

Supporting Information

One-pot synthesis of porous “carbon foam” derived from corn straws: atrazine adsorption equilibrium and kinetics

Fan Yang, Lili Sun, Wei Zhang, Ying Zhang*

College of resource and environment, Northeast Agricultural University, 150030, China

Contents:

1. Tables
2. Figures

1. Tables

Table S1. Textural properties of the as-prepared products calcined at 800 °C with different mass ratio of NaHCO₃ to corn straw.

Mass ration of NaHCO ₃ to corn straw	S _{BET} (m ² g ⁻¹)	Total pore volume (cm ³ g ⁻¹)	V _{mic} /V _{total}
0*	11.2648	0.0358	0.064
1	1891.9	0.845	0.823
2	1210.7	0.844	0.510
6	1103.1	0.688	0.572

[*] 0 represented corn straw was calcined without NaHCO₃.

Table S2. Textural properties of the as-synthesized products* calcined at different temperature

Temperature (°C)	S _{BET} (m ² g ⁻¹)	Total pore volume (cm ³ g ⁻¹)	V _{mic} /V _{total}
800	1891.9	0.845	0.823
900	1231.3	0.833	0.507
1000	1370	0.778	0.601

[*] Mass ratio of NaHCO₃ to corn straws is 1.

Table S3. The yield and EA results of the as-synthesized products* calcined at different temperature.

Temperature (°C)	Yield (%)	C (%)	H (%)	O (%)	N (%)	H/C	O/C	(O+N)/C
800	12.02	72.64	0.66	7.13	0.18	0.11	0.073	0.074
900	10.58	74.21	0.27	4.41	0.16	0.043	0.045	0.050
1000	8.39	75.65	0.35	2.12	0.21	0.055	0.021	0.023

[*]Mass ratio of NaHCO₃ to corn straws is 1.

Table S4. The yield and EA results of the as-synthesized products calcined at 800 °C with different mass ratio of NaHCO₃ to cellulose.

Mass ration of NaHCO ₃ to corn straw	Yield (%)	C (%)	H (%)	O (%)	N (%)	H/C	O/C	(O+N)/C
0*	13.66	70.30	0.32	3.32	0.36	0.055	0.035	0.040
1	12.02	72.64	0.66	7.13	0.18	0.11	0.073	0.074
2	9.21	74.24	0.38	3.83	0.28	0.061	0.039	0.059
6	7.56	74.80	0.56	5.47	0.20	0.090	0.055	0.069

[*] 0 represented corn straw was calcined without NaHCO₃.

Table S5. Kinetic parameters of Modified Freundlich model for atrazine sorption on CSs at 25 °C.

Conc. (mg/L)	k (L/(g h))	m	q _{e,exp} (mg/g)	q _{e,cal} (mg/g)	OF
35	1.18	15.00	53.4	57.6	9.82
40	1.27	16.97	63.7	68.2	9.85
50	0.99	10.22	77.3	80.8	10.07
75	0.97	9.37	118.6	124.2	14.50
100	0.60	5.28	137.2	154.9	31.19

Table S6. Kinetic parameters of Modified Freundlich model for atrazine sorption on PCFs at 25 °C.

Conc. (mg/L)	k (L/(g h))	m	q _{e,exp} (mg/g)	q _{e,cal} (mg/g)	OF
--------------	-------------	---	---------------------------	---------------------------	----

35	1.98	15.67	88.5	95.4	18.5
40	1.90	15.22	98.1	105.6	17.21
50	1.82	14.36	117.6	128.9	27.60
75	1.75	14.69	175.2	184.6	22.72
100	1.59	12.87	226.4	234.6	25.71

Table S7. Kinetic parameters of Modified Freundlich model for atrazine sorption on PCFs at 35 °C.

Conc. (mg/L)	k (L/(g h))	m	q _{e,exp} (mg/g)	q _{e,cal} (mg/g)	OF
35	2.08	17.94	93.3	96.2	11.13
40	1.98	16.70	100	106.9	15.49
50	1.89	14.76	122	132.7	27.37
75	1.97	17.69	183.7	196.1	30.13
100	1.72	13.96	236.5	246.3	21.46

Table S8. Kinetic parameters of Modified Freundlich model for atrazine sorption on PCFs at 45 °C.

Conc. (mg/L)	k (L/(g h))	m	q _{e,exp} (mg/g)	q _{e,cal} (mg/g)	OF
35	2.16	19.36	91.7	97.9	14.2
40	2.11	19.35	102.4	109.3	15.4
50	1.97	15.95	127.2	134.8	14.2
75	1.97	17.92	186.1	195.4	19.8

100	1.79	15.81	240.2	245.7	13.35
-----	------	-------	-------	-------	-------

Table S9. Intraparticle diffusion model of CSs at different initial concentrations.

		k_1	C_1	OF	k_2	C_2	OF
Conc.(mg/L)	35	6.84	31.89	6.18	0.11	52.15	53.58
	40	7.66	40.42	6.44	0.26	60.96	54.36
	50	9.42	36.68	5.74	1.07	64.15	72.75
	75	16.08	51.37	11.16	2.06	94.26	113.50
	100	25.87	22.63	6.18	3.78	96.83	197.18

Table S10. Intraparticle diffusion model of PCFs at different initial concentrations.

		k_1	C_1	OF	k_2	C_2	OF
Conc.(mg/L)	35	15.71	50.04	12.82	0.48	83.70	2.57
	40	15.01	57.15	12.02	0.61	92.25	4.59
	50	23.62	61.24	13.52	0.30	114.85	3.36
	75	22.66	102.81	18.57	1.80	155.90	7.99
	100	34.81	116.91	13.06	3.30	188.68	6.44

Table S11. Isotherm parameters for atrazine sorption on CSs and PCFs.

	CSs	PCFs		
	298.15K	298.15K	308.15K	318.15K

Langmuir	$q_{\max}$	150.11	306.37	340.74	345.72
	K_L	0.0287	0.148	0.183	0.266
	OF	31.46	76.40	83.12	101.65
Freundlich	K_f	14.65	76.39	88.90	102.14
	n	1.89	2.99	2.91	2.92
	OF	48.98	83.11	83.74	72.56

Table S12. Comparison of the performance of atrazine on the as-prepared PCFs with other representative materials.

Materials	Sources	Activating agent	q_e (mg/L)	Ref.
Biochar	Corn straw	$\text{NH}_4\text{H}_2\text{PO}_4$	53.85	1
Activated carbon	Sludge	None	45.49	2
O-MWNTs	CH_4/H_2	H_2SO_4	17.35	3
Biochar	Sludge	/	16.8	4
Biochar	Wheat straw	/	12.0	5
Biochar	Corn straw	NaHCO_3	97.9	This work

References

1. Zhao, X.; Ouyang, W.; Hao, F.; Lin, C.; Wang, F.; Han, S.; Geng, X., Properties comparison of biochars from corn straw with different pretreatment and sorption behaviour of atrazine. *Bioresource Technology* 2013, 147, 338-344.
2. Lladó, J.; Lao-Luque, C.; Ruiz, B.; Fuente, E.; Solé-Sardans, M.; Dorado, A. D.,

Role of activated carbon properties in atrazine and paracetamol adsorption equilibrium and kinetics. *Process Safety and Environmental Protection* 2015, 95, 51-59.

3. Chen, G.-C.; Shan, X.-Q.; Zhou, Y.-Q.; Shen, X.-e.; Huang, H.-L.; Khan, S. U., Adsorption kinetics, isotherms and thermodynamics of atrazine on surface oxidized multiwalled carbon nanotubes. *Journal of Hazardous Materials* 2009, 169 (1–3), 912-918.

4. Zhang, W.; Zheng, J.; Zheng, P.; Qiu, R., Atrazine immobilization on sludge derived biochar and the interactive influence of coexisting Pb(II) or Cr(VI) ions. *Chemosphere* 2015, 134, 438-445.

5. Wang, P.; Yin, Y.; Guo, Y.; Wang, C., Preponderant adsorption for chlorpyrifos over atrazine by wheat straw-derived biochar: experimental and theoretical studies. *RSC Advances* 2016, 6 (13), 10615-10624.

Figures

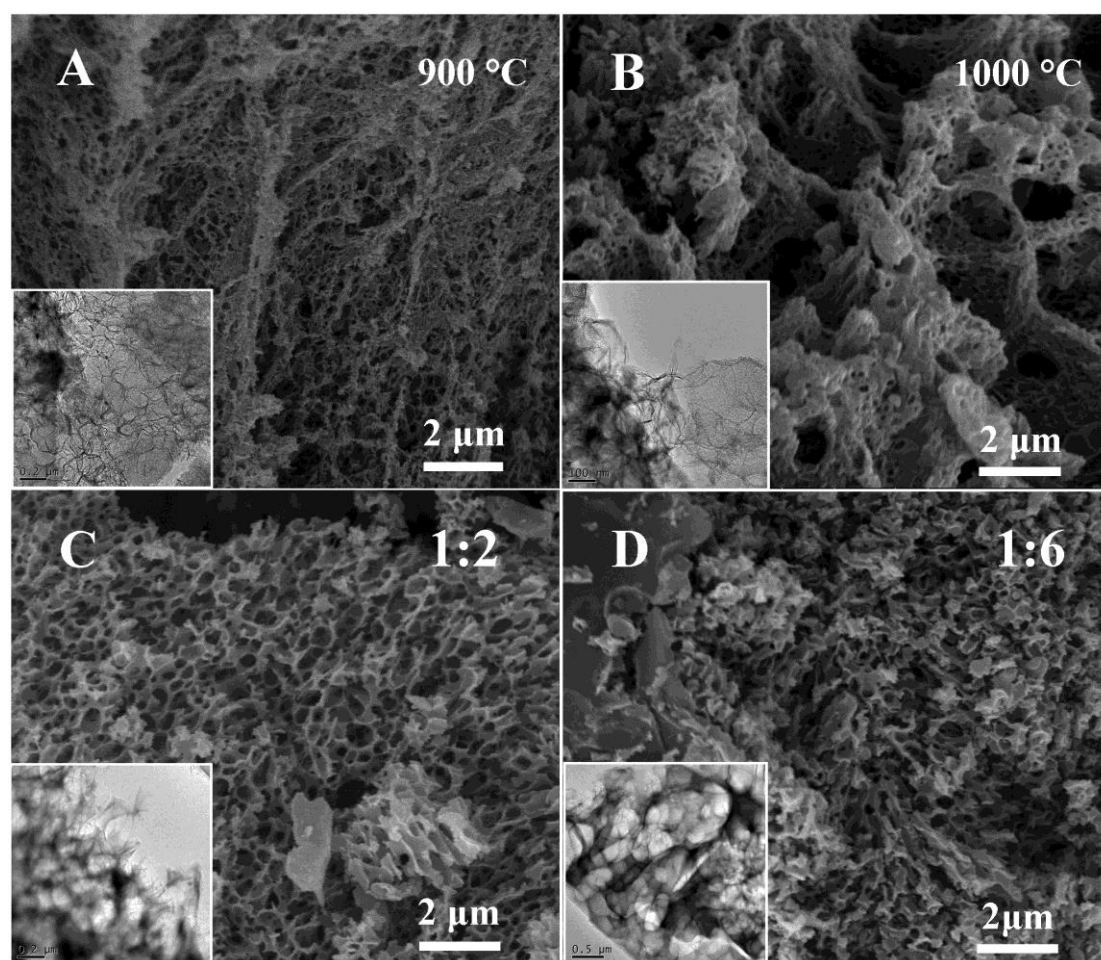


Figure S1. The SEM and TEM images of PCFs prepared with different temperature of 900 °C (A) ,1000 °C (B) and different mass ratio (precursor/NaHCO₃) of 1:2 (C), 1:6 (D).

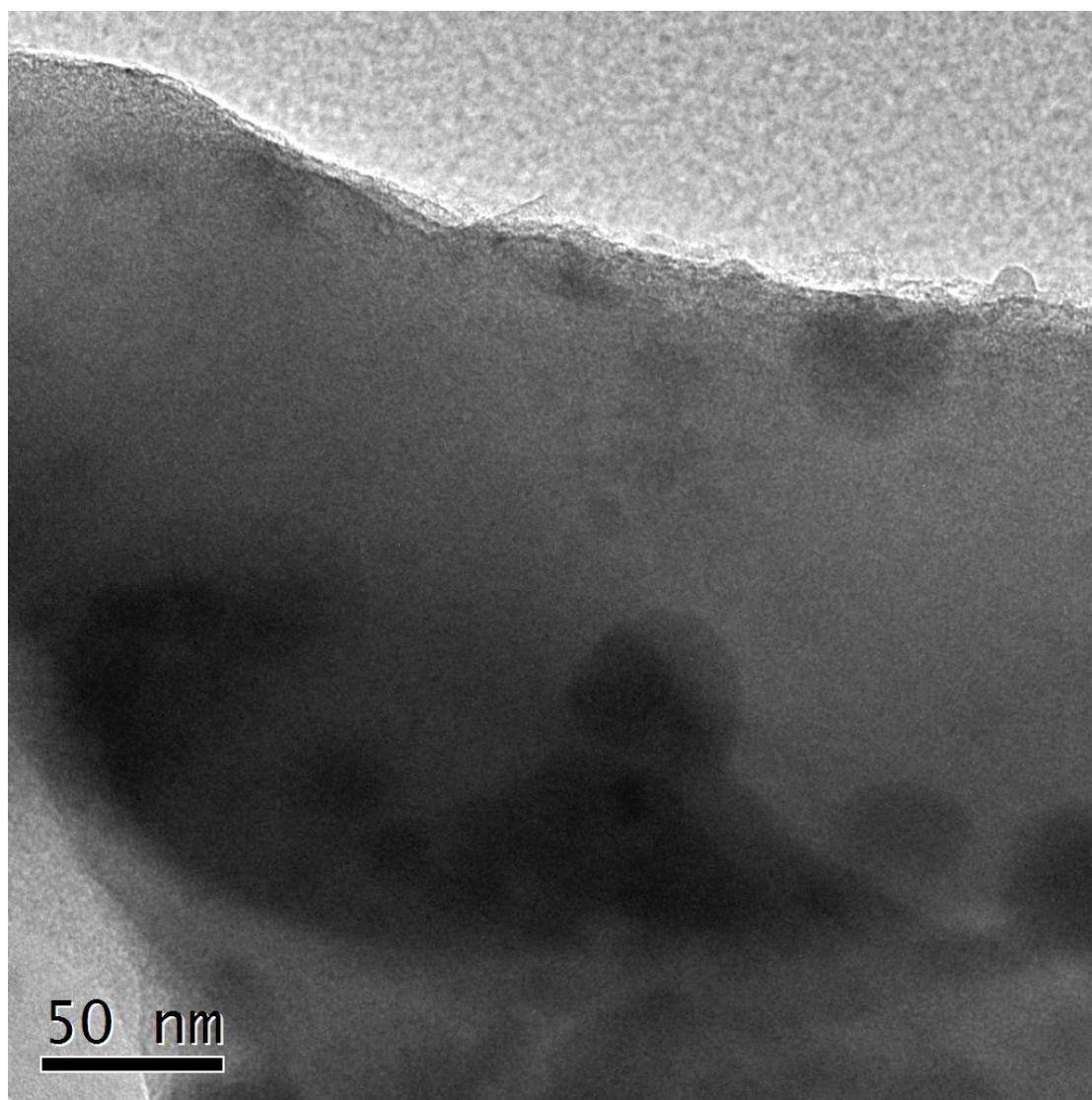


Figure S2. The TEM images of CSs prepared via the direct pyrolysis of corn straws.

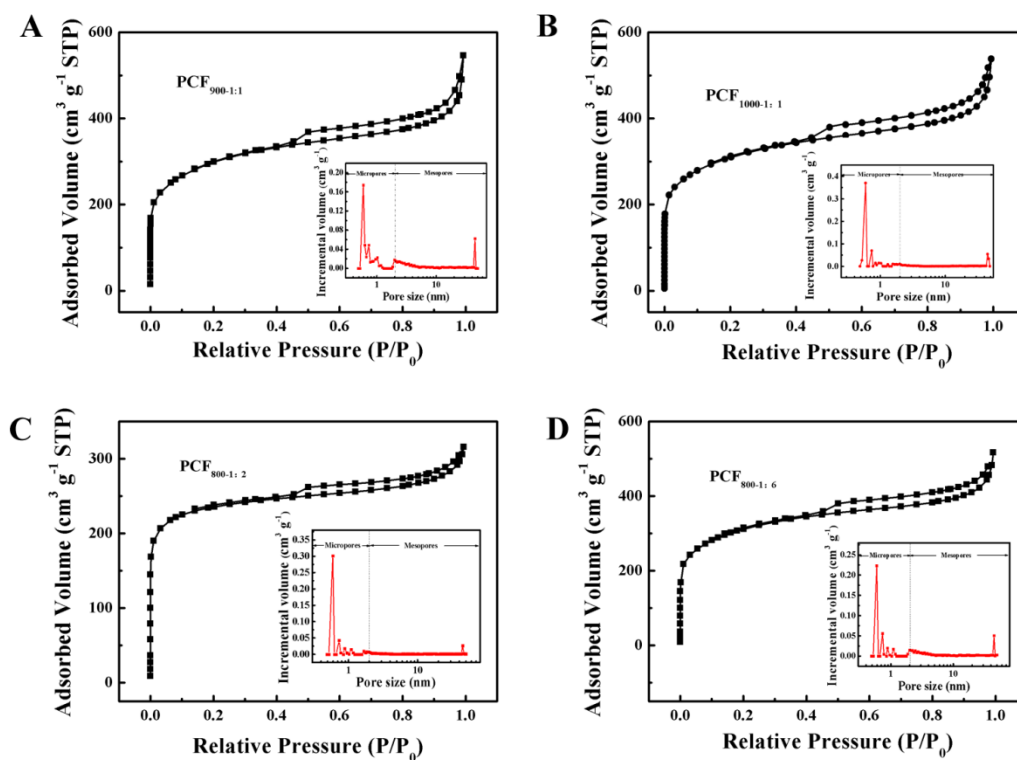


Figure S3. N_2 isotherms of PCFs and CSs prepared at different conditions. (Insert is the PSDs of PCFs and CSs).

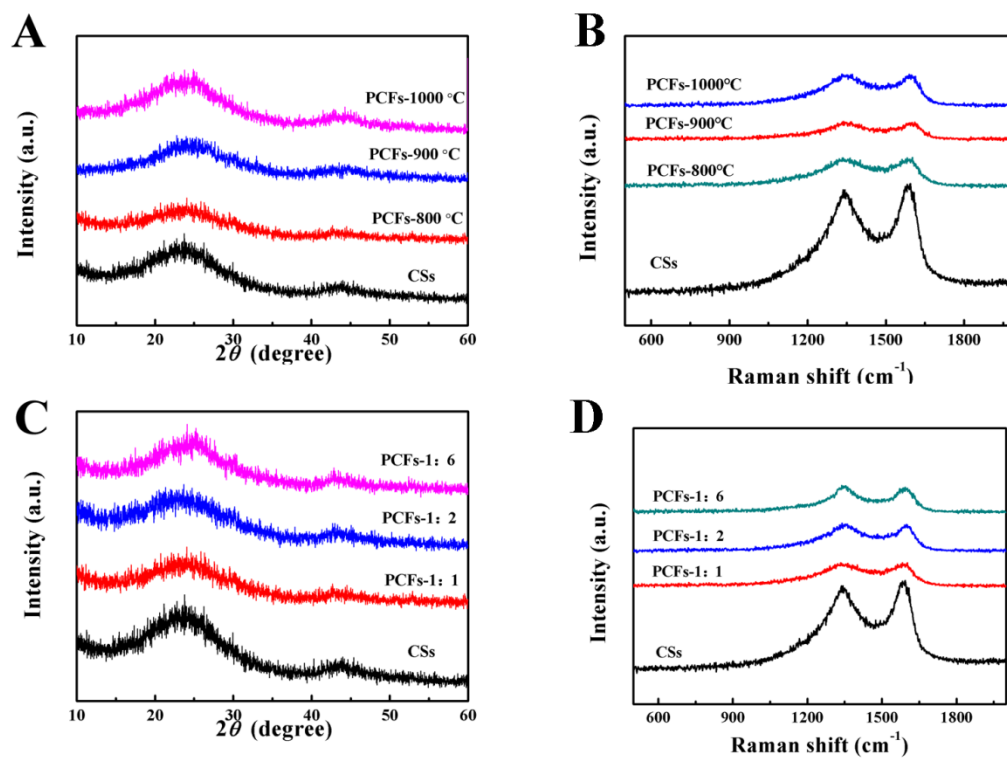


Figure S4. (A) XRD results and (B) Raman spectras using 532 nm excitation of PCFs

with different temperature and CSs; (C) XRD results and (D) Raman spectras using 532 nm excitation of samples calcined at 800 °C with different mass ratio of NaHCO_3 to corn straws.

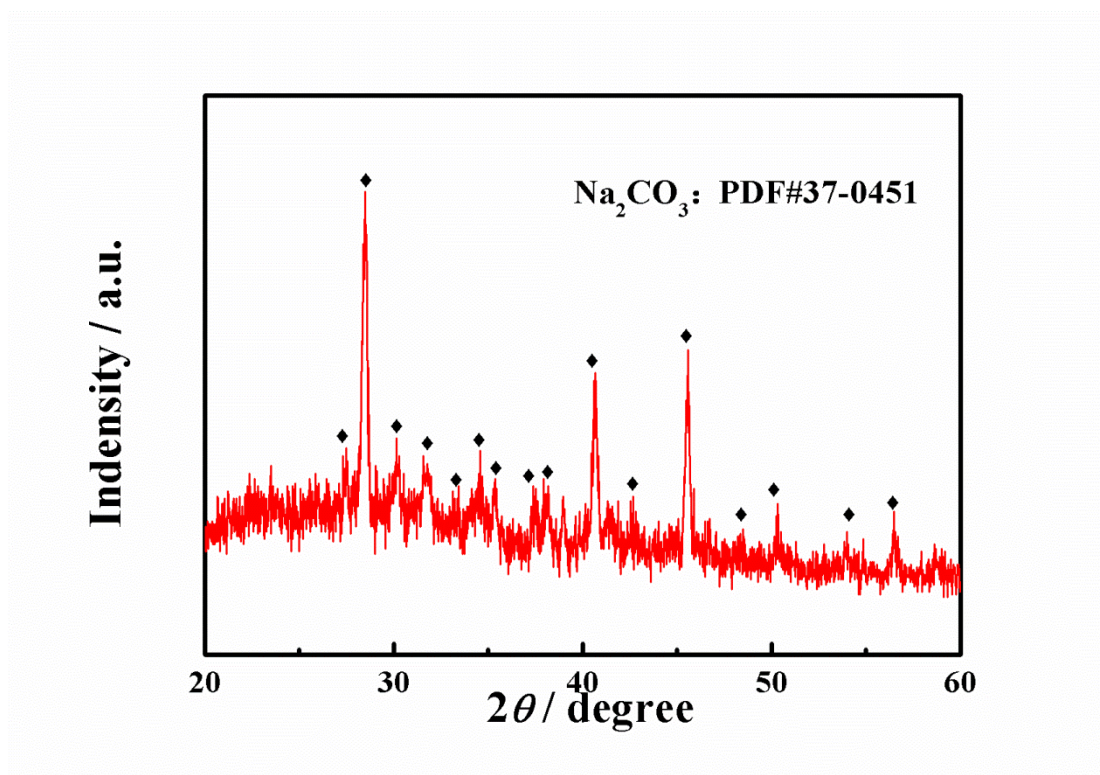


Figure S5. XRD spectrum of PCFs before washing with HCl solutions.

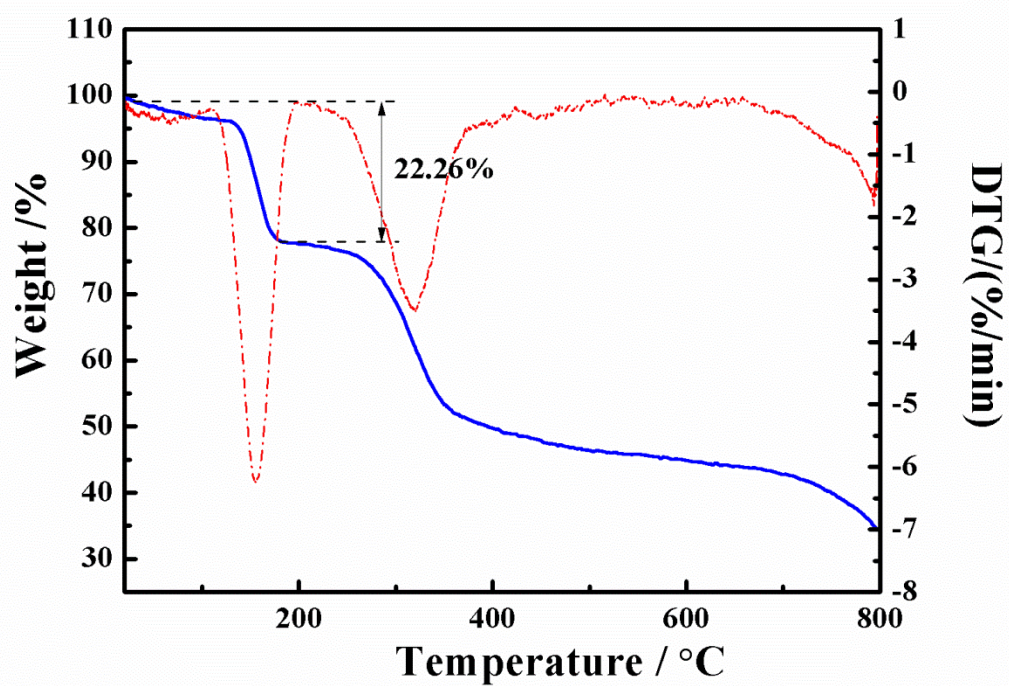


Figure S6. TG results for the mixture of cellulose and NaHCO_3 (1:1). The TG was measured at $5\text{ }^\circ\text{C min}^{-1}$ under the atmosphere of N_2 .

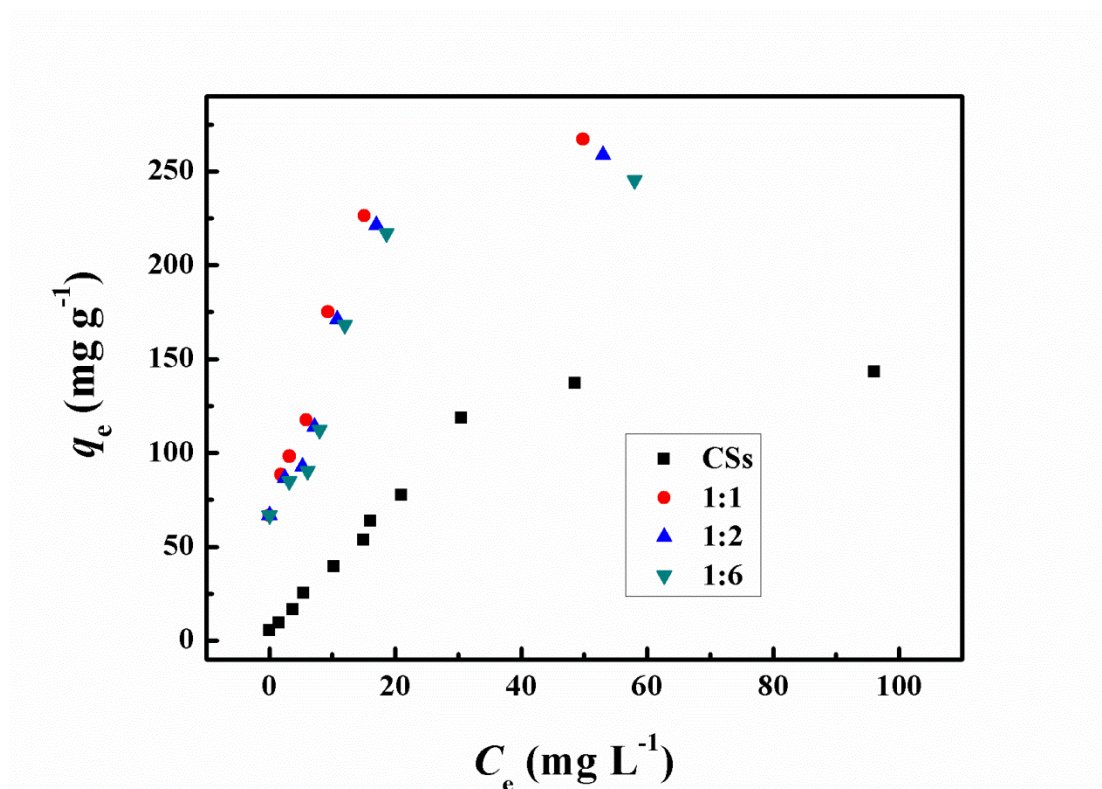


Figure S7. Sorption isotherms of atrazine on CSs and PCFs prepared at different mass ratio of precursor/NaHCO₃ with the temperature of 800 °C.

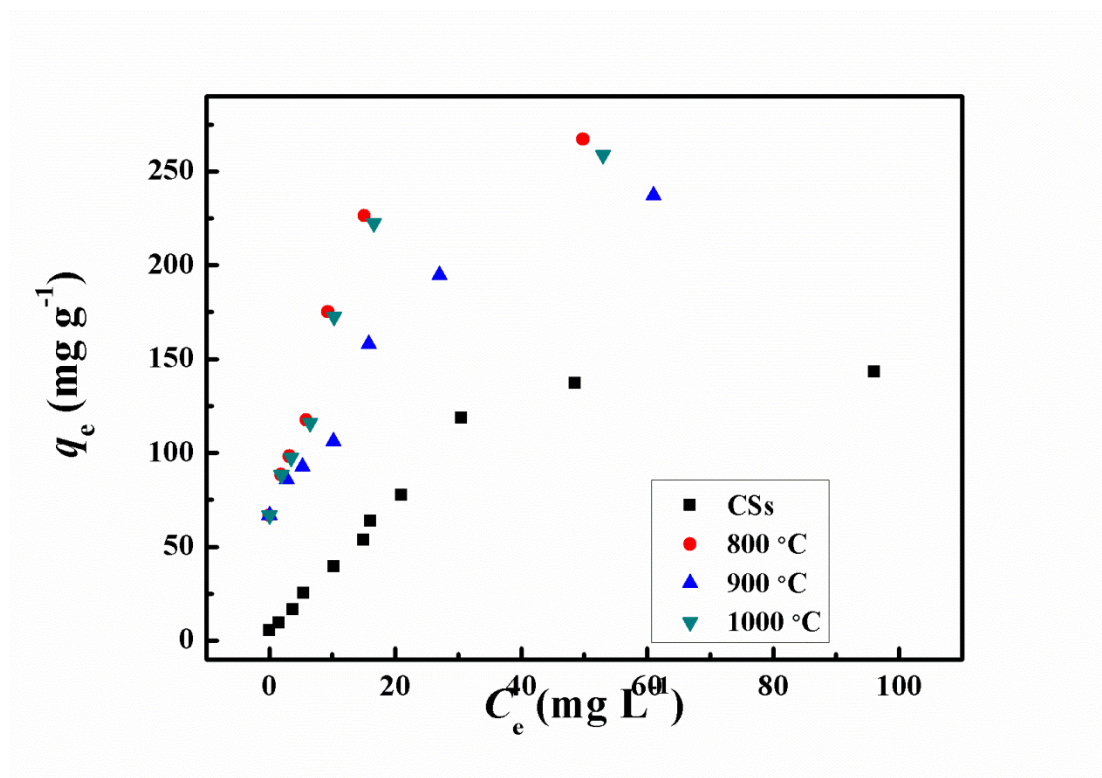


Figure S8. Sorption isotherms of atrazine on CSs and PCFs prepared at different temperature with the precursor/ NaHCO_3 of 1:1 in mass ratio.

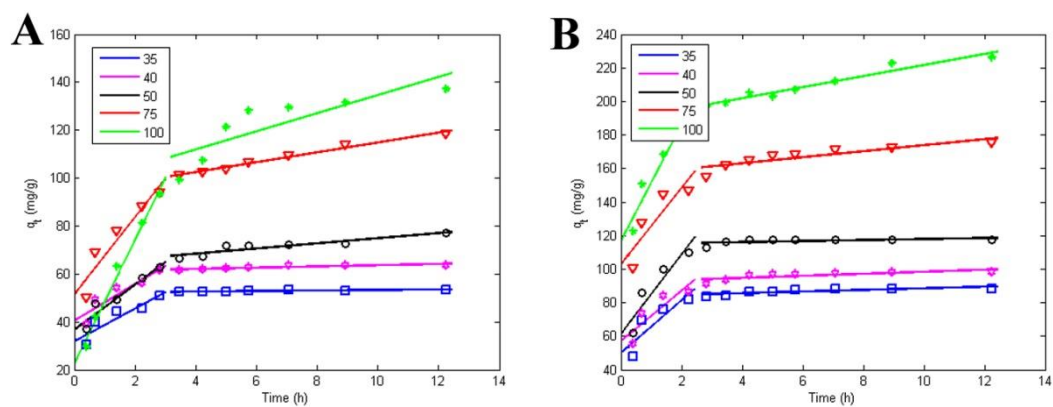


Figure S9. Intraparticle diffusion model of CSs (A) and PCFs samples (B) at the temperature of 25 °C.