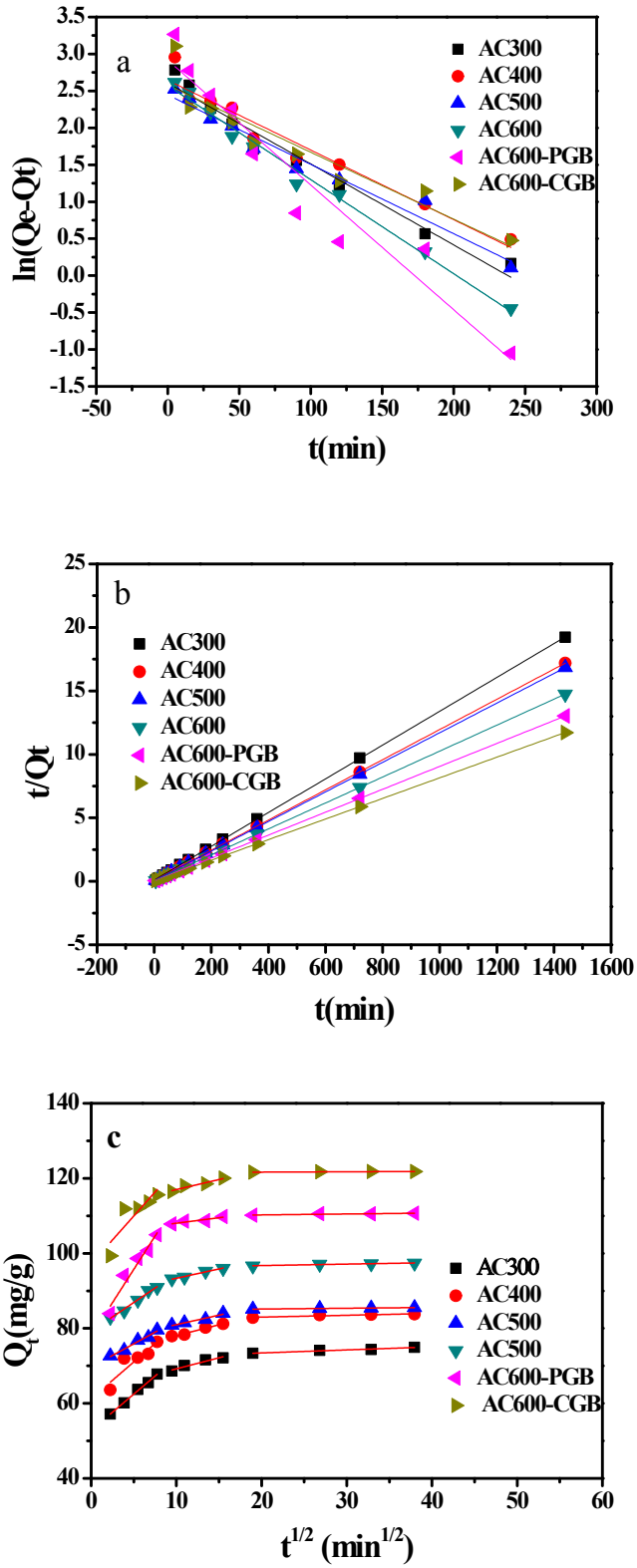

Fig. S4. Pseudo-first-order kinetic model (a),Pseudo-second-order kinetic model (b) and Particle diffusion equation(c) for CBD onto the samples (temperature=20±0.5℃; initial pH=7.00±0.10; time=360±5min）

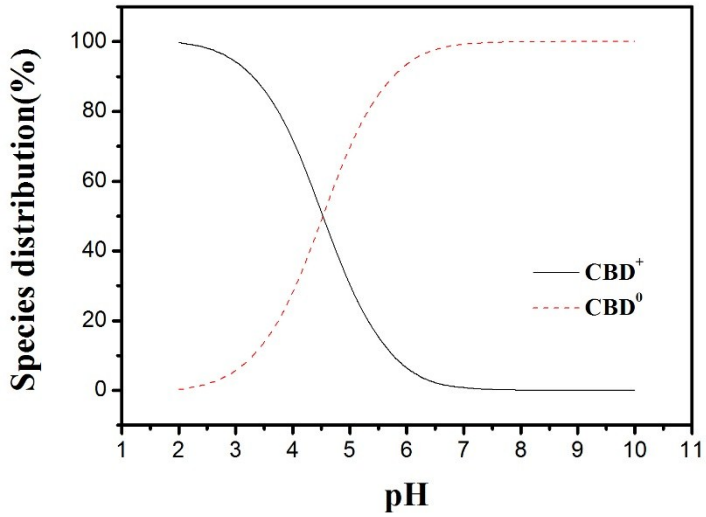

Fig. S5. Solution speciation of CBD as a function of pH

Table S1 Textural properties of the samples

Samples	S_{BET}(m^2/g)	S_{mic}(m^2/g)	S_{ext}(m^2/g)	V_{tot}(cm^3/g)	V_{mic}(cm^3/g)	V_{ext}(cm^3/g)	D_p(nm)
AC300	951	275	676	0.47	0.14	0.33	3.70
AC400	1490	35	1455	1.40	0.02	1.38	4.75
AC500	1164	75	1089	1.17	0.04	1.13	4.58
AC600	1053	79	974	1.06	0.04	1.02	4.18
AC600-PGB	1122	89	1033	1.08	0.05	1.03	4.16
AC600-CGB	1120	90	1030	0.99	0.04	0.95	4.69

Table S2 Etimated kinetic model constants for the sorption of CBD onto the samples

Model	Parameter	Adsorbent					
		AC300	AC400	AC500	AC600	AC600-PGB	AC600-CGB
pseudo-first-order	*Qe*,exp(mg/g)	13.57	14.06	11.54	13.10	18.46	13.16
	Qe,cal(mg/g)	73.33	82.33	85.12	96.64	110.14	121.64
	K_1(1/min)	0.0110	0.0094	0.0094	0.0127	0.0169	0.0097
	R^2	0.9656	0.9409	0.9623	0.9890	0.9260	0.8734

pseudo-second-order	Qe,exp(mg/g)	75.02	84.10	85.76	97.56	110.86	122.10
	Qe,cal(mg/g)	73.33	82.33	85.12	96.64	110.14	121.64
	K_2(g/(mgmin)10^{-3})	1.9616	2.0119	2.7397	2.8576	3.0749	2.6636
	h(mg/(g min))	11.04	14.23	20.15	27.19	37.79	39.71
	R^2	0.9999	0.9999	0.9999	0.9999	0.9999	0.9999
intra-particle diffusion	K_{p1}(mg/g $min^{1/2}10^{-3}$)	1.9278	1.9617	1.2411	1.5397	3.5510	2.5550
	C_1	52.83	61.24	69.68	79.20	77.98	91.19
	$(R_1)^2$	0.9964	0.7706	0.9761	0.9803	0.9354	0.6889
	K_{p2} (mg/g $min^{1/2}10^{-3}$)	0.5874	0.5739	0.5057	0.4966	0.2921	0.5344
	C_2	63.34	72.27	75.94	88.39	105.11	111.66
	$(R_2)^2$	0.9265	0.9743	0.9449	0.9739	0.8549	0.8969
	K_{p3}(mg/g $min^{1/2}10^{-3}$)	0.0805	0.0487	0.0211	0.0387	0.0246	0.0091
	C_3	71.84	82.02	84.73	95.97	109.76	121.47
	$(R_3)^2$	0.9683	0.8277	0.9924	0.9030	0.6451	0.9849

Table S3 Thermodynamic parameters of samples sorption on CBD

Samples	temperature (K)	ΔG (kJ/mol)	ΔH (kJ/mol)	ΔS (kJ/mol)
AC300	293	-1.02	-15.60	-49.92
	303	-0.37		
	313	-0.01		
AC400	293	-1.54	-16.48	-50.88
	303	-1.08		
	313	-0.52		
AC500	293	-2.04	-17.01	-51.03
	303	-1.55		
	313	-1.01		
AC600	293	-3.37	-11.59	-28.07
	303	-3.06		
	313	-2.80		
AC600-PGB	293	-6.34	-20.44	-48.07
	303	-5.86		
	313	-5.37		
AC600-CGB	293	-7.60	-20.36	-43.67
	303	-7.01		
	313	-6.71		

Table S4 Dual-mode model fitting results of CBD sorption on the samples

Samples	Q^0	a	K_p	R^2	C_e=10 mg/L		C_e=300 mg/L	
					Q_{ad}	Q_p	Q_{ad}	Q_p
AC300	87.0±11	0.023	0.016	0.993	16.3	0.16	83.4	4.8
AC400	112.3±37	0.018	0.019	0.980	17.1	0.19	106.4	5.7
AC500	106.2±18	0.026	0.023	0.988	21.9	0.23	102.3	6.9
AC600	106.8±12	0.057	0.072	0.985	38.8	0.72	105.0	21.6
AC600-PGB	99.6±12	0.242	0.215	0.958	70.5	2.15	99.2	64.5
AC600-CGB	103.8±9	0.739	0.273	0.962	91.4	2.73	103.7	81.9

Text S1 Thermodynamic adsorption analysis

The standard free energy change ($\Delta G^{0)}$ can be calculated from the following equation (S1):

$$\Delta G^0 = -RT ln\, K^0 \qquad \text{(S1)}$$

where R is the universal gas constant (8.314 J $mol^{-1}K^{-1}$), T is the temperature in Kelvin. The sorption equilibrium constant, K^0, can be calculated by plotting lnK_d versus C_e and extrapolating C_e to zero. The standard enthalpy change (ΔH^0) and the standard entropy change (ΔS^0) are calculated from the following equation (S2):

$$lnK^0 = \frac{\Delta S^0}{R} - \frac{\Delta H^0}{RT} \qquad \text{(S2)}$$

The thermodynamic parameters are calculated from the plot of lnK^0 vs 1/T using equations (S1) and (S2).