Supplementary material

Adsorption of arsenite to polystyrene microplastics in the presence of humus

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1. Material and Methods

1.4 Mathematical model

The following formula represents the content of adsorption:

$$Q = (C_0 - C_e) \times V/m \quad (2)$$

where Q ($mg \cdot g^{-1}$) indicates the amount of As(III) adsorbed by PSMPs; C_0 and C_e ($mg \cdot L^{-1}$) represent the initial concentration and equilibrium concentration in solution; V (L) represents the total volume, and m (g) represents the mass of PSMPs in the reaction system.

The adsorption kinetics were fitted using an intraparticle diffusion model.[1,2]

Intraparticle diffusion: $Q = k_p t^{1/2}$ (3)

Where k_p ($g \cdot mg^{-1} \cdot min^{-0.5}$) is the intraparticle diffusion rate coefficient, indicating the adsorption rate.

The Langmuir,[3] Sips,[4] and Toth models[5] were used to fit the adsorption isotherms.

Langmuir: $Q = (Q_m C_e K_L)/(1 + C_e K_L)$ (4)

Sips: $Q = Q_m (K_S C_e)^s/(1 + (K_S C_e)^s)$ (5)

Toth: $Q = Q_m C_e K_T/(1 + (K_T C_e)^t)^{1/t}$ (6)

Where K_L ($L \cdot mg^{-1}$), K_S ($L \cdot mg^{-1}$), and K_T ($L \cdot mg^{-1}$) are the isotherm constants of Langmuir, Sips, and Toth, respectively; t and s represent Toth and Sips model heterogeneity parameters, respectively; Q_m represents the maximum adsorption capacity.

The Gibbs–Helmholtz and van't Hoff equations were used to analyze thermodynamic parameters.[6]

Gibbs–Helmholtz: $\Delta G = -RTlnk$ (7)

van 't Hoff: $\Delta G = \Delta H - T\Delta S$ (8)

Where R is the gas constant (8.314 $J \cdot mol^{-1} \cdot K^{-1}$), T (K) is the temperature, and k is the equilibrium constant; ΔG ($kJ \cdot mol^{-1}$), ΔH ($kJ \cdot mol^{-1}$) and ΔS ($kJ \cdot mol^{-1} \cdot K^{-1}$) represent Gibbs free energy, enthalpy, and entropy changes, respectively.

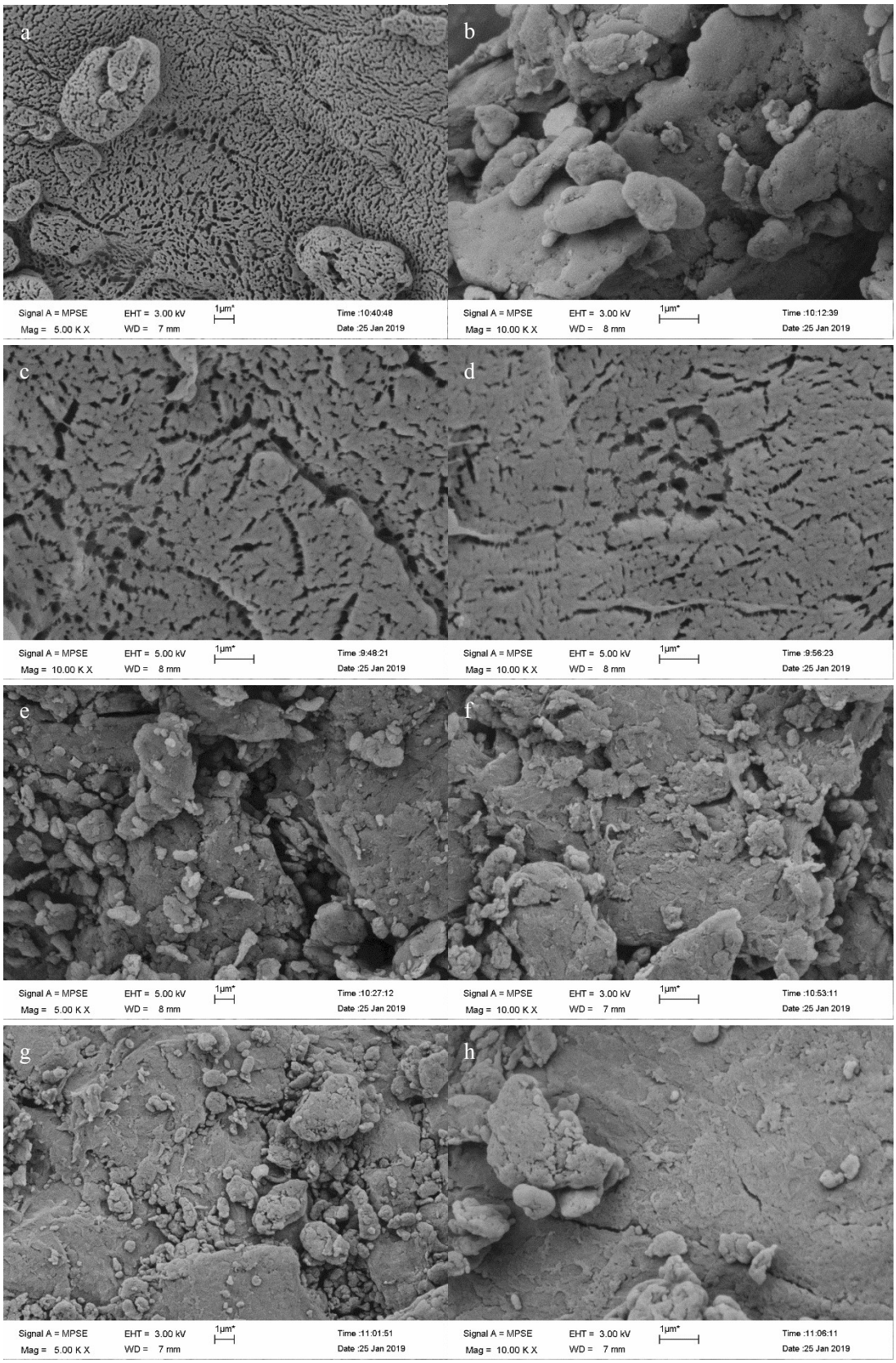

Figure. S1. Scanning electron microscope of PSMP before adsorption (a) and after adsorption under HAFA0 (b), HA20 (c), FA20 (d), HA40 (e), FA40 (f), HA60 (g), and FA60 (h) treatment.

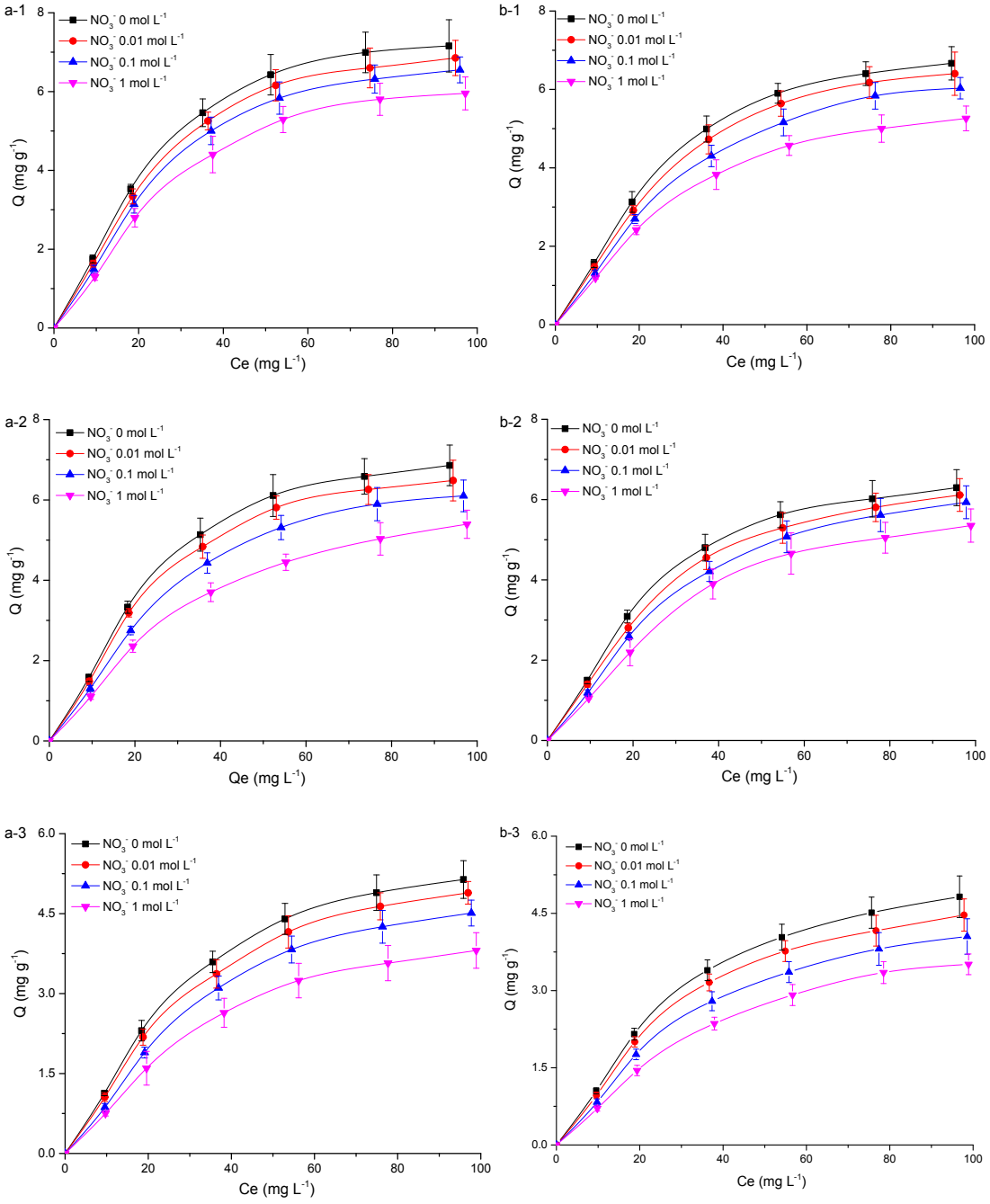

Figure. S2. Effect of ionic strength on the adsorption of As(III) on PSMP in fulvic and humic acid presence; a-1, a-2 and a-3 indicate HA concentrations of 20, 40 and 60 mg L^{-1}, b-1, b-2 and b-3 indicate FA concentrations of 20, 40 and 60 mg L^{-1}

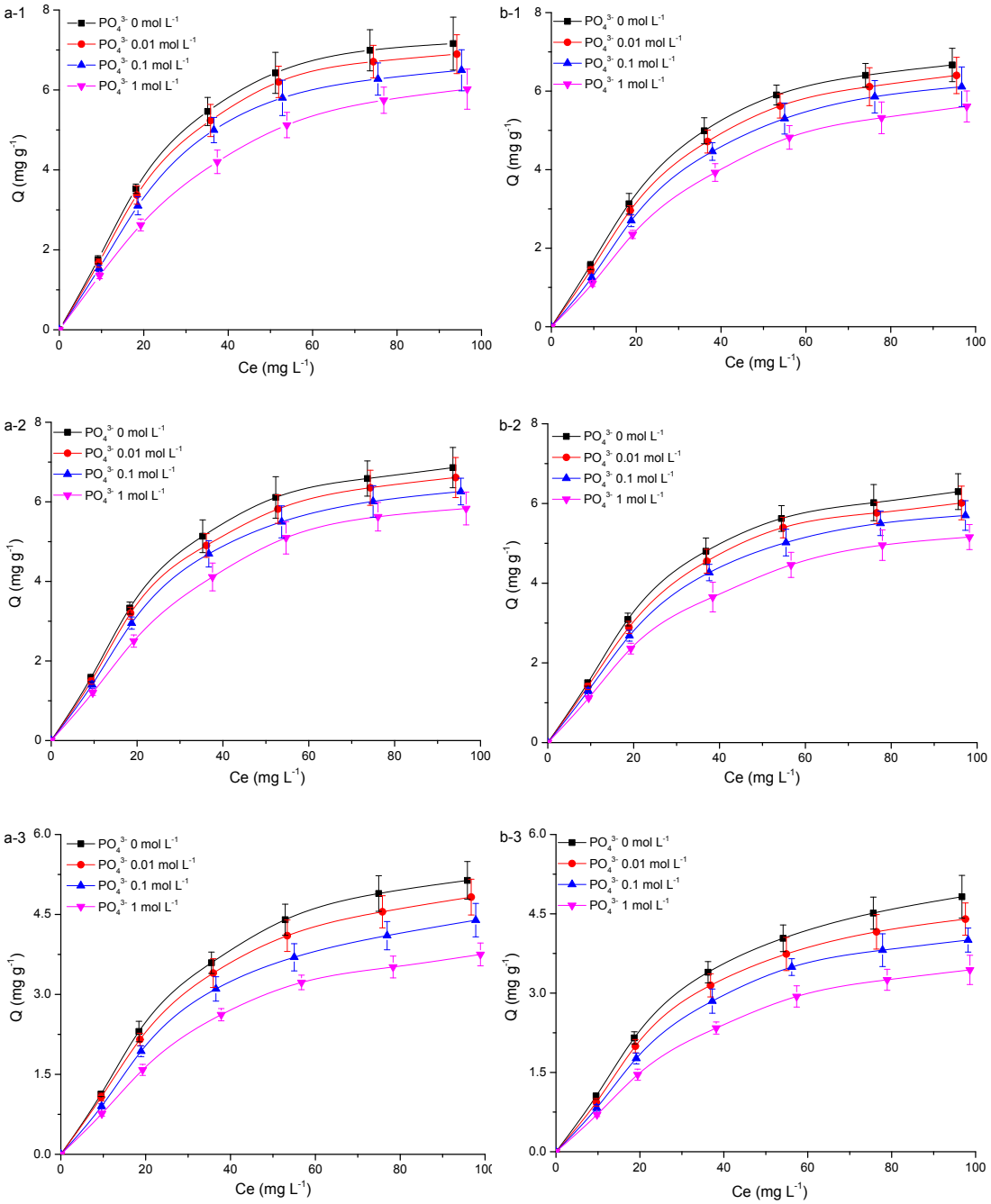

Figure. S3. Effect of competitive ion on the adsorption of As(III) on PSMP in fulvic and humic acid presence; a-1, a-2 and a-3 indicate HA concentrations of 20, 40 and 60 mg L^{-1}, b-1, b-2 and b-3 indicate FA concentrations of 20, 40 and 60 mg L^{-}

Table S1 Characteristics of PSMP of As(III) adsorption on PSMP in humic and fulvic acid presence

	pH_{PZC}	SSA ($m^2 g^{-1}$)	APD (nm)	PV ($cm^3 g^{-1}$)
PSMP	5.1±0.4	8.51	18.89	$2.83*10^{-3}$
HAFA0	4.7±0.3	8.28	18.22	$2.71*10^{-3}$
HA20	4.5±0.3	7.92	16.93	$2.52*10^{-3}$
HA40	4.0±0.3	7.41	16.12	$2.20*10^{-3}$
HA60	3.6±0.2	6.58	14.83	$2.08*10^{-3}$
FA20	4.8±0.3	8.11	17.31	$2.61*10^{-4}$
FA40	4.4±0.2	7.58	16.48	$2.36*10^{-4}$
FA60	3.8±0.4	6.82	15.05	$2.17*10^{-4}$

PSMP represents the PSMP before adsorption, HAFA0, HA20 (FA20), HA40 (FA40), and HA60 (FA60), respectively, representing the PSMP after adsorption of As under the conditions of 0, 20, 40, and 60 mg L^{-1} HA (FA).

Table S2 Intraparticle diffusion model parameters of As(III) adsorption on PSMP in humic and fulvic acid presence

		HAFA0	HA20	HA40	HA60	FA20	FA40	FA60
stage1	k_p ($g \cdot mg^{-1} \cdot min^{-0.5}$)	0.006	0.113	0.110	0.046	0.078	0.070	0.037
	R^2	0.869	0.992	0.998	0.897	0.980	0.964	0.879
stage2	k_p ($g \cdot mg^{-1} \cdot min^{-0.5}$)	0.027	0.246	0.233	0.144	0.221	0.199	0.130
	R^2	0.637	0.879	0.870	0.795	0.845	0.789	0.787
stage3	k_p ($g \cdot mg^{-1} \cdot min^{-0.5}$)	0.035	0.208	0.199	0.131	0.193	0.181	0.119
	R^2	-541.7	-12911	-2342	-431.7	-314.2	-3588	-3013

Table S3 Thermodynamics parameters for the adsorption of As(III) on PSMP in humic and fulvic acid presence

	k			ΔG (kJ mol^{-1})			ΔH	ΔS
	288	298	308	288	298	308	(kJ mol^{-1})	(kJ mol^{-1})
HA20	0.682	0.619	0.755	-0.916	-1.190	-0.720	-0.39	-0.010
HA40	0.667	0.670	0.797	-0971	-0.993	-0.581	-6.66	-0.020
HA60	0.638	0.781	0.885	-1.076	-0.614	-0.312	-12.06	-0.038
FA20	0.670	0.680	0.839	-0.959	-0.955	-0.451	-8.36	-0.025
FA40	0.639	0.668	0.961	-1.088	-1.001	-0.103	-15.40	-0.049
FA60	0.667	0.808	0.915	-0.968	-0.528	-0.227	-11.62	-0.037

Reference

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