J. Chem. Eng. Data **1998,** *43,* 843−845

Adsorption of Benzene and Toluene Vapors on Activated Carbon Fiber at 298, 323, and 348 K

Jeong-Ho Yun,* Kyung-Yub Hwang, and Dae-Ki Choi

Division of Environment & CFC Technology, Korea Institute of Science & Technology, P.O. Box 131,
Cheongryang, Seoul 130-650, Korea

The adsorption equilibria for benzene and toluene vapors on commercially available activated carbon fiber were measured by a static volumetric technique. The equilibrium measurements were made at 298.15, 323.15, and 348.15 K and pressures up to 8.7 kPa for benzene and 3.4 kPa for toluene, respectively. The results were correlated by the Dubinin−Astakhov equation, which is a fundamental theoretical relation for describing the filling of micropores.

Introduction

Because of their environmental significance, removal of volatile organic compounds (VOCs) from a bulk gas stream by an adsorption processes a common engineering practice. Activated carbons are the key elements in a number of control technologies designed to remove and recover VOCs from a bulk gas stream. A particularly common application of carbon adsorption is solvent recovery (Ruhl, 1993). For this purpose, activated carbon fiber has been used because of its attractive features, e.g., higher rate of adsorption, higher amount of adsorption than those of granular activated carbon, and ease of handling (Takeuchi et al., 1993).

Among VOCs, benzene derivatives that escape through leakage during operations are harmful to the environment and human health (Macek, 1991; Ruhl, 1993). To design the adsorption facilities, thermodynamic data on adsorption equilibria must be known over a wide range of temperatures. However, there appears to be relatively little information in the literature concerning adsorption of benzene and toluene on activated carbon fiber at various temperatures. In this regard, the present study is devoted to the measurement of adsorption isotherms of benzene and toluene on activated carbon fiber at 298, 323, and 348 K. Also, it should be noted that the data presented were obtained as a part of a continuing study of adsorption of aromatic VOCs on microporous solid (Yun and Choi, 1997).

Experimental Section

Materials. The activated carbon fiber (Toyobo type KF-1500), in felt type, was used as the adsorbent in this study. The physical properties of the activated carbon fiber can be found elsewhere (Tokunaga et al., 1988). Prior to measurement, the sample was kept in a drying vacuum oven at 423 K for more than 24 h to remove impurities.

The benzene and toluene were obtained from J. T. Baker, and the purity of these materials was 99.9%.

Apparatus and Procedure. The experimental apparatus used was a static volumetric type. The total quantity of gas admitted to the system and the amount of gas in the vapor remaining after adsorption equilibrium was established were determined by appropriate $P-V-T$ measurements. The system pressure measurements were made using a Baratron absolute pressure transducer (MKS type 690A13TRA) with a high-accuracy signal conditioner (MKS type 270D). Its pressure range was from 0 to 133.33 kPa and its reading accuracy was ±0.05% within the useable measurement range. During adsorption, the adsorption cell was placed in a water bath and the temperature was maintained constant within ±0.02 K by a refrigerated circulating thermostat (Haake type F3). The experimental temperature was measured with a T-type thermocouple.

To eliminate any trace of pollutants, the activated carbon fiber was kept in a drying oven at 423 K for more than 24 h. Its mass was determined with an accuracy of ±10 μg, and the fiber was introduced into the adsorption cell. Prior to each isotherm measurement, the charged activated carbon fiber was regenerated at 473 K under a high vacuum for 12 h. An oil diffusion pump and a mechanical vacuum pump in combination (Edward type Diffstak 63/150M) provided a vacuum down to 10^{-3} Pa, and the evacuation was monitored by both an ion gauge and a convection gauge with a vacuum gauge controller (Granville-Phillips type 307). The volume of the adsorption cell was determined by expansion of helium gas at the experimental temperature. Details of the equipment and the operating procedures used are described in the previous publication of Yun and Choi (1997).

Results and Discussion

Adsorption of gases and vapors by microporous solids has attracted much attention because of its great practical importance in the fields of gas separation, gas purification, and environmental problems. The design of adsorption facilities requires primarily a knowledge of thermodynamic data on the adsorption equilibria. This information is used to calculate the operation time of a specific bulk concentration level and to derive the optimum size of adsorbers and operating conditions (Yang, 1987). Also, information concerning the relevant adsorption equilibria is an essential requirement for the process simulation.

In this study, the adsorption isotherm data for benzene and toluene on activated carbon fiber at 298, 323, and 348 K were obtained at pressures up to 8.7 kPa for benzene and 3.4 kPa for toluene, respectively. The experimental

---

* To whom correspondence should be addressed. E-mail: jhyun@kistmail.kist.re.kr.

S0021-9568(98)00069-7 CCC: $15.00

Table 1. Experimental Isotherm Data for Benzene on Activated Carbon Fiber (KF-1500)

P/kPa	N/mmol g^{-1}	P/kPa	N/mmol g^{-1}
298.15 K			
0.0036	0.719	0.3100	5.234
0.0073	1.124	0.3572	5.424
0.0100	1.402	0.4944	5.768
0.0124	1.652	0.6029	5.987
0.0199	2.106	0.7677	6.173
0.0201	2.162	0.8556	6.272
0.0303	2.533	1.1576	6.427
0.0311	2.592	1.1744	6.443
0.0480	3.005	1.4373	6.532
0.0484	3.067	1.7413	6.578
0.0748	3.543	2.3040	6.695
0.0859	3.670	2.5987	6.706
0.1316	4.176	3.5573	6.820
0.1348	4.226	3.6253	6.846
0.2095	4.750	4.5347	6.918
0.2223	4.837		
323.15 K			
0.0045	0.459	0.4575	3.951
0.0119	0.961	0.6883	4.382
0.0196	1.172	0.7376	4.428
0.0249	1.300	1.0927	4.971
0.0361	1.608	1.1744	5.014
0.0579	1.973	1.5493	5.323
0.0637	2.079	1.5640	5.378
0.0956	2.441	2.0573	5.654
0.1012	2.464	2.2067	5.765
0.1519	2.714	2.7853	5.966
0.1727	2.860	3.2000	6.091
0.2141	3.080	4.0213	6.273
0.2848	3.427	4.6360	6.322
0.3031	3.527	5.5933	6.445
0.4511	3.890	7.2413	6.616
348.15 K			
0.0072	0.428	0.9243	3.302
0.0275	0.873	1.5067	3.843
0.0668	1.256	2.4147	4.404
0.1325	1.652	3.6760	4.913
0.2117	1.970	5.3093	5.375
0.3053	2.253	6.6800	5.646
0.4171	2.523	8.7146	5.905
0.5600	2.797		

equilibrium data are presented in Tables 1 and 2. The adsorption equilibrium isotherms of benzene and toluene on activated carbon fiber at 298 and 348 K are shown in Figures 1 and 2. At the high-pressure region, the adsorption amount is higher for benzene compared with toluene. At the low-pressure region, however, the adsorption amount is higher for toluene compared with benzene, implying that the adsorption affinity is higher for toluene compared with benzene.

For practical applications, the adsorption equilibrium data should be represented by mathematical equations. Adsorption of gases and vapors by microporous solids such as activated carbon fiber can be described by the equation of Dubinin and Astakhov (Stoeckli et al., 1982). It has been reported that the Dubinin–Astakhov equation has found utility in interpreting adsorption by capillary condensation or pore filling (Stoeckli et al., 1982; Agarwal and Schwarz, 1988)

$$W = W^0 \exp\left[-\left(\frac{\epsilon}{\beta E^0}\right)^r\right], \quad W = NV^0 \qquad (1)$$

where W is the specific volume of adsorbate condensed in micropores at temperature T and relative pressure P^*/P (P^* is the equilibrium saturation vapor pressure at T), W^0 is the limiting specific volume of the adsorbed space, which equals the micropore volume, N is the moles adsorbed at equilibrium, $\epsilon = \Delta G = RT\ \ln(P^*/P)$, β is the affinity coefficient, V^0 is the saturated liquid molar volume, and r and E^0 are the specific parameters of the system investigated.

Table 2. Experimental Isotherm Data for Toluene on Activated Carbon Fiber (KF-1500)

P/kPa	N/mmol g^{-1}	P/kPa	N/mmol g^{-1}
298.15 K			
0.0035	1.470	0.6613	5.758
0.0069	2.344	0.9241	5.798
0.0153	3.257	1.1604	5.817
0.0349	4.083	1.4733	5.835
0.0867	4.877	1.6280	5.847
0.3285	5.533	1.8267	5.857
0.3435	5.550		
323.15 K			
0.0073	1.369	0.6704	5.089
0.0151	2.090	0.8959	5.248
0.0295	2.585	0.9497	5.270
0.0568	3.212	1.2779	5.373
0.1100	3.747	1.3400	5.393
0.1852	4.178	1.8013	5.488
0.2904	4.545	2.3787	5.563
0.4388	4.805	2.4467	5.585
0.4497	4.854	3.0920	5.684
0.6239	5.075		
348.15 K			
0.0145	1.241	0.4953	3.827
0.0165	1.264	0.6609	4.022
0.0349	1.779	0.6815	4.101
0.0405	1.879	0.8821	4.271
0.0756	2.295	0.9024	4.347
0.0757	2.317	1.1431	4.496
0.1323	2.694	1.1539	4.553
0.1373	2.752	1.4893	4.713
0.2096	3.092	1.5293	4.765
0.2140	3.120	2.1040	4.957
0.3273	3.432	2.6720	5.117
0.3377	3.506	3.4347	5.335
0.4716	3.734		

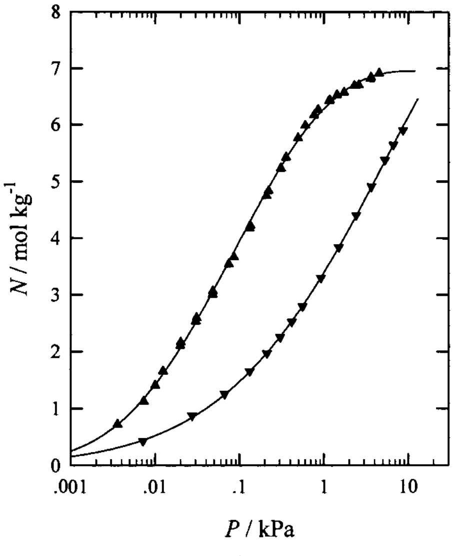

Figure 1. Adsorption isotherms for benzene on activated carbon fiber (KF-1500) at 298 and 348 K: ▲, 298 K; ▼, 348 K; —, Dubinin–Astakhov equation.

For the nonpolar and weakly polar adsorbates, the adsorption interaction is strongly dependent on the polarizability of the molecules. Since the polarizability of a molecule is approximately proportional to the molar volume of the saturated liquid, the affinity coefficient can be expressed as (Noll et al., 1989)

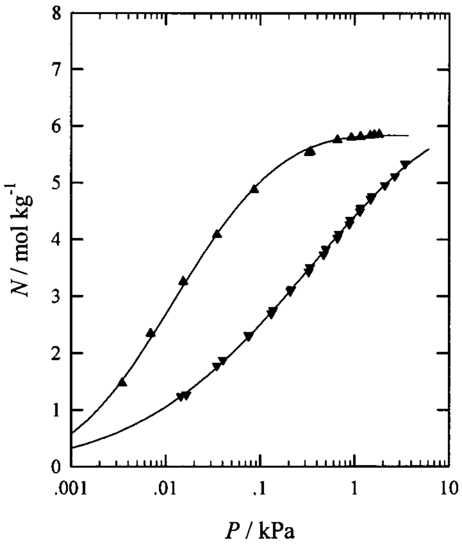

Figure 2. Adsorption isotherms for toluene on activated carbon fiber (KF-1500) at 298 and 348 K: ▲, 298 K; ▼, 348 K; —, Dubinin–Astakhov equation.

$$\beta = V^0/V^0_{\mathrm{ref}} \tag{2}$$

where V^0_{ref} is the saturated liquid molar volume of the reference vapor. In this study, benzene vapor was chosen as the reference vapor. To calculate the saturated liquid molar volume, the modified Rackett equation was used (Reid et al., 1986).

The parameters of the Dubinin–Astakhov equation were determined from the best fit to the experimental data, and they are summarized in Table 3 along with the average absolute deviation parameter *D*.

$$D = \frac{1}{k}\sum_{i=1}^{k}\left|\frac{N_i^{\mathrm{obs}} - N_i^{\mathrm{cal}}}{N_i^{\mathrm{obs}}}\right|, \quad k = \text{number of data} \tag{3}$$

The solid lines in Figures 1 and 2 denote the calculated adsorption isotherms from the Dubinin–Astakhov equation. As can be seen, the agreement of the experimental data points with the calculated isotherms is excellent.

The correlation by the Dubinin–Astakhov equation has a great utility in that it can provide a determination of the total micropore volume of the adsorbent. As shown in Figure 3, the total micropore volume can be estimated according to the Dubinin–Astakhov equation, and its value is approximately 625 $\mathrm{cm^3\ kg^{-1}}$.

Conclusion

The adsorption equilibria for benzene and toluene at 298, 323, and 348 K were measured on activated carbon fiber at pressures up to 8.7 kPa for benzene and 3.4 kPa for toluene, respectively. The experimental equilibrium data were satisfactorily correlated using the Dubinin–Astakhov equation, which is a fundamental theoretical relation for describing the filling of micropores. Also, the Dubinin–Astakhov equation was used to determine an estimate of the total micropore volume of activated carbon fiber from the measurements.

Table 3. Dubinin–Astakhov Equation Parameters and Physical Properties of Benzene and Toluene on Activated Carbon Fiber (KF-1500)

	T/K	W^0/ $\mathrm{cm^3\ kg^{-1}}$	*E*/ $\mathrm{kJ\ mol^{-1}}$	*r*	β	V^0/ $\mathrm{cm^3\ mol^{-1}}$	100*D*
benzene	298.15	624.5	14.86	2.654	1.000	89.74	1.305
	323.15	665.7	15.11	2.077	1.000	92.43	1.984
	348.15	760.4	14.20	1.636	1.000	95.43	0.803
toluene	298.15	623.5	15.86	3.328	1.190	106.8	1.143
	323.15	628.1	17.62	2.646	1.187	109.8	0.899
	348.15	676.6	17.88	2.058	1.184	113.0	0.787

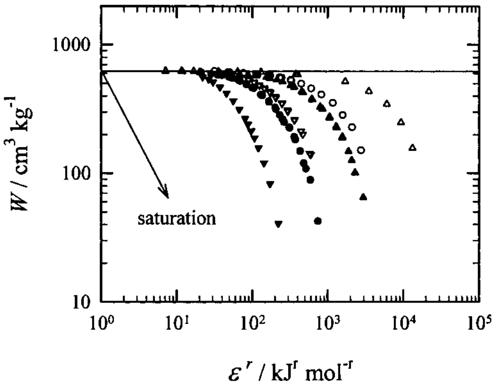

Figure 3. Saturation volume of activated carbon fiber (KF-1500) for benzene and toluene at various temperatures: (▲) 298 K, benzene; (●) 323 K, benzene; (▼) 348 K, benzene; (△) 298 K, toluene; (○) 323 K, toluene; (▽) 348 K, toluene.

Literature Cited

Agarwal, R. K.; Schwarz, J. A. Analysis of High-Pressure Adsorption of Gases on Activated Carbon by Potential Theory. *Carbon* **1988**, *26*, 873–887.

Macek, S. J. Economical Solvent Recovery. *Chem. Process.* **1991**, March, 28–30.

Noll, K. E.; Wang, D.; Shen, T. Comparison of Three Methods to Predict Adsorption Isotherms for Organic Vapors from Similar Polarity and Nonsimilar Polarity Reference Vapors. *Carbon* **1989**, *27*, 239–245.

Reid, R. C.; Prausnitz, J. M.; and Poling, B. E. *The Properties of Gases & Liquids*, 4th ed.; McGraw-Hill: New York, 1988.

Ruhl, M. J. Recover VOCs via Adsorption on Activated Carbon. *Chem. Eng. Prog.* **1993**, *89*, 37–41.

Stoeckli, H. F.; Lavanchy, A.; Kraehenbuehl, F. Recent Developments in the Context of the Dubinin–Astakhov Equation. *Adsorption at the Gas–Solid and Liquid–Solid Interface*; Elsevier: New York, 1982; pp 201–209.

Takeuchi, Y.; Shigeta, A.; Iwamoto, H. Adsorption of Solvent Vapor Mixture in Air by Activated Carbon Fiber Bed. *Sep. Technol.* **1993**, *3*, 46–52.

Tokunaga, N.; Abe, M.; Nitta, T.; Katayama, T. Adsorption Isotherms of Ethane, Ethylene, and Carbon Dioxide on Activated Carbon Fiber at Elevated Pressures. *J. Chem. Eng. Jpn.* **1988**, *21*, 315–318.

Yang, R. T. *Gas Separation by Adsorption Processes*; Butterworth: Boston, MA, 1987.

Yun, J.-H.; Choi, D.-K. Adsorption Isotherms of Benzene and Methylbenzene on Activated Carbon. *J. Chem. Eng. Data* **1997**, *42*, 894–896.

Received for review March 12, 1998. Accepted June 10, 1998.

JE980069A