Supporting Information

Enhanced phosphate sequestration by Fe(III) modified

biochar derived from coconut shell

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Appendix A

<div align="center">Table S1 List of isotherm models and kinetic models in this study</div>

Kinetic models [1]	Parameters	Isotherm models [2]	Parameters
First-order: $$\frac{dq_t}{dt} = k_1(q_e - q_t)$$ $$\ln(q_e - q_t) = \ln q_e - k_1 t$$	q_e, q_t, k_1, R^2;	**Freundlich** $$q_e = K_f C_e^{1/n}$$	K_F, n, R^2;
Second-order: $$\frac{dq_t}{dt} = k_2(q_e - q_t)^2$$ $$\frac{t}{q_t} = \frac{1}{k_2 q_e^2} + \frac{t}{q_e}$$	q_e, q_t, k_2, R^2;	**Langmuir** $$q_e = \frac{K_l q_m C_e}{1 + KC_e}$$	K_L, q_m, R^2;
Richie n-th-order: $$\frac{dq_t}{dt} = k_n(q_e - q_t)^n$$ $$q_t = q_e - ((n-1)k_n t + q_e^{1-n})^{\frac{1}{1-n}}$$	q_e, q_t, k_n, n, R^2;	**Langmuir- Freundlich** $$q_e = \frac{K_{lf} q_m C_e^n}{1 + K_{lf} C_e^n}$$	K_{LF}, q_m, n, R^2;
Elovich: $$\frac{dq_t}{dt} = a\,exp(-bq_t)$$ $$q_t = \frac{1}{b} ln(abt + 1)$$	a, b, q_t, R^2		

Table S2 Kinetic parameters of phosphate sorption to CSBs based on the intra-particle diffusion model [3]

Adsorbents	K_{p1} (mg/g•h$^{1/2}$)	C_1 (mg/g)	R^2	K_{p2} (mg/g•h$^{1/2}$)	C_2 (mg/g)	R^2
CSB	1.023	0.463	0.797	0.049	1.886	0.895
Fe-CSB	0.806	1.212	0.905	0.323	2.092	0.923

The intraparticle diffusion model: $q_t = k_p • t^{1/2} + C$; where K_p is the intraparticle diffusion rate constant (mg/g•h$^{1/2}$), and C is a constant that reflects the thickness of the boundary layer.

Table S3 Thermodynamic parameters of P adsorption for CSB and Fe-CSB

Materials	T (K)	Parameters			
		K_0 (L/mg)	ΔG^0 (kJ/mol)	ΔH^0 (kJ/mol)	ΔS^0 (J/mol/K)
CSB	298	0.13	-12.06		
	308	0.15	-12.82	21.58	111.43
	318	0.20	-14.01		
Fe-CSB	298	1.43	-18.00		
	308	1.54	-18.79	26.54	82.11
	318	1.63	-19.56		

Thermodynamic parameters are determined by the following equations [4]:

$K_0 = \dfrac{q_e}{C_e}$ (1); $\Delta G = - RT \ln K_0$ (2); $\Delta G = \Delta H - T\Delta S^0$ (3); $\ln K_0 = \dfrac{\Delta H^0}{RT} - \dfrac{\Delta S^0}{R}$ (4);

where K_0 is the adsorption coefficient, R is gas constant (kJ/mol K), and T is the absolute temperature (K), respectively.

Table S4 Comparison of maximum P sorption capacities for various Fe-based materials

Adsorbents	Solution pH	Contact time (h)	Temperature (℃)	Fe (wt %)	Equilibrium Ce (mg/g)	Max q_m (mg/g)	Ref.
Fe-CSB	7.0	24	25	11.2%	2-100	36.0	This work
Fe(III)-Bentonite	7.0	96	25	2.78%	0.05-5.0	11.2	[5]
Granulated ferric hydroxide	5.5	24	20	31.4%	0.3-4.0	23.3	[6]
Magnetic water hyacinth biochar	7.0	24	25	15.0-27.1%	0.2-150	5.1	[7]
Fe-impregnated woodchip biochar	5.6	24	24	2-4%	10-200	3.2	[8]
Fe-doped activated carbon	7.0	24	RT[a]	18.6%	15-640	8.1	[9]
Fe^{3+}/Fe^{2+} modified WAS biochar	7.0	2	22	24.2%	5-1000	34.2	[10]
Magnetic Fe-Zr binary oxide	4.0	24	25	26.62%	0-100	13.7	[11]
Ferrihydrite	7.0	24	25	31.4%	0-250	22.2	[12]

a: RT, room temperature;

Table S5 Chemical reactions between phosphate and metal ions in this study

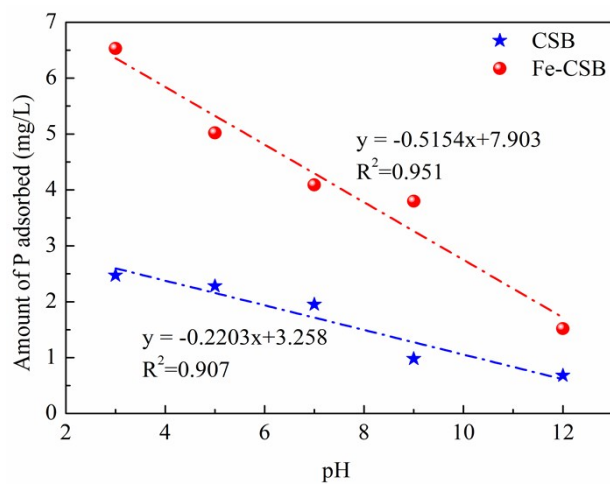| Solid formed	Chemical equation	Solubility equation constant (log K)	Ref.
Ferric phosphate	$Fe^{3+} + PO3- 4 \leftrightarrow FePO_{4(s)}$	21.9	[13]
Iron (III) hydrogen phosphate	$2Fe^{3+} + 3HPO2- 4 \leftrightarrow Fe_2(HPO_4)_{3(s)}$	30.9	[14]
Iron (II) dihydrogen phosphate	$Fe^{3+} + 3H_2PO- 4 \leftrightarrow Fe(H_2PO_4)_{3\ (s)}$	26.6	[14]
Aluminum phosphate	$Al^{3+} + PO3- 4 \leftrightarrow AlPO_{4(s)}$	21.0	[13]
Aluminum hydrogen phosphate	$2Al^{3+} + 3HPO2- 4 \leftrightarrow Al_2(HPO_4)_{3(s)}$	Particles	[15]
Calcium hydrogen phosphate	$Ca^{2+} + HPO2- 4 \leftrightarrow CaHPO_{4(s)}$	6.66	[16]
Calcium dihydrogen phosphate	$Ca^{2+} + 2H_2PO- 4 \leftrightarrow Ca(H_2PO_4)_{2(s)}$	1.14	[16]
Tricalcium phosphate	$3Ca^{2+} + 2PO3- 4 \leftrightarrow Ca_3(PO_4)_{2(s)}$	24.0	[16]
Hydroxyapatite	$5Ca^{2+} + 3PO3- 4 + OH^- \leftrightarrow Ca_5(PO_4)_3OH_{(s)}$	55.9	[16]
Magnesium phosphate	$3Mg^{2+} + 2PO3- 4 \leftrightarrow Mg_3(PO_4)_{2(s)}$	25.2	[1]
Magnesium hydrogen phosphate	$Mg^{2+} + HPO2- 4 \leftrightarrow MgHPO\ 4_{(s)}$	5.82	[1]
Magnesium dihydrogen phosphate	$Mg^{2+} + 2H_2PO- 4 \leftrightarrow Mg(H_2PO\ 4)_{2(s)}$	Particles	[1]

Fig. S1 Linear correlations between the initial pH and the P adsorption amount of CSB and Fe-CSB
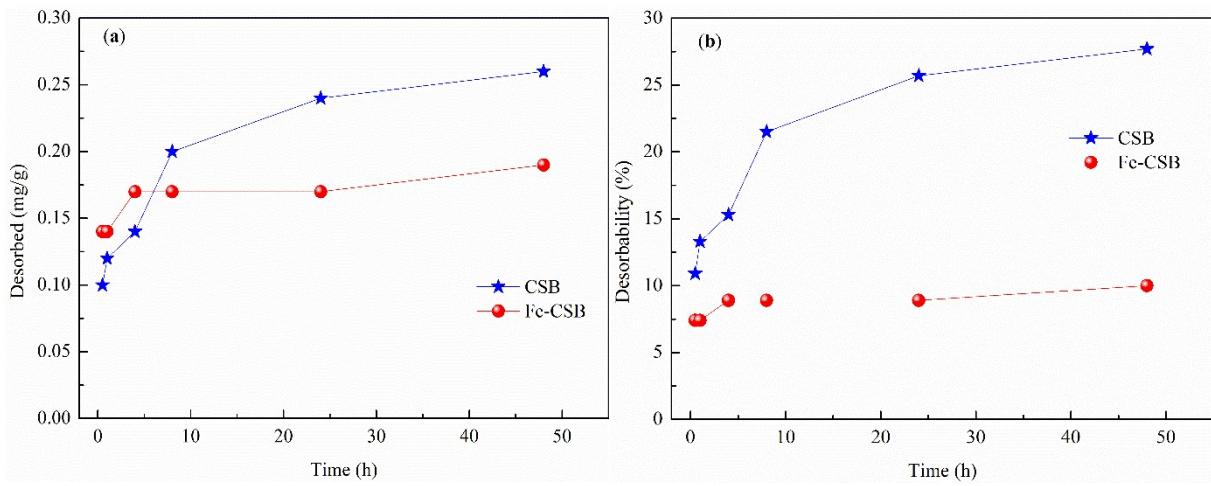
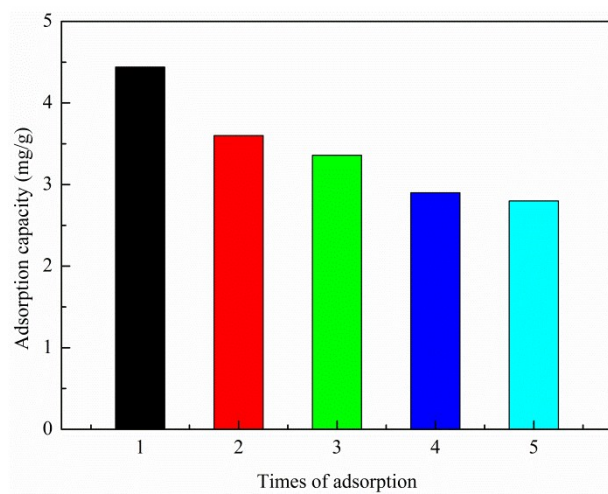Fig. S2 Desorbed amount (a) and Desorbability (b) of the adsorbed P from the CSB and Fe-CSB

Fig. S3. The adsorption capacity of phosphate by Fe-CSB during five successive cycles

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