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Article

Effects of salinity, pH, and Cu (II) on the adsorption behaviors of tetracycline onto polyvinyl chloride microplastics: the site energy distribution analysis

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Supplementary Materials

Text. S1 SED frequency function F(E*)

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$$F(E^*) = \frac{Q_g n(k_{LF}C_s)^n}{RT} \exp\left(\frac{-nE^*}{RT}\right)[1 + (k_{LF}C_s)^n \exp\left(\frac{-nE^*}{RT}\right)]^{-2} \quad \text{(S1)}$$

Eq. (S1) can be used to determine the SED curves (F(E*)-E*). In general, the number of adsorption sites can be determined by calculating the area under the SED curve, which also represents the maximum adsorption capacity. The SED curve's peak value F(E0*) denotes the most dispersed energy at the adsorption site. The peak value corresponds to the horizontal axis value of E0*, which de-notes the most distributed energy on the adsorbent surface. E0* can be calculated using the formula Eq (S2).

$$E_0{}^* = RT\ln(k_{LF}C_s) \quad \text{(S2)}$$

Additionally, there are two types of adsorption sites on the adsorbent surface, namely high-energy and low-energy sites. Here, the right side of E_0* is the high-energy area and the left side is the low-energy area.

Text. S2. The calculation of relative crystallinity

The crystallinity was calculated via relative crystallinity equation (Eq. S3).

$$Xc = lc\ (lc + la) \times 100\% \quad \text{(S3)}$$

Where, lc is the diffraction integral intensity of the crystalline part, la is the diffraction integral intensity of the amorphous part.

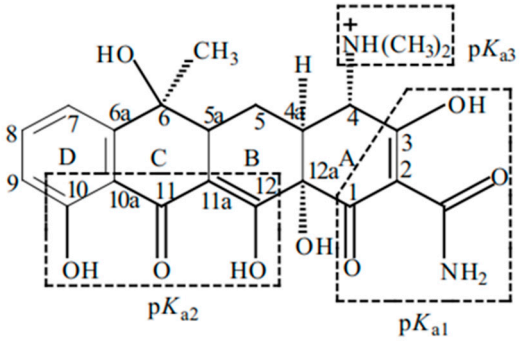

Figure S1. Molecular structure of tetracycline (TC).

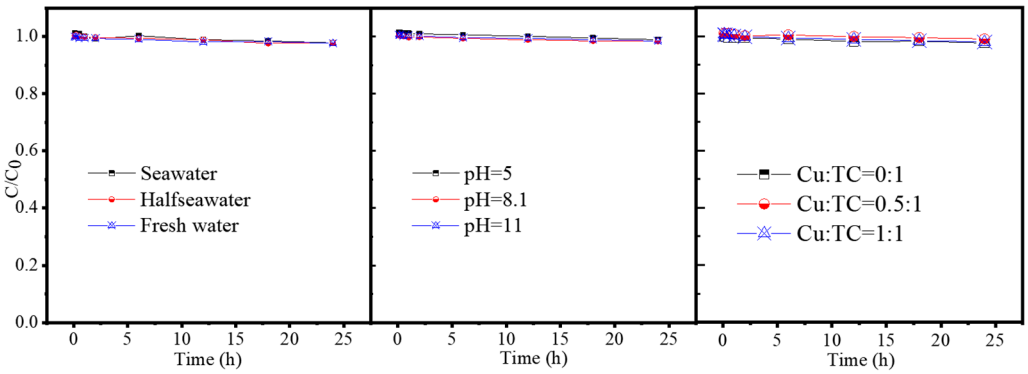

Figure S2. The control experiments for all explored conditions.

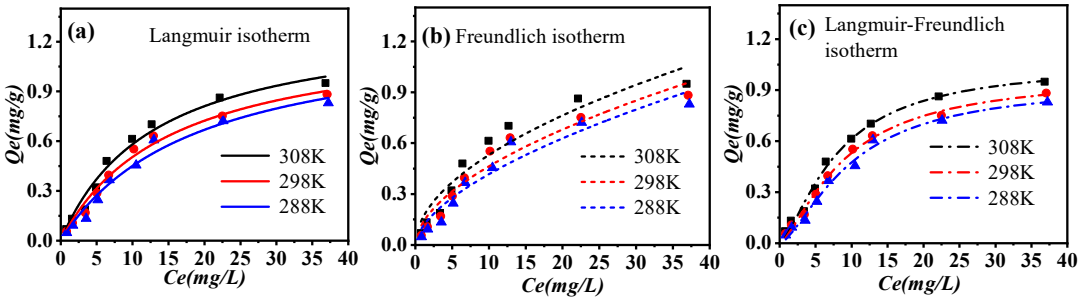

Figure S3. The sorption isotherm of virgin and aged PVC MPs at three temperatures.

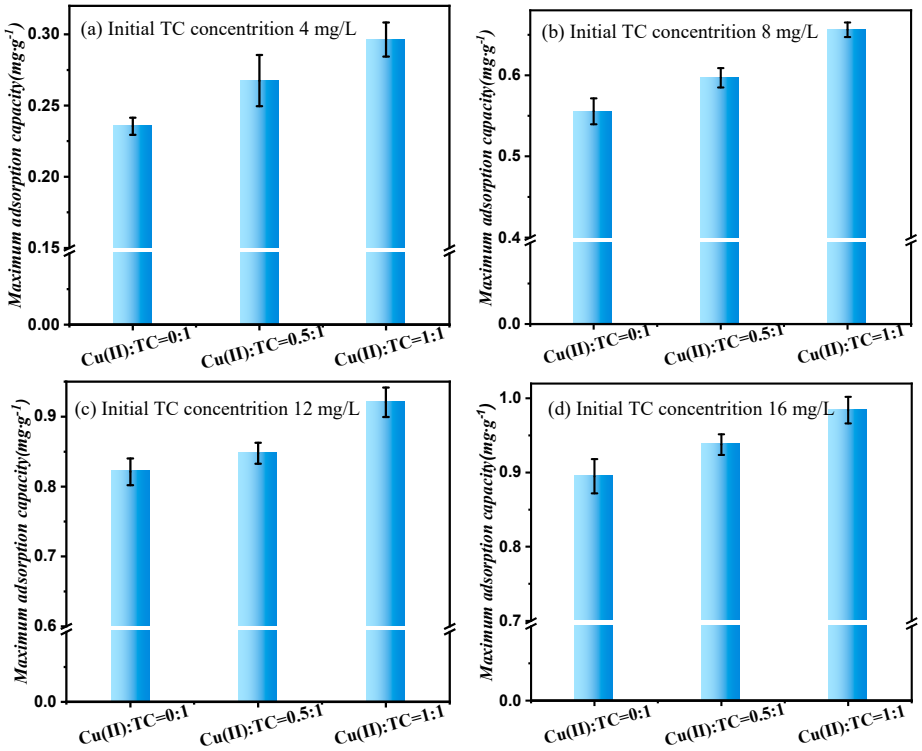

Figure S4. The adsorption of TC onto PVC MPs in the presence of Cu^{2+}.

Table S1. The results of BET test.

Microplastics	BET surface area (m^2/g)	Single point pore volume (cm^3/g)	Average pore size (nm)
PVC-MPs	1.9413	0.003113	6.4147

Table S2. Parameters for three sorption isotherms of virgin and aged PVC MPs and TC at three temperatures.

T (K)	Langmuir Isotherm				Freundlich Isotherm				Langmuir- Freundlich Isotherm				
	Q_m/mg·g^{-1}	k_L/L·mg^{-1}	R^2	Adjust R^2	k_F/mg·g^{-1}	1/n	R^2	Adjust R^2	Q_g/mg·g^{-1}	n	K_{LF}/L·mg^{-1}	R^2	Adjust R^2
288K	1.293	0.0536	0.978	0.971	0.107	0.591	0.939	0.919	0.943	1.507	0.101	0.990	0.987
298K	1.275	0.0656	0.985	0.980	0.129	0.554	0.943	0.924	0.990	1.423	0.111	0.995	0.993
308K	1.339	0.0768	0.980	0.973	0.159	0.524	0.930	0.907	1.061	1.447	0.124	0.991	0.988

Table S3. The parameters of sorption kinetics for PVC MPs adsorbing TC.

MPs	T (K)	Pseudo-first order				Pseudo-second order			
		k_1/h^{-1}	Q_e/mg·g^{-1}	R^2	Adjust R^2	k_2/mg·(g·h$^{0.5}$)$^{-1}$	Q_e/mg·g^{-1}	R^2	Adjust R^2
PVC	288K	3.726	0.367	0.670	0.56	14.696	0.387	0.868	0.824
	298K	3.225	0.400	0.767	0.689	11.440	0.423	0.919	0.892
	308K	3.564	0.481	0.713	0.617	10.811	0.507	0.895	0.860

Table S4. The SED parameters of PVC MPs adsorbing TC in three salinity systems.

MPs	Salinity	E_0^*	$F(E_0^*)$	$\mu(E^*)$	$\sigma(E^*)$
PVC	Freshwater	19.974	174.532	20.971	2.729
	Half of seawater	19.871	160.967	20.969	2.718
	Seawater	19.740	142.153	20.948	2.702