Supporting Information

Binary adsorption equilibrium and breakthrough of *n*-butyl acetate and *p*-xylene on granular activated carbon

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Table S1. Physical properties of VOC species.

i component	Formula	Molar mass (g/mol)	Boiling point[a] (℃)	Vapor pressure at 20℃[a] (kPa)	Dipolar moment[b] (D)	Density at 20℃[a] (g/cm^3)
n-butyl acetate	$C_6H_{12}O_2$	116.16	127	1.07	1.85	0.88
p-xylene	C_8H_{10}	106.17	138	0.89	0.02	0.86

[a] data obtained from GESTIS Substance Database.

[b] data obtained from Shanghai Institute of Organic Chemistry of CAS. Chemistry Database [DB/OL].

Table S2. Operating conditions about pure component adsorption (temperature, T, 25 ℃; adsorbent mass, W, 4.9 g; feed flow rate, Q, 0.75 Ndm^3/min ; inlet pressure, P, 120 kPa).

Single adsorbate	Inlet concentration (ppm)
n-butyl acetate	800, 1200, 1800, 2400, 2800, 4600, 5300
p-xylene	800, 1200, 1400, 1800, 2400, 2800, 4200

Table S3. Operating conditions about *n*-butyl acetate/*p*-xylene mixture adsorption (temperature, T, 25 ℃; adsorbent mass, W, 4.9 g; inlet pressure, P, 120 kPa).

Feed flow rate (Ndm^3/min)	Total concentration C_{t0} [a] (ppm)	Feed fraction y_{10} [b]
0.75	2800	0.25
0.75	2800	0.32
0.75	2800	0.39
0.75	2800	0.61
0.75	2800	0.71
0.75	2800	0.82
0.75	2800	0.50
0.75	3400	0.50
0.75	2200	0.50
0.75	1600	0.50
0.45	2800	0.50
0.60	2800	0.50
0.90	2800	0.50

[a] C_{t0} is the sum of the inlet *n*-butyl acetate concentration C_{10} and the inlet *p*-xylene concentration C_{20}.

[b] y_{10} is the mole ratio of *n*-butyl acetate concentration C_{10} to the total concentration C_{t0} in the feed.

Table S4. The fitting parameters of the Y-N model and the predicted penetration time.

VOC species	Initial concentration	k_{YN} ($\times 10^{-3}$ min^{-1})	τ (min)	R^2	t_P [a] (min)
n-butyl acetate	1800	25.5	344	0.998	129
	2400	28.3	307	0.998	104
	4600	42.1	205	0.995	54
	5300	46.3	163	0.999	22
p-xylene	1400	20.5	512	0.996	225
	1800	27.1	363	0.994	139
	2400	34.2	305	0.996	118
	4200	45.4	220	0.999	67

The isosteric heats of adsorption of *n*-butyl acetate and *p*-xylene on activated carbon

Based on the adsorption isotherms of *n*-butyl acetate and *p*-xylene with different temperatures (288 K, 298 K, 308 K), the isosteric heats of adsorption on the activated carbon were calculated by using the Clausius-Clapeyron equation. **Figure S1** shows the isosteric heats of adsorption plotted as a function of adsorption uptake. It is noted that the isosteric heat of adsorption of *p*-xylene on the activated carbon decreases with the increase in the adsorption capacity because of the energetic heterogeneity of the adsorbent surface[1]. However, the isosteric heat of adsorption of *n*-butyl acetate increases with loading, suggesting that the lateral interactions between adsorbed *n*-butyl acetate molecules dominate while the adsorbate-adsorbent interaction energy relatively maintain steady. A similar result for C_2H_6 adsorption on NaX zeolite were reported by Dunne et al.[2]. Most importantly, the adsorption heat of *p*-xylene (47.1-64.2 $kJ \cdot mol^{-1}$) is apparently larger than that of *n*-butyl acetate (9.0-27.5 $kJ \cdot mol^{-1}$). This result indicates that the adsorption affinity of *p*-xylene is greater than that of *n*-butyl acetate on granular activated carbon.

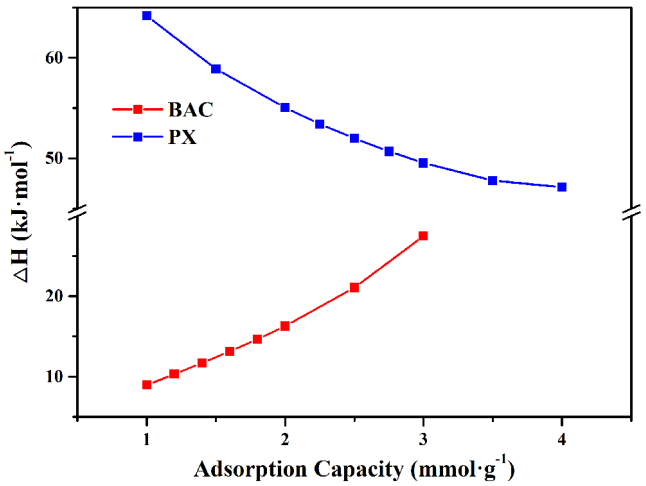

Figure S1. The isosteric heats of adsorption on activated carbon.

Reference

1. Sircar, S.; Cao, D. Heat of adsorption. *Chem. Eng. Technol.* **2002,** *25* (10), 945-948.

2. Dunne, J.; Rao, M.; Sircar, S.; Gorte, R.; Myers, A. Calorimetric heats of adsorption and adsorption isotherms. 2. O2, N2, Ar, CO2, CH4, C2H6, and SF6 on NaX, H-ZSM-5, and Na-ZSM-5 zeolites. *Langmuir* **1996,** *12* (24), 5896-5904.