

Supporting Information

Performance of mesoporous silicas (MCM-41 and SBA-15) and carbon (CMK-3) in removal of gas-phase naphthalene: adsorption capacity, rate and regenerability

Yingshu Liu^a, Ziyi Li^{a,*}, Xiong Yang^a, Yi Xing^{b,**}, Chuenjinn Tsai^c, Quan Yang^a, Zhanying Wang^a, Ralph T. Yang^d

^aSchool of Mechanical Engineering, University of Science and Technology Beijing, Beijing, 100083, China

^bSchool of Civil and Environmental Engineering, University of Science and Technology Beijing, Beijing, 100083, China

^cInstitute of Environmental Engineering, National Chiao Tung University, University Road, Hsinchu, 30010, Taiwan

^dDepartment of Chemical Engineering, University of Michigan, Ann Arbor, Michigan 48109-2136, United States

*Corresponding author

(T) +86-10-62332751; (F) +86-10-62334210. Email: masterlazy@163.com.

**Co-corresponding author:

(T) +86-10-62332206; (F) +86-10-62347649. E-mail address: xing_bkd@163.com.

NO. OF PAGE: 7

NO. OF FIGURES: 2

NO. OF TABLES: 4

S1. Experimental conditions and parameters

The experimental conditions and main parameters are summarized in Table S1 of the Supporting Information.

Table S1. Experimental conditions and main parameters for the adsorption tests.

Parameters	Experimental conditions		
T , bed temperature (K)	398.2		
H , packed length of adsorbents (mm)	100		
d_b , bed diameter (mm)	3.0		
u_0 , gas superficial velocity ($\text{m}\cdot\text{s}^{-1}$)	0.024		
μ , gas dynamic viscosity ($\text{Pa}\cdot\text{s}$)	2.42×10^{-5}		
	MCM-41	SBA-15	CMK-3
ρ_s , solid density ($\text{kg}\cdot\text{m}^{-3}$)	2181	2075	2790
ρ_a , apparent density ($\text{kg}\cdot\text{m}^{-3}$)	730.7	670.3	440.8
ρ , bed density ($\text{kg}\cdot\text{m}^{-3}$)	67.76	79.35	24.66
ε , bed porosity	0.907	0.882	0.944
d_s , adsorbent size (mm)	0.32	0.24	0.12
a , mass-transfer area per unit volume of the bed ($\text{m}^2\cdot\text{m}^{-3}$)	1854	3550	3354

S2. Calibration of flame ionization detector FID measurement

The naphthalene concentrations generated at different saturator temperatures were directly measured by the previous calibrated FID. The calibration procedure is described as follows. A tiny amount of solid naphthalene was weighted and placed in the saturator, M (mg). Then, the temperature of the saturator was increased up to the selected temperature for vapor generation and kept until all the solid was evaporated. In this way, a trapezoid-like curve was obtained with FID, and then the total area under the curve, A (mV·min), can be calculated by the integration method. The area corresponding to 1 μg of evaporated naphthalene, defined as the calibration parameter, F (mV·min· μg^{-1}), was determined to be by averaging the results of five runs as shown in Table S2. Once the FID signal, S (mV), for the vapor naphthalene generated at certain temperature was measured, the feed concentration, C_0 (mol·m⁻³), can be calculated by the equation of $C_0 = S/Q/F/128.18$, with the known Q of 10 ml/min. The FID-determined result for the concentration at the selected generation temperatures in the adsorption text are listed in Table S3.

Table S2. Determinations of FID calibration parameter in five runs.

	1	2	3	4	5	average	RSD (%)
M (mg)	2.96	2.64	2.71	3.17	2.83	—	—
A (mV·min)	86846	68957	74471	95163	78787	—	—
F (mV·min/ μg)	29.34	26.12	27.84	30.02	27.48	28.16	4.92

Table S3. Determinations of the naphthalene concentration at selected generation temperatures.

Temperature (°C)	FID signal (mV)				C_0 (mol·m ⁻³)	RSD (%)
	1	2	3	average		
-10	4.97	5.33	5.18	5.16	1.43×10^{-4}	2.86
0	13.36	11.85	12.83	12.68	3.52×10^{-4}	4.93
10	33.56	34.67	34.4	34.21	9.49×10^{-4}	1.38
15	57.89	61.45	60.72	60.02	1.66×10^{-3}	2.56
20	96.34	101.22	101.33	99.63	2.76×10^{-3}	2.34
25	155.67	161.78	163.48	160.31	4.44×10^{-3}	2.09
30	270.43	278.2	275.23	274.62	7.61×10^{-3}	1.17
40	668.78	689.34	666.82	674.98	1.87×10^{-2}	1.51
50	1653.24	1703.45	1667.83	1674.84	4.64×10^{-2}	1.26

S3. Sensitivity analysis for mass-transfer parameters on the breakthrough curve

A sensitivity analysis was performed to study the effects of mass-transfer parameters on the breakthrough curve. The sensitivity to k_f and k_p on the example case of naphthalene on SBA-15 at feed concentration of $0.352 \times 10^{-3} \text{ mol/m}^3$ are shown in Figs. S1 and S2, respectively. The values of both k_f and k_p were varied from 0.5 to 2 times of the base values while other parameters were kept unchanged. It shows that the breakthrough curve is very sensitive to the internal mass transfer, while increasing or decreasing the value of k_f within the tested range has little effect on the breakthrough curve. This implies that the overall mass transfer for naphthalene adsorption is controlled by internal mass transfer, suggesting the more important internal mass transfer resistance compared to the external mass transfer resistance.

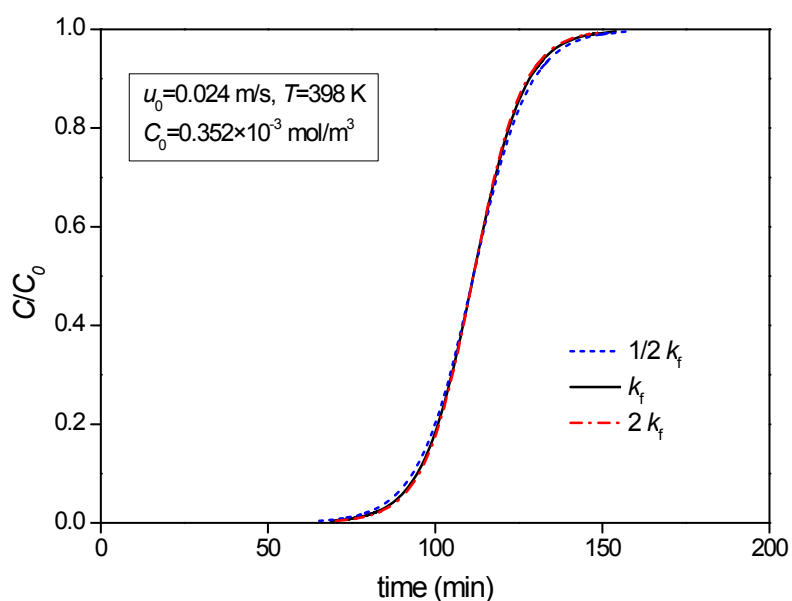


Fig. S1. Sensitivity of predicted breakthrough curves to k_f for naphthalene in SBA-15 packed beds.

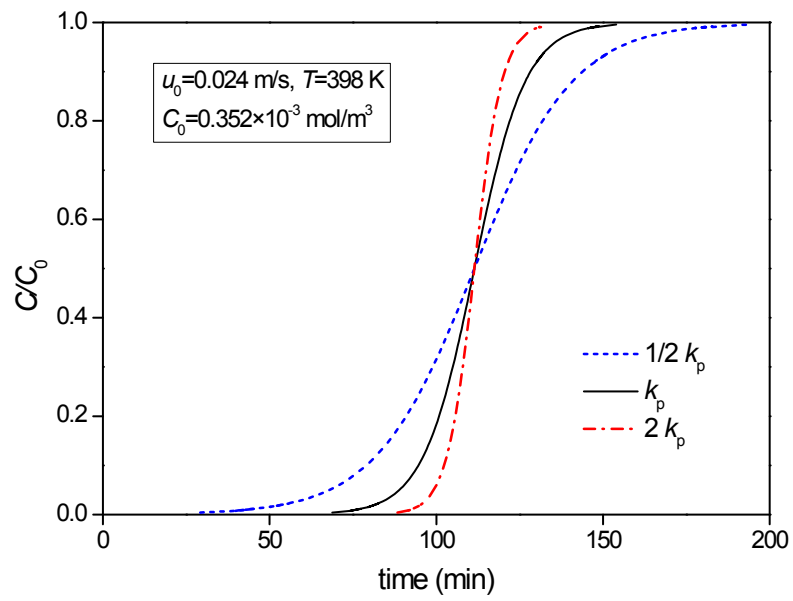


Fig. S2. Sensitivity of predicted breakthrough curves to k_p for naphthalene in SBA-15 packed beds.

S4. Comparisons of the internal mass-transfer from previous studies

The internal mass-transfer coefficients for the current adsorption of naphthalene on mesoporous adsorbents are compared with those for smaller VOCs on traditional adsorbents. The results are listed in Table S4.

Table S4. Comparison of internal mass-transfer coefficient (k_p) between the present results and literature data.

Studies	Samples		C_0 (mol/m ³)	u_0 (m/s)	k_p (s ⁻¹)
	Adsorbate	Adsorbent			
present	naphthalene	MCM-41			7.51×10^{-3}
		SBA-15	2.76×10^{-3}	0.024	9.95×10^{-3}
		CMK-3			7.90×10^{-3}
A ¹	toluene	activated carbon fiber (ACF)	3.04×10^{-3}	0.06	2.54×10^{-5}
B ²	toluene	non-woven ACF	22.9×10^{-3}	0.37	4.69×10^{-5}
	acetone		6.00×10^{-3}		2.42×10^{-4}
C ³	heptane	zeolite	6.00×10^{-3}	0.29	2.71×10^{-4}
	octane		10.0×10^{-3}		1.99×10^{-4}

References

1. X. Zhang, S. Chen and H. T. Bi, *Carbon*, 2010, **48**, 2317-2326.
2. C. Lorimier, A. Subrenat, L. Le Coq and P. Le Cloirec, *Environ. Technol.* 2005, **426**, 1217-1230.
3. S. Brosillon, M. H. Manero and J. N. Foussard, *Environ. Sci. Technol.*, 2001, **35**, 3571-3575.