Supplementary Information

Performance of a Zeolite modified with *N,N*-dimethyl dehydroabietylamine Oxide (DAAO) for Adsorption of Humic Acid Assessed in Batch and Fixed Bed Columns

Shaogang Liu[a], Wenzhen Zhang[a] Xuecai Tan [a], Fang Zhao[a], Wanting Huang[a], Hanchun Du[b], Bernard A. Goodman [c], Fuhou Lei[a], Kaisheng Diao[a]*

[a] *Guangxi Key Laboratory of Chemistry and Engineering of Forest Products, Guangxi Colleges and Universities Key Laboratory of Food Safety and Pharmaceutical Analytical Chemistry, School of Chemistry and Chemical Engineering, Guangxi University for Nationalities, Nanning 530008, Guangxi, China*

[b] *Guangxi Center for Analysis and Test Research, Nanning 530022, China.*

[c] *College of Physical Science and Engineering, Guangxi University, Nanning 530004, Guangxi, China*

Table S1

Table S1 Carbon contents of the natural zeolite and DAAO-modified zeolites

Samples	Carbon content (%)
natural zeolite	0.095
SMZ1	2.92
SMZ 2	3.69
SMZ 3	4.75
SMZ 4	5.90
SMZ 5	6.92
SMZ 6	7.52
SMZ 7	7.75

Table S2

Table S2 Isotherm parameters for adsorption of HA on SMZ6 at 20, 30, and 40 °C.

Model	Parameter	Temperature (°C)		
		20	30	40
Langmuir	q_m (mg g^{-1})	126.56	123.12	119.83
	k_L (L g^{-1})	0.38	0.19	0.16
	R^2	0.99	0.99	0.99
Freundlich	K_f	36.14	26.24	23.35
	1/n	0.37	0.43	0.42
	R^2	0.96	0.95	0.96
Temkin	K_T	6.42	2.72	2.24
	B	20.90	22.82	21.74
	R^2	0.98	0.95	0.96

Table S3

Table S3 Thermodynamic parameters for HA adsorption on SMZ6

ΔH^{o}_{ads} (kJ mol^{-1})	ΔS^{o}_{ads} (J K^{-1} mol^{-1})	ΔG^{o}_{ads} (kJ mol^{-1})			R^2
		20 °C	30 °C	40 °C	
−27.93	−71.78	−6.95	−6.04	−5.52	0.985

Table S4

Table S4 Model parameters for SMZ6 fixed-bed columns of different depths

	Adams-Bohart model			Thomas model			Yoon-Nelson model		
Z (cm)	N_0 (mg L^{-1})	$k_{AB} \times 10^{-6}$ (L mg^{-1} min^{-1})	R^2	q_0 (mg g^{-1})	$K_{Th} \times 10^{-4}$ (L mg^{-1} min^{-1})	R^2	$K_{YN} \times 10^{-2}$ (min^{-1})	T (min)	R^2
10	20.78	0.15	0.594	10.77	2.22	0.987	7.54	734	0.981
20	13.98	0.14	0.625	7.61	1.64	0.981	0.55	1040	0.977
30	10.77	0.13	0.647	6.64	1.16	0.976	0.40	1370	0.973

Table S5

Table S5 The calculated constants of BDST model for the adsorption of HA (C_0 = 40 mg L^{-1})

C_t/C_0	a (min cm^{-1})	b (min)	K_a (L mg^{-1} min^{-1})	N_0 (mg L^{-1})	R^2
0.1	17.8	689.1	1.7×10^{-5}	2848	0.998
0.9	91.5	546.9	-2.1×10^{-5}	14640	0.985

Figure S1

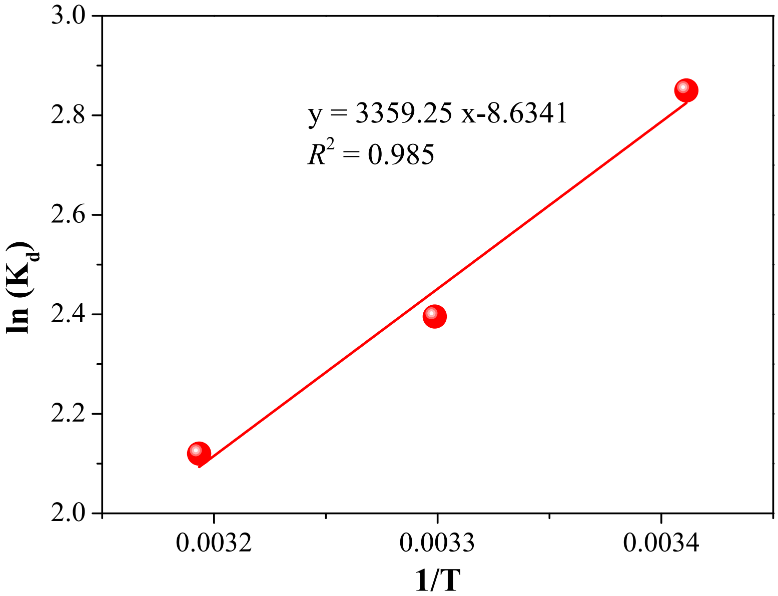

Fig S1. Plots of $\ln K_d$ versus 1/T for adsorption of HA by SMZ6.

Figure S2

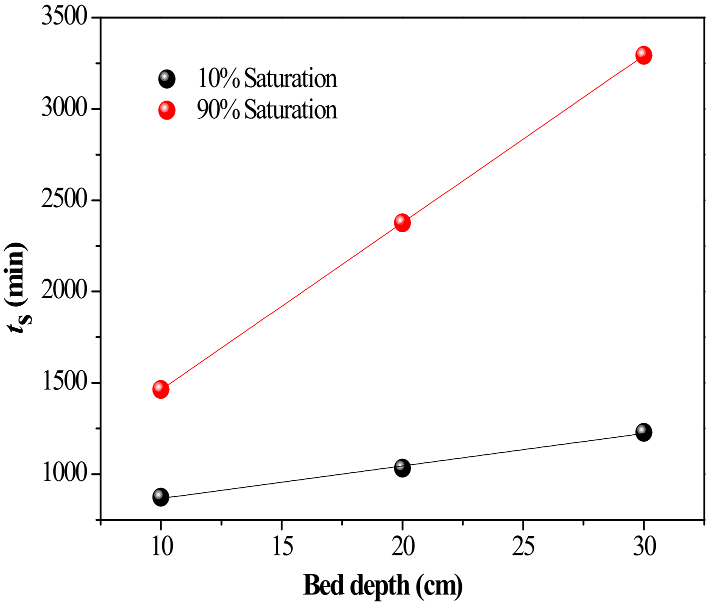

Fig. S2. Bed depth versus service times plots for 10 and 90% saturation of a SMZ6 column with HA. Experimental conditions: [HA] = 40 mg L^{-1}, 5.6 mL min^{-1}

Figure S3

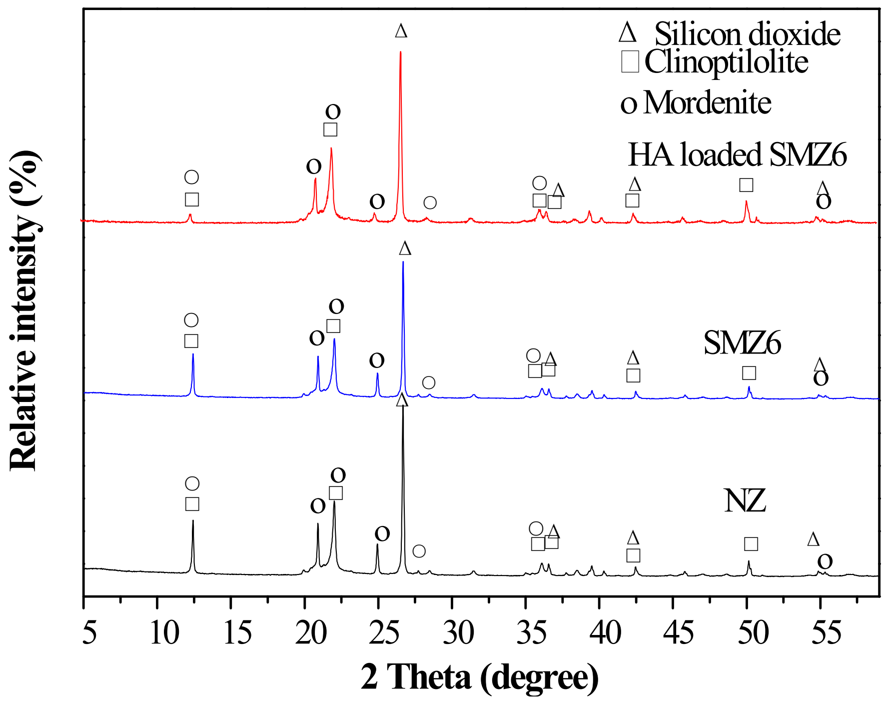

Fig. S3. XRD patterns of the SMZ6 and HA-loaded SMZ6.

Text S1

The Thomas, Adams-Bohart, and Yoon-Nelson models were used to predict the performance of adsorption columns.

Thomas model [1]:

$$\frac{C_t}{C_0} = \frac{1}{1+\exp(K_{\mathrm{Th}} q_0 m / Q - K_{\mathrm{Th}} C_0 t)} \tag{S1}$$

Yoon-Nelson model [2]:

$$\frac{C}{C_0} = \frac{\exp(K_{\mathrm{YN}} t - \tau K_{\mathrm{YN}})}{1+\exp(K_{\mathrm{YN}} t - \tau K_{\mathrm{YN}})} \tag{S2}$$

Adams-Bohart model [3]:

$$\frac{C_{\mathrm{t}}}{C_0} = \exp\left(k_{\mathrm{AB}} C_0 t - k_{\mathrm{AB}} N_0 \frac{Z}{F}\right)$$

(S3) where, K_{Th}, K_{YN}, and k_{AB} are the Thomas rate constant (mL min^{-1} mg^{-1}), Yoon-Nelson rate constant (min^{-1}), and the Adams-Bohart rate constant (min^{-1}), respectively; q_0 is column adsorption capacity (mg g^{-1}), Q is the flow rate (L min^{-1} or mL min^{-1}), and m is the mass of the adsorbent (g). C_0 is the inlet HA concentration (mg L^{-1}), C_{t} is the outlet concentration at time t (mg L^{-1}). τ is the time required for 50% adsorbate breakthrough (min). t is the filtration time (min). N_0 is the saturation concentration of the bed (mg L^{-1}); t_{b} is the service time at breakthrough (h).

References

[1] H.C. Thomas, Heterogeneous ion exchange in a flowing system, *J. Am. Chem. Soc.,* 1944, 66, 1664-1666.

[2] Y. H. Yoon, J.H. Nelson, Application of gas adsorption kinetics—II. A theoretical model for respirator cartridge service life and its practical applications, *Am. Ind. Hyg. Assoc. J.,* 1984, 45, 517-524.

[3] G.S, Bohart, E.Q, Adams, Some aspects of the behavior of charcoal with respect to chlorine, *J. Am. Chem. Soc.,* 1920, 42, 523-544.