Supporting information

Enhanced peroxydisulfate (PDS) Activation for Sulfamethoxazole (SMX) Degradation by Modified Sludge Biochar: Focusing on the Role of Functional Groups

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Text S1 Materials and chemicals

Initially, a mixture of 20 g of sludge and 3 g of tannin extract was prepared in 30 ml of deionized water. The pH of this mixture was carefully adjusted to 8 using 0.1 mol/L hydrochloric acid. The mixture was then stirred at 180 rpm for 2 hours. The resulting mixture was then dried at 105°C and ground to a fine powder, passing through a 100-mesh sieve, to yield the biochar precursor. This precursor powder was then pyrolyzed in a tube furnace at 700°C for 2 hours (controlled heating rate of 10°C/min, nitrogen flow of 100 mL/min). The resulting biochar was thoroughly washed with 1 mol/L hydrochloric acid and deionized water to a neutral pH of 7 was achieved. Finally, the TSBC was dried to constant weight in an oven at 105°C. SDBC was generated employing the aforementioned pyrolysis technique, excluding the incorporation of tannin extracts.

Text S2 Experimental procedures

Based on the degradation experiments steps, the effect of various factors on the catalytic degradation performance of sulfamethoxazole (SMX) was further investigated. These factors include initial pH values (3.88, 5.76, 8.19, and 10.22) and reaction temperatures (25°C, 35°C, 45°C, and 55°C). It is noteworthy that 0.1 mol/L hydrochloric acid was used for pH adjustment. Further investigations were carried out to assess the influence of environmental variables in the water matrix, specifically inorganic anions (Cl^-, NO_3^-, HCO_3^-) and humic acid (HA), on the degradation of SMX. It is important to note that these compounds were introduced after the adsorption-desorption equilibrium (reached after 30 minutes).

Text S3 Analytical methods

Quantitative analysis of SMX: The mass concentration of SMX in the samples was measured by a liquid chromatograph (LC-20AT) equipped with a C18 column (ZORBAX Eclipse Plus C18) and a UV detector. The UV detection wavelength was 269 nm and the mobile phase was 70% methanol and 30% ultrapure water (v v^{-1}) at a flow rate of 1 mL min^{-1} with an injection volume of 20 μL. To improve the reliability of the test results, the standard curve of SMX was determined using the following procedure: 0.4 g of SMX was weighed and made up to 1 L with ultrapure water to prepare a stock solution. Pipette 0.5, 1, 2, 3, 4, 5 mL of the above stock solution into a 50 mL colorimetric tube and add ultrapure water to dilute the volume to form a standard solution with a concentration gradient of 2, 4, 8, 12, 16, 20 mg/L and then determine the concentration by HPLC. The SMX standard curve derived from the tested peak areas is shown in Figure S1. The correlation coefficient of the linear regression equation between peak area and SMX mass concentration was R^2=0.9996, indicating that the determination of SMX mass concentration in the range of 0-20 mg L^{-1} was highly reliable.

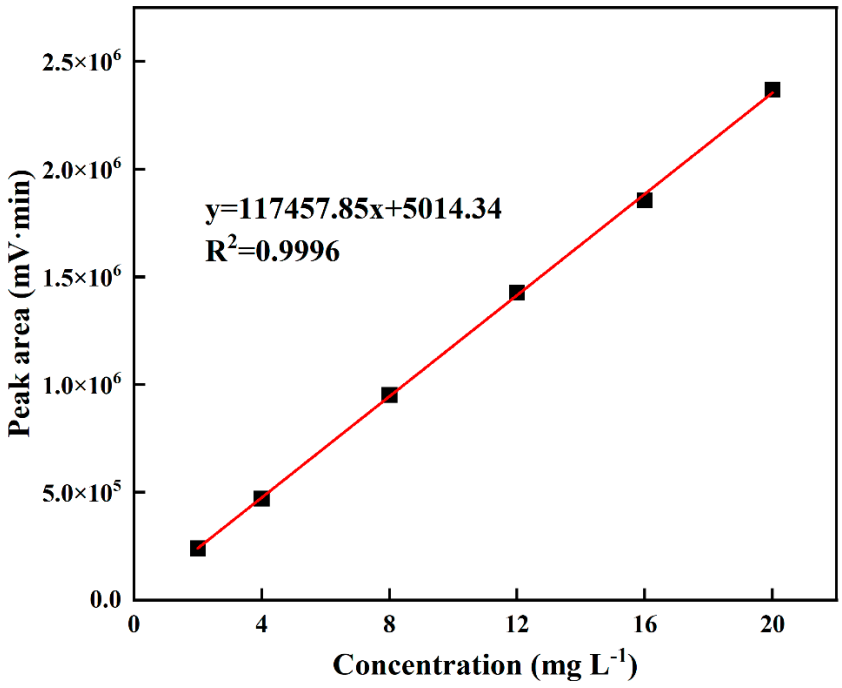

Figure S1 Calibration curve of SMX

Characterization methodology: The surface morphologies of the samples were examined using ultra-high resolution field emission scanning electron microscopy (SEM, Verios G4, Thermo Fisher). Quantitative analysis of the elemental composition, in particular C, H, N, and O, in the samples was carried out using an elemental analyzer (EA, Vario EL Cube, Ementar). Surface functional groups of TSBC, both before and after the reaction, were characterized using Fourier Transform Infrared Spectrometer (FTIR, Nicolet is50, ThermoFisher) with an Attenuated Total Reflection (ATR) module. Samples were uniformly compressed into pellets and positioned in the ATR module. Spectral scanning was performed 36 times over a wave number range of 500 to 4000 cm^{-1}. The resulting infrared absorption spectra were obtained by subsequent data fitting. The changes in the crystal structure before and after the TSBC reaction were systematically analyzed using an X-ray diffractometer (XRD, MiniFlex 600, Rigaku). The analysis was carried out under the following conditions: CuKα radiation, an acceleration voltage of 40 kV, a current of 15 mA, and a scan rate of 5º/min within a 2θ range of 5º to 80º.

Zeta potential test: Zeta potential values were determined over a range of pH values (3, 5, 7, 9, and 11) using a particle size and zeta potential analyzer (Nanoplus-3, Micromeritics). The pH of a 50 mL aqueous solution was adjusted to the desired value using 0.1 mol/L HCl or NaOH to prepare the samples. Then 5 mg of the TSBC sample was added. The mixture was then sonicated for 5 minutes to ensure homogeneity prior to analysis.

Electron paramagnetic resonance (EPR) testing: EPR spectroscopy was used for the qualitative analysis of reactive oxygen species in the TSBC/PDS system. Specifically, 2,2,6,6-tetramethylpiperidine (TEMP) at a concentration of 20 mmol/L was used as a spin trap to capture the singlet oxygen generated in the system.

Table S1 Element composition of SDBC and TSBC

Samples	Element composition					
	C (%)	H (%)	O (%)	N (%)	H/C	O/C
SDBC	6.10	0.66	8.91	0.34	0.11	1.46
TSBC	25.94	0.91	7.45	0.66	0.04	0.29

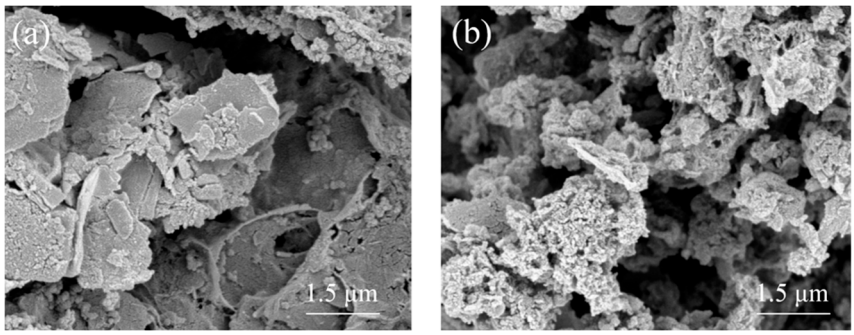

Figure S2 SEM images of SDBC (**a**) and TSBC (**b**)

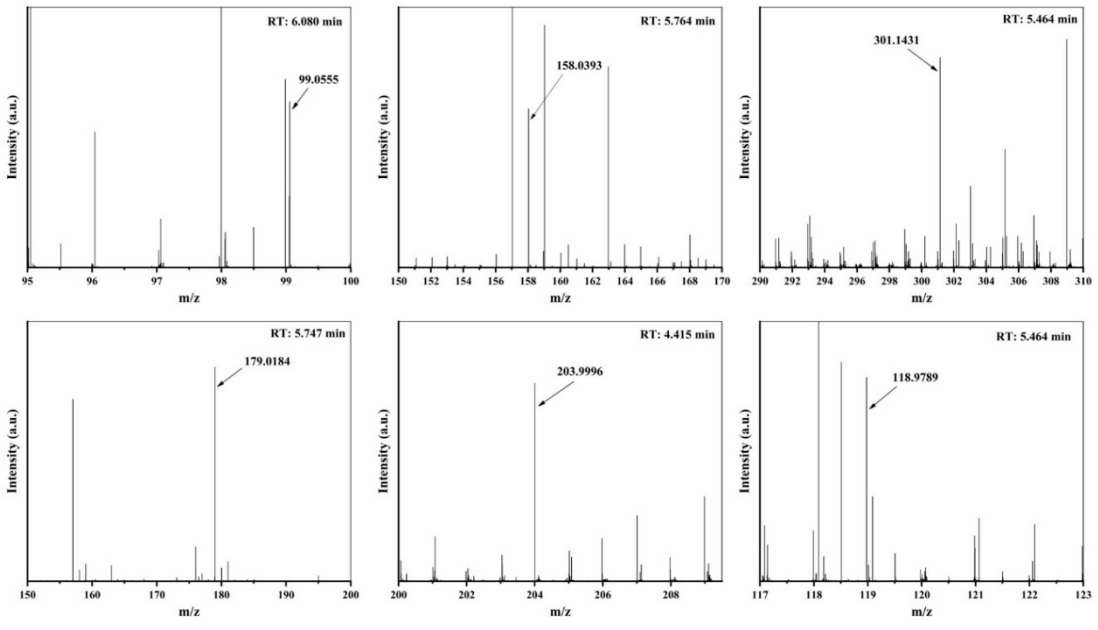

Figure S3 SMX intermediates detected in TSBC/PDS system