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Supporting information

Quantitative evaluation for the relationship of adsorption and partition of atrazine on biochar-amended soils with biochar characteristics

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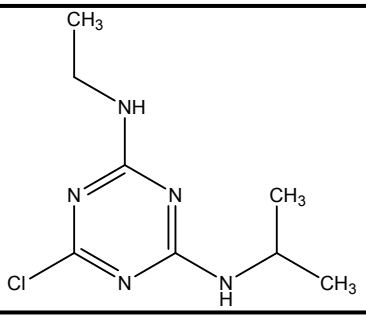
Table S1 Molecular structure and physicochemical properties of atrazine (ATZ).

Molecular structure	
Molecular formula	$C_8H_{14}N_5Cl$
Molar weight (g mol^{-1})	216
Water solubility (mg L^{-1})	33
log K_{ow}[a]	2.70
Melting point (℃)	171

[a]logK_{ow}, octanol-water partition coefficient.

Table S2 Fitting parameters for the Freundlich model and the single point K_{OC} for atrazine adsorption.

Sample	Freundlich sorption				LogK_{oc} at C_e (mL/g)		
	K_F	n	R^2	K_{FOC}	=0.005S_W	=0.05S_W	=0.5S_W
RC300	0.676	0.647	0.978	1.231	2.326	1.032	0.458
RC400	0.745	0.685	0.991	1.355	2.388	1.157	0.561
RC500	1.788	0.348	0.991	3.137	10.161	2.263	0.504
RC600	3.048	0.260	0.992	4.983	18.909	3.440	0.626
RC700	7.898	0.195	0.976	12.467	53.172	8.331	1.305
BC300	0.0429	0.723	0.989	0.0588	0.0969	0.0512	0.0270
BC400	0.105	0.630	0.994	0.135	0.262	0.112	0.0477
BC500	0.274	0.509	0.980	0.332	0.805	0.260	0.0839
BC600	0.780	0.389	0.979	0.887	2.665	0.653	0.160
BC700	5.828	0.239	0.965	6.486	25.573	4.430	0.767
MC300	0.506	0.773	0.994	1.106	1.664	0.987	0.585
MC400	0.684	0.708	0.980	1.511	2.558	1.305	0.666
MC500	1.098	0.454	0.976	2.587	6.919	1.968	0.560
MC600	3.858	0.273	0.999	8.700	32.234	6.045	1.134
MC700	4.765	0.242	0.974	11.388	44.666	7.789	1.358

[a]The adsorption data fitted the Freundlich model well (R^2 = 0.965–0.999), $Q_e = K_f C_e^n$, where Q_e (mg kg^{-1}) and C_e (mg L^{-1}) represents the solid-phase concentration and equilibrium solution-phase concentration, respectively. K_f ((mg/kg)/(mg/L)^n) is Freundlich adsorption coefficient and n is an index of isotherm nonlinearity. Log K_{oc} (log K_{oc} = log $Q_e/(C_e f_{oc})$) is organic carbon-normalized adsorption coefficient of ATZ on biochars.

Table S3 Fitting parameters for the Freundlich model for atrazine adsorption on biochar-amended soil.

Sample	Biochar	Freundlich sorption		
		K_F	n	R^2
Paddy soil (PS)	0	2.110	0.979	0.985
	2% RC300	14.989	0.682	0.995
	2% RC500	35.892	0.531	0.992
	2% RC700	98.265	0.374	0.991
	2% BC300	2.925	0.875	0.995
	2% BC500	27.893	0.431	0.988
	2% BC700	82.458	0.320	0.971
	2% MC300	12.779	0.811	0.996
	2% MC500	23.115	0.539	0.990
	2% MC700	69.823	0.413	0.989
Black soil (BS)	0	6.724	0.776	0.998
	2% RC300	18.168	0.678	0.999
	2% RC500	41.476	0.472	0.997
	2% RC700	112.876	0.359	0.982
	2% BC300	7.301	0.729	0.994
	2% BC500	25.710	0.462	0.998
	2% BC700	80.501	0.319	0.984
	2% MC300	15.129	0.778	0.997
	2% MC500	27.409	0.523	0.993
	2% MC700	75.561	0.403	0.986

Fig. S1 X-ray diffraction patterns of biochars from different biomass.

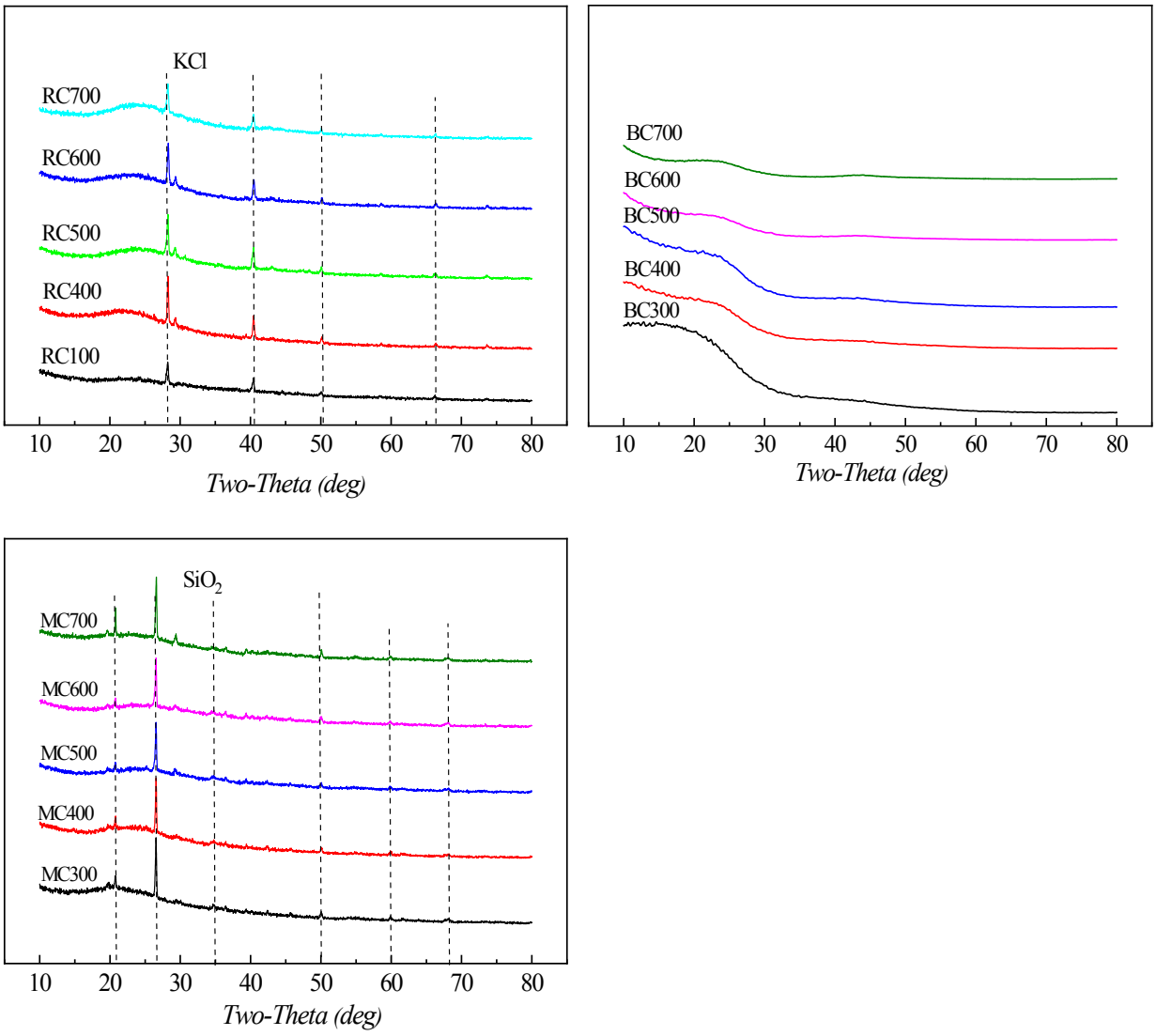


Fig. S2 Van Krevelen diagram for biochar produced from different feedstocks at 300°C–700°C.

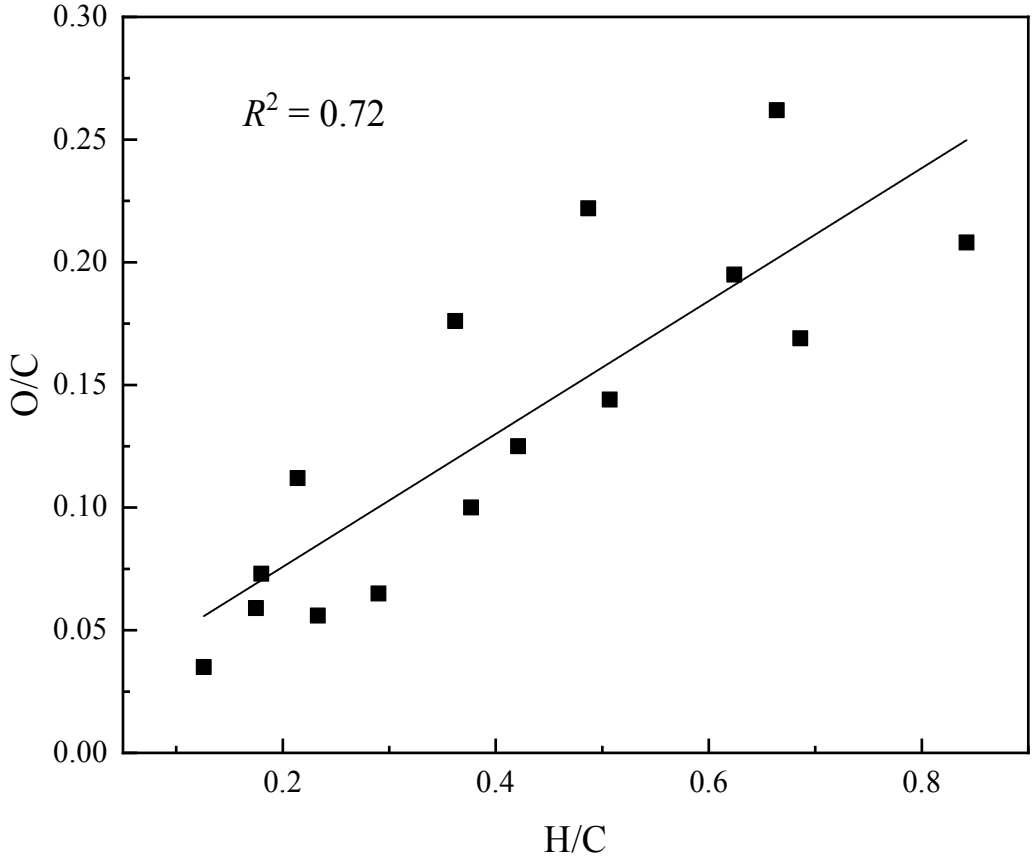


Fig. S3 FTIR spectra of the biochars from different biomass.

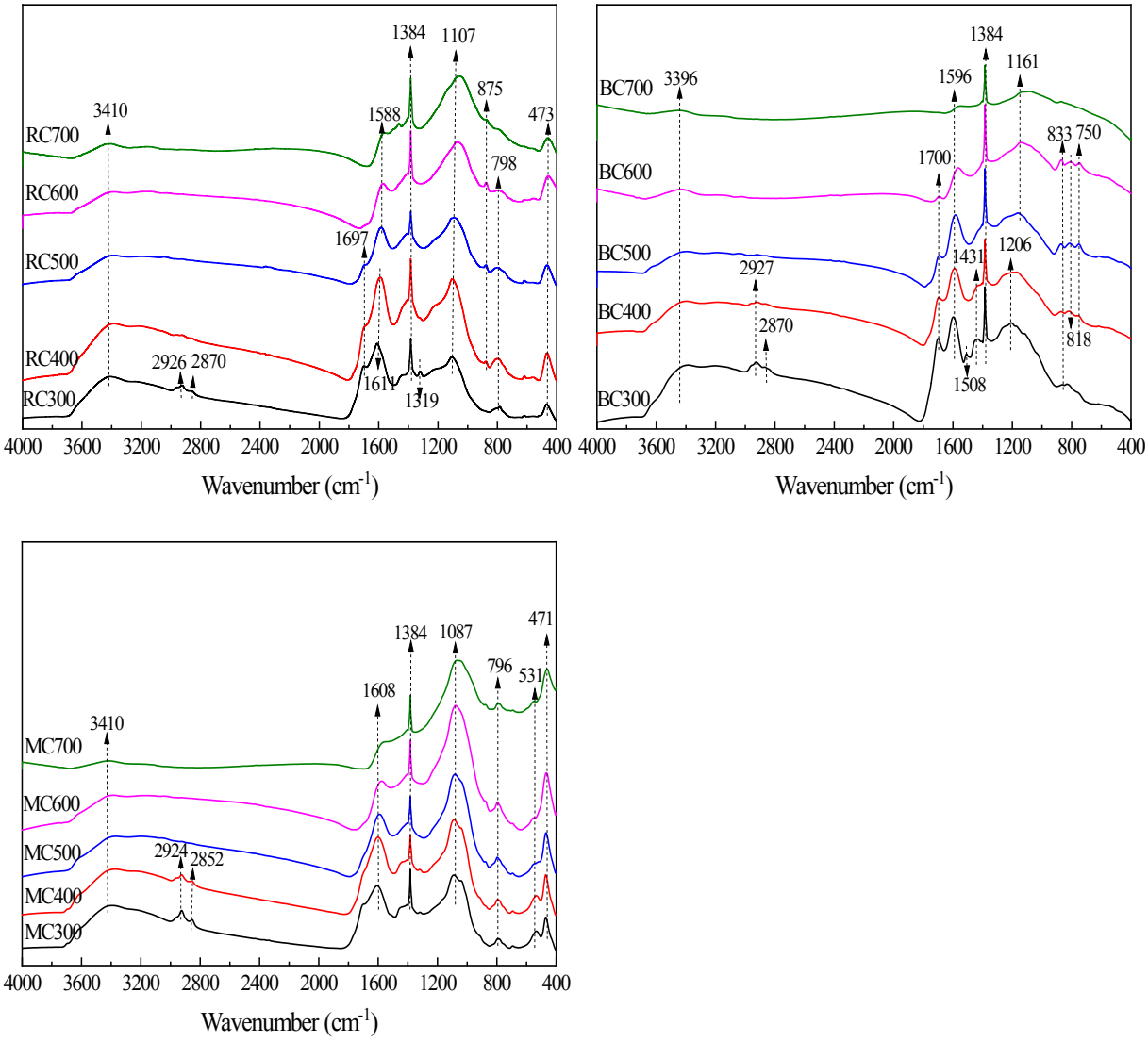


Fig. S4 Adsorption isotherms of ATZ on RC300–700, BC300–700, and MC300–700.

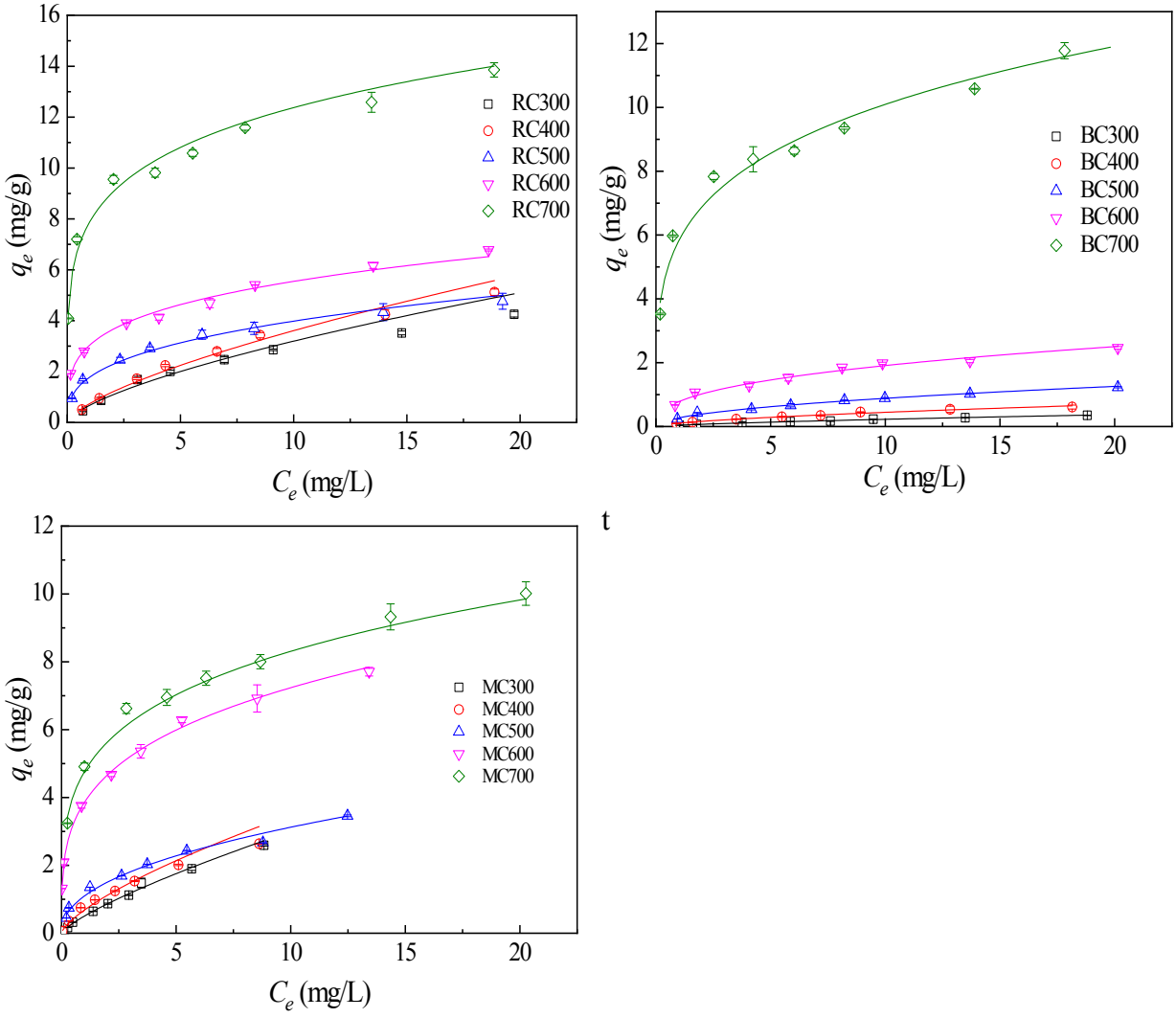


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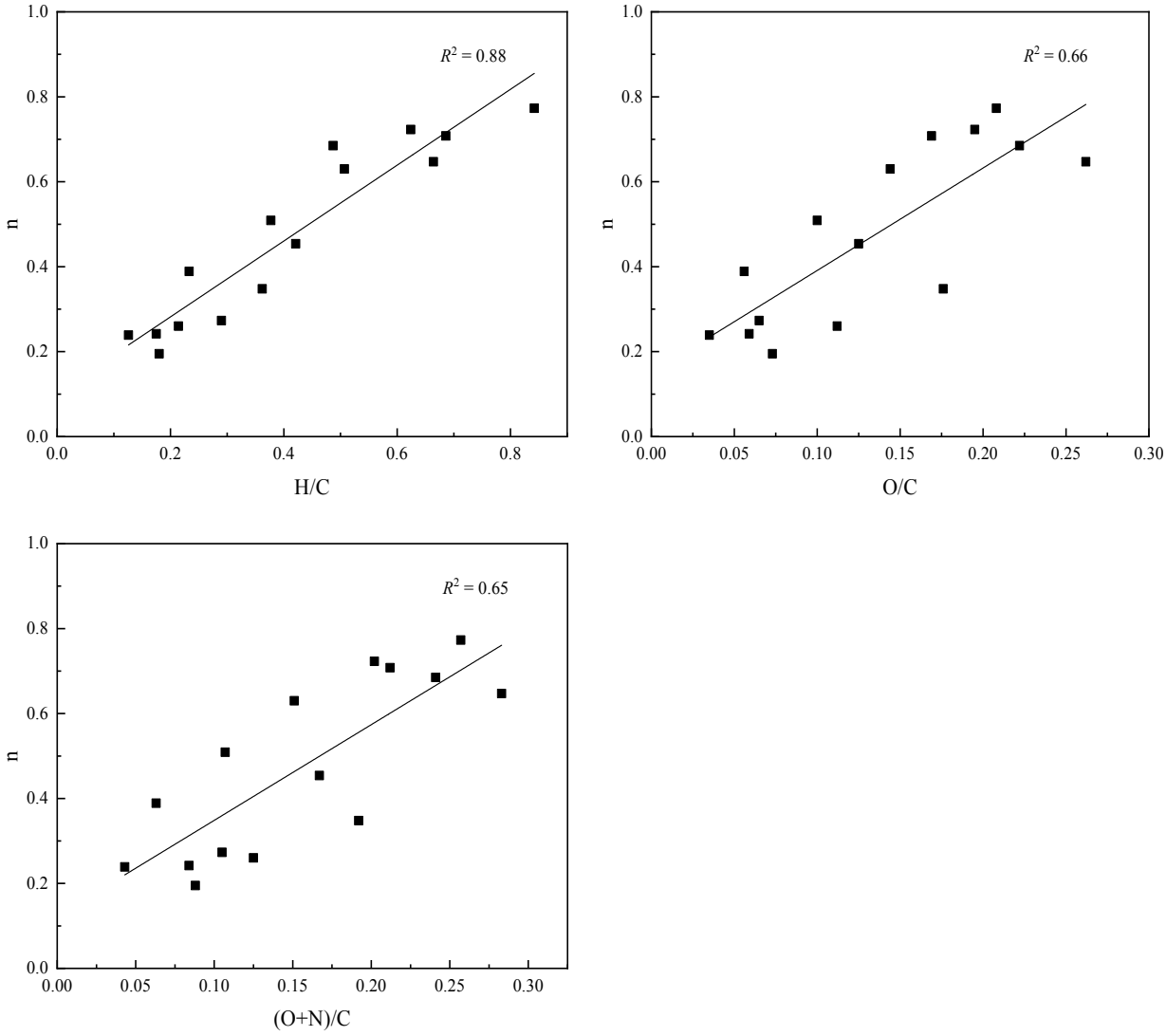
Fig. S5 Correlations between n values of ATZ adsorption on biochars and H/C, O/C, and (O + N)/C atomic ratio of the biochars.



Biochars production. Briefly, the ground rice straws, bamboo, and cow manure were placed into a lab-scale tubular reactor within a muffle furnace and pyrolyzed at 300–700°C under a N_2 atmosphere with a heating rate of 15°C min^{-1}. The solid residues in the reactor were rinsed with deionized water several times to remove water-soluble matter, dried at 105°C for 24 h and homogenized to pass through a 0.15 mm sieve. The obtained biochars were denoted as RCX, BCX, and MCX, where RC, BC, and MC referred to rice straw biochar, bamboo biochar, and cow manure biochar, respectively, and X referred to the pyrolysis temperature.