Supplementary Information (SI) for RSC Advances.
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Supporting Information

Enhancing Wastewater Treatment: A study on Steam Explosion-Biochar Derived from Chinese Herbal Medicine Residue for NOR Adsorption

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Text S1

Characterization

The Bruner-Emmett-Teller (BET) surface area, pore size, and total pore volume of each of these materials were determined by using the Specific Surface Area and Pore Size Analysis (Quantachrome IQ2, Quantachrome)) instrument. The surface morphology and composition of activated carbon were examined by scanning electron microscopy (SEM,Zeiss Gemini). The elemental contents of C, H, O, and N in the sample were measured using an organic element analyzer (EA, Elementar UNICUBE). The functional groups of activated carbon were determined with BRUKER TENSOR2-FTIR spectrometer, recording spectra from 4000 cm-1 to 500 cm-1. The powder diffraction measurements were performed using X-ray diffraction (XRD, Bruker D8), with 2θ ranging from 10° to 90°. The fundamental properties of activated carbon were determined by using a Raman spectrometer (Thermo Scientific DXR 3Xi), X-ray photoelectron spectroscopy (XPS, Thermo-Scientific K-Alpha) analysis. The pHpzc of activated carbon was measured using a Zeta Potential and particle size analyzer (90 Plus PALS).

Text S2

Determination of NOR concentration, calculation of adsorption capacity and removal rate.

In the adsorption test, the concentration of residual NOR was determined using an ultraviolet spectrophotometer (U-3900H, Japan) at 273 nm. The experimental NOR adsorption capacity (qe, mg· g^{-1}) and removal rate (R) on the activated carbon obtained can be determined using the following two equations.

$$q_e = \frac{(C_0 - C_e)V}{m} \tag{1}$$

$$R = \frac{(C_0 - C_e)}{C_0} \times 100\% \tag{2}$$

where q_e (mg/g) and R (%) are separately the equilibrium adsorption capacity and removal rate of NOR. C_0 (mg/L) is the initial mass concentration of NOR; C_e (mg/L) is the equilibrium mass concentration; V (mL) is the volume of NOR solution; m (g) is the mass of activated carbon.

Figure captions

Table captions

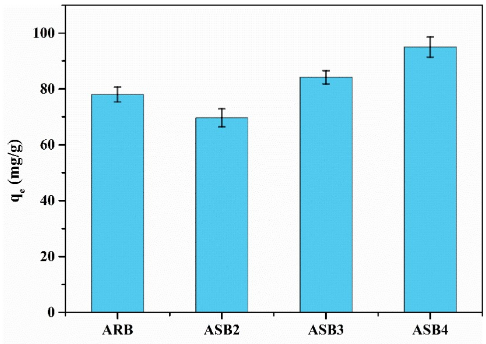
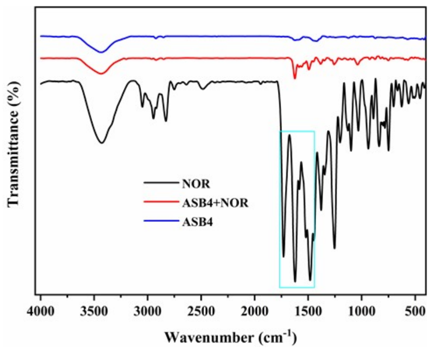
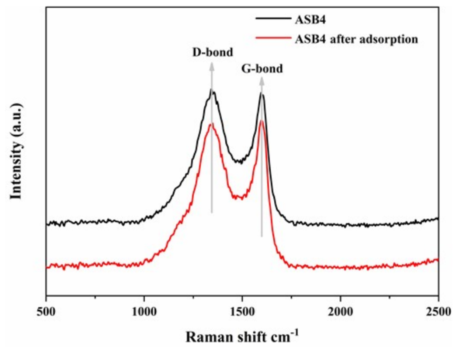


Fig.S1. Adsorption of NOR by different adsorbents. (pH=8, C_0=50 mg/L)



(a)



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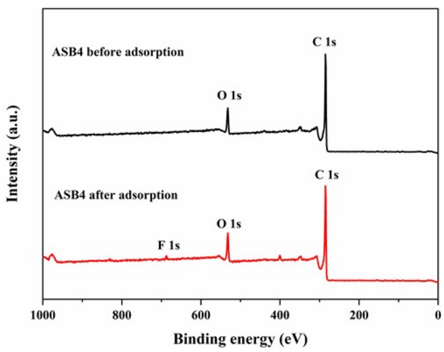

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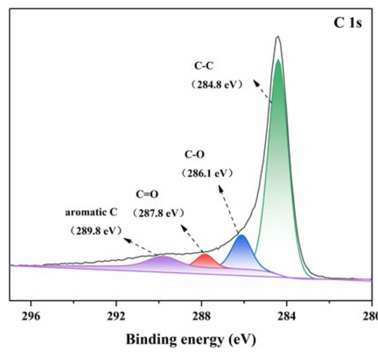

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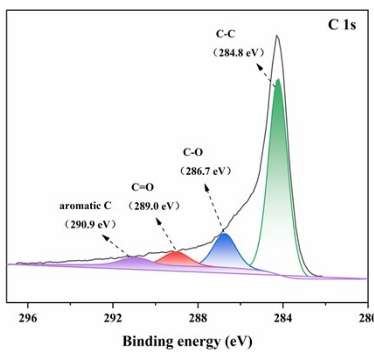

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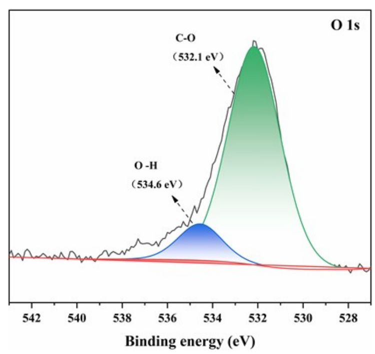

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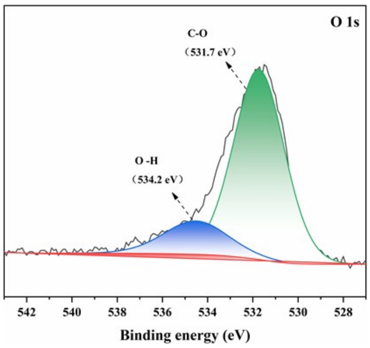

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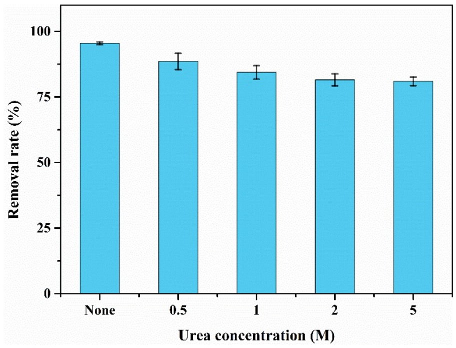
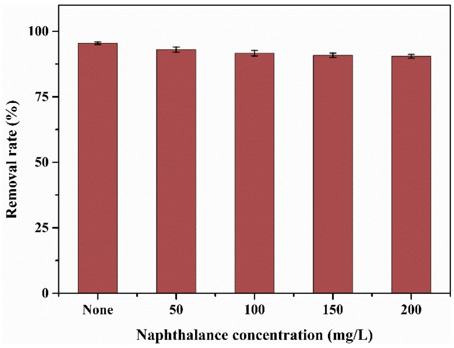
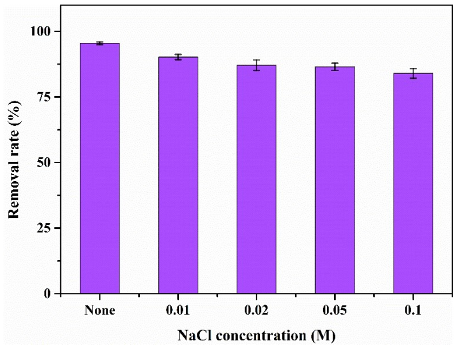


(h)

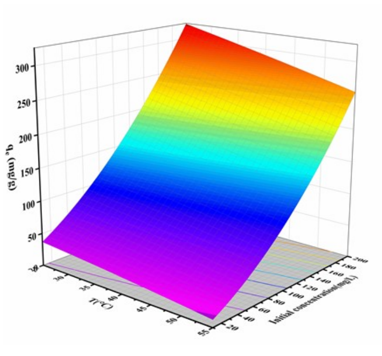


(i)

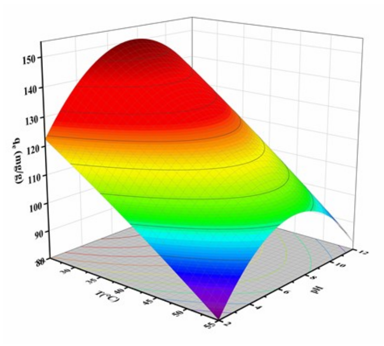


(j)

Fig. S2. (a) FTIR spectra of ASB4 before and after adsorption and NOR, (b) Raman spectrum of ASB4 before and after adsorption, (c) XPS spectra of ASB4 before and after adsorption, (d) C 1s XPS analysis of ASB4, (e) C 1s XPS analysis of ASB4 after adsorption, (f) O 1s XPS analysis of ASB4, (g) O 1s XPS analysis of ASB4 after adsorption, Adsorption capacity of NOR on ASB4 in different concentrations of (h) urea solution, (i) naphthalene solution and (j) NaCl solution. (pH=8, C_0=50 mg/L)



(a)



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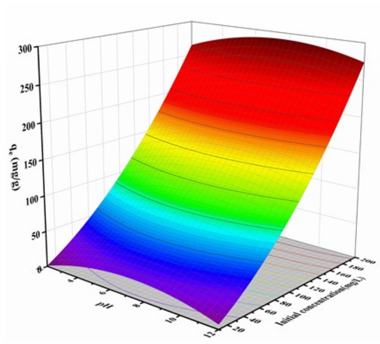
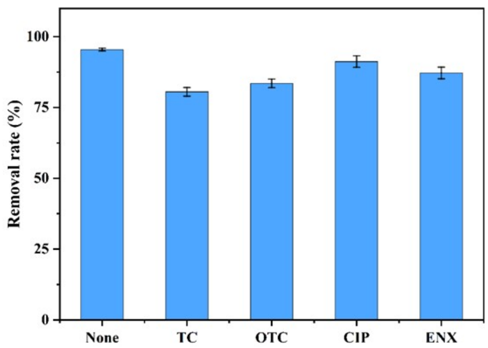
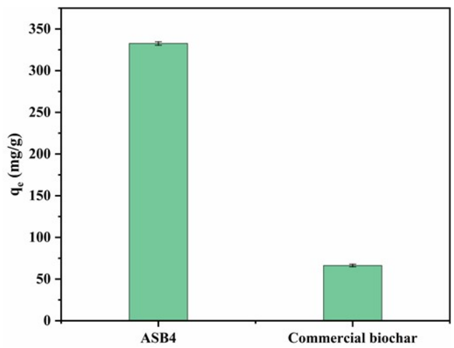


(c)

Fig. S3. Response surface plots of different factors to NOR removal (a) temperature and concentration, (b) temperature and pH, and (c) pH and concentration.



(a)



(b)

Fig. S4. Effect of different antibiotics on NOR adsorption (a) (pH=8, C_0=50 mg/L) and NOR adsorption effect comparison of ASB4 and commercial biochar (b) (pH=8, C_0=200 mg/L).

Table S1. Adsorption kinetics, isotherm models and thermodynamic equations.

Adsorption model	Type	Equation*	Parameters
Kinetics	PFO	$q_t = q_e\left(1-e^{-k_1 t}\right)$	q_e and q_t (mg/g) are the adsorbed amount at an equilibrium concentration, (C_e, mg/g) and a predetermined time (t, min), k_1 (min^{-1}) is the rate constants.
	PSO	$q_t = \frac{k_2 q_e^2 t}{1+k_2 q_e t}$	k_2 (min^{-1}) is the rate constants for the pseudo-second order.
	Elovich	$q_t = \frac{1}{\beta}\ln(1+\alpha\beta t)$	α (mg/(g·min)) is the initial rate constant, β (mg/g) is the desorption constant.
	IPD	$q_t = \mathrm{k}_i t^{0.5} + C_i$	k_i (mg/(g·min$^{0.5}$)) is the adsorption rate constants of intraparticle diffusion model and C_i is the constant for film thickness of the intra-particle diffusion model.
Isotherm	Langmuir	$q_e = \frac{q_m K_L C_e}{1+K_L C_e}$	q_m (mg/g) is the maximum adsorption capacity of the adsorbent, q_e (mg/g) is the adsorption capacity at equilibrium, C_e (mg/L) is the adsorbate concentration at equilibrium, K_L (L/mg) is the constant for the affinity between the adsorbate and the adsorbent.
	Sips	$q_e = \frac{q_m K_s {C_e}^n}{1+K_s {C_e}^n}$	C_e (mg/L) is the equilibrium concentration, q_m (mg/g) is the maximum adsorption capacity of the adsorbent, K_S (L/mg)^n is the adsorption equilibrium constant, n is indicative of the surface site heterogeneity of the adsorbent.
	Freundlich	$q_e = K_F C^{1/n}$	K_F ((mg^{1-n}·L^n)/g), $1/n$ is the Freundlich constant, n is a dimensionless Freundlich intensity parameter.
Thermodynamic	Van der Hoff equation	$\Delta G = \Delta H - T\Delta S$ $\ln K_e = \frac{\Delta S}{R} - \frac{\Delta H}{RT}$ $K_e = \frac{(1000 \cdot K_S \cdot \mathrm{MW}_{\mathrm{adsorbate}}) \cdot [\mathrm{Adsorbate}]^0}{\gamma}$ $\Delta G = -RT\ln K_e$	ΔG (kJ/mol) is the Gibbs energy; K_e is the dimensionless equilibrium constant of adsorption; γ is the activity coefficient and equal to 1.00, [Adsorbate]^0 represents the standard concentration which is equal to 1 mol·L^{-1}; K_s (L·mg^{-1})^n is the equilibrium constant of the best model for isotherm fitting; $\mathrm{MW}_{\mathrm{adsorbate}}$ is the relative molecular weight of the adsorbate (g/mol); R is the ideal gas constant, whose value is 8.314 J/(mol·K); T (K) is absolute temperature; ΔH (kJ/mol) is the activate denthalpy; and ΔS is the change in entropy (J/mol/K).

Table S2. Lists of maximum NOR adsorption capacity on various biochar and other adsorption materials.

Raw material	BET (m^2/g)	Total pore Volume (cm^3/g)	Adsorbent dosage (g/L)	NOR concentration (mg/L)	q_e (mg/g)	Ref.
Original kaolin	44	0.233	0.5	20	30.47	[1]
Cocoa shells	328.45	1.856	1	300	134	[2]
Coffee grounds	46.32	-	1.32	24.69	69.8	[3]
Algal biochar-clay composite	221.04	0.24	0.4	200	192.80	[4]
Longan seed	420.58	0.277	0.6	50	139.27	[5]
Apple branch	331.02	0.215	0.4	20	81.08	[6]
Astragalus residue	512	0.534	0.5	200	332	This study

Table S3. Thermodynamic parameters for NOR adsorption.

Material	ΔG (kJ/mol)		ΔH (kJ/mol)	ΔS (J/mol/K)
ASB4	298 K	-26.06	-38.52	-41.24
	303 K	-25.82		
	313 K	-25.25		
	323 K	-24.99		

Table S4. Pore character of ASB4 before and after adsorption.

Samples	S_{BET} (m^2/g)	$S_{Langmuir}$ (m^2/g)	V_{Micro} (cm^3/g)	V_{Total} (cm^3/g)	Average pore diameter (nm)
ASB4	512	745	0.066	0.534	4.16
after adsorption	146	222	NA	0.158	4.33

Table S5. ANOVA for quadratic models.

Source	Sum of squares	df	Mean square	F value	p-value
Model	1.518×10^5	9	16862.66	61.39	< 0.0001
A-Temperature	4465.13	1	4465.13	16.25	0.0050
B-initial concentration	112.50	1	112.50	0.41	0.5427
C-pH	1.412×10^5	1	1.412E+005	513.90	< 0.0001
AB	25.00	1	25.00	0.091	0.7717
AC	462.25	1	462.25	1.68	0.2358
BC	4.00	1	4.00	0.015	0.9074
A^2	5.81	1	5.81	0.021	0.8885
B^2	1932.76	1	1932.76	7.03	0.0329
C^2	3872.02	1	3872.02	14.09	0.0071
Residual	1923.95	7	274.85		
Lack of Fit	1422.75	3	474.25	3.87	< 0.1156
Pure Error	501.20	4	125.30		
Cor Total	1.532×10^5	16			

Table S6. Direct Operating Costs analysis of ASB4 production.

Sample	Material	Specification	Price ($/kg)[a]	Amount (kg)	Total ($/kg)
ASB4	AR residue		0.02	2.85	0.52
	Water	18.2 MΩ	0.005	20	0.1
				Total DOC ($/kg)	0.62

[a] Price was based on: Made-in-China, Focus Technology Co., Ltd. (https://www.made-in-china.com).

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