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APPENDIX

APPENDIX A

CALCULATION

1. CONCENTRATIONS OF TOLUENE AND O-XYLENE VAPORS

The concentrations of toluene and o-xylene vapors are calculated from the ratio of vapor pressure and total pressure of the system.

For toluene vapor,

vapor pressure of toluene at 30 °C (Perry,1987)		= 50.72 cmH_2O
total pressure of the system is the summation of the atmospheric pressure and the difference level of manometer		= 1037.50 cmH_2O
then, the mole fraction of toluene is	50.72/1037.50	= 0.0489
		≈ 4.89 %mol

For o-xylene vapor,

vapor pressure of o-xylene at 30 °C (Perry, 1987) = 5.60 cmH_2O

total pressure of the system = 1033.50 cmH_2O

then, the mole fraction of o-xylene is 5.60/1033.50 = 0.0054

≈ 0.54 %mol

2. CALCULATION OF ADSORPTION EQUILIBRIUM CONSTANT

From equation 2-19,

$$t_R = \frac{L}{v}\left(1+\left(\frac{1-\varepsilon}{\varepsilon}\right)K\right)$$

The plot of the t_R versus L/v provided the slope, $1 + [(1-\varepsilon)/\varepsilon]K$ which was used adsorption equilibrium constant calculation.

An example of the plot between t_R and L/v are illustrated in Figure A-1.

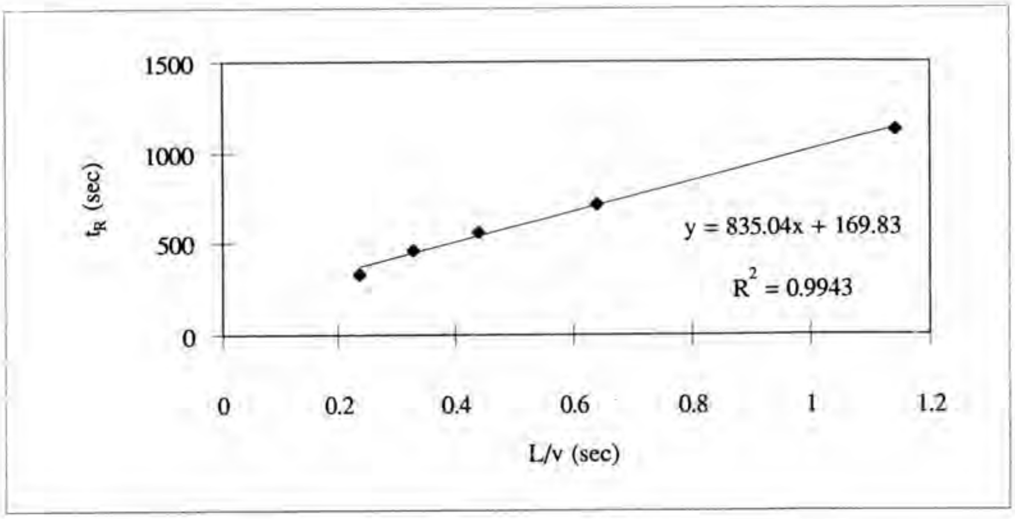

Figure A-1 First moment plot of adsorption of o-xylene on synthesized 4A at 80 °C

Therefore, the adsorption equilibrium constant could be obtained from :

$$K = \frac{slope}{1 + (1-\varepsilon)/\varepsilon}$$

The bed porosity of synthesized the 4A is 0.461, the adsorption equilibrium constant of o-xylene on the synthesized 4A is

$$K = \frac{835.04}{1 + (1-0.461)/0.461}$$

$$= 713.34$$

3. CALCULATION OF HEAT OF ADSORPTION

From the van't Hoff equation (Equation 2-3)

$$\frac{d\ln K}{dT} = \frac{\Delta H}{RT^2}$$

This equation could be integrated with an assumption of constant heat of adsorption (-ΔH) to yeild

$$K = K_0 \exp(-\Delta H / RT)$$

or $$\ln K = \ln K_0 + (-\Delta H / RT)$$

Thus, the heat of adsorption could be obtained from the slope of the plot of ln K with 1/T , as illustrated in Figure A-2.

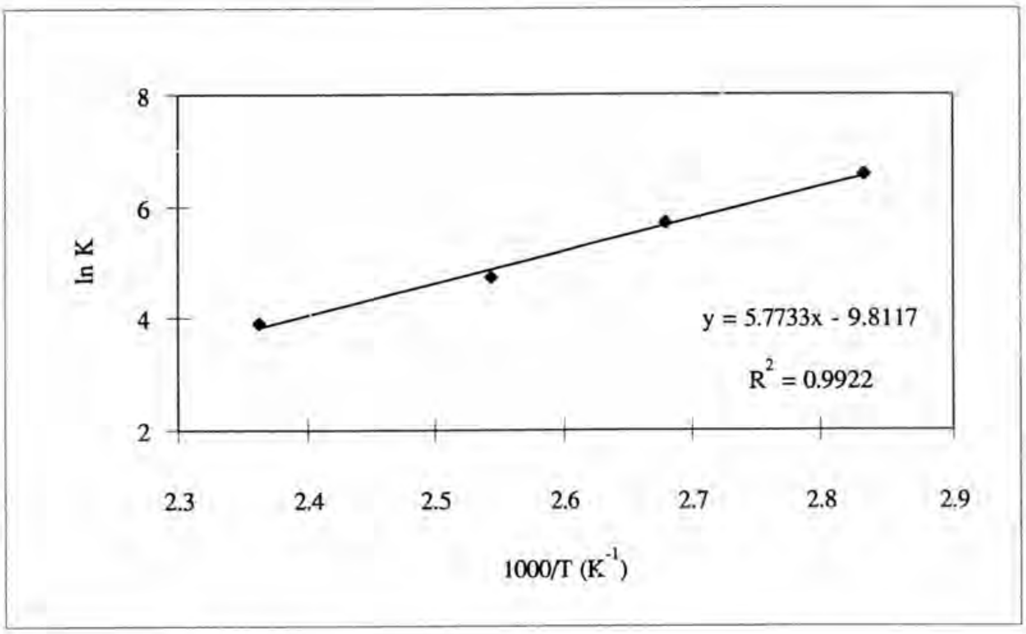

Figure A-2 Adsorption equilibrium constants of o-xylene on synthesized 4A

$$-\Delta H = slope \times R$$

$$= (5773.3\ K) \times (8.314\ J/mol\ K^{-1})$$

$$= 48.00\ kJ/mol$$

4. CALCULATION OF OVERALL MASS TRANSFER COEFFICIENT

According to equation 2-20,

$$\frac{\sigma^2}{2t_R^{\ 2}} = \frac{D_L}{vL} + \frac{v}{L}\left(\frac{\varepsilon}{1-\varepsilon}\right)\frac{1}{kK}\left(1+\frac{\varepsilon}{(1-\varepsilon)K}\right)^{-2}$$

The plots of $(\sigma^2/2t_R^2)(L/v)$ versus $1/v^2$ has yield a straight line providing 2 independent information, i.e. slope of the straight line and 0-intercept. The overall mass transfer coefficient could be determined from the intercept while the slope of the plot has provided useful information for the axial dispersion coefficient determination, as illustrated in Figure A-3.

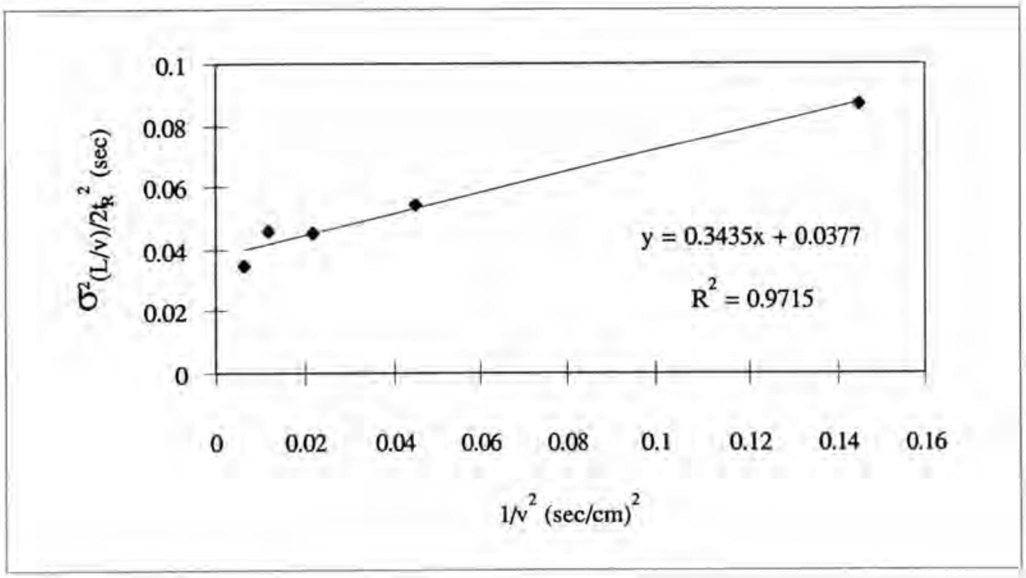

Figure A-3 The second moment plot of adsorption of o-xylene on synthesized 4A

$$\frac{\sigma^2}{2t_R^2}\frac{L}{v} = \frac{D_L}{v^2} + \left(\frac{\varepsilon}{1-\varepsilon}\right)\frac{1}{kK}\left(1+\frac{\varepsilon}{(1-\varepsilon)K}\right)^{-2}$$

$$\text{intercept} = \left(\frac{\varepsilon}{1-\varepsilon}\right)\frac{1}{kK}\left(1+\frac{\varepsilon}{(1-\varepsilon)K}\right)^{-2}$$

$$k = \frac{1}{\text{intercept}}\left(\frac{\varepsilon}{1-\varepsilon}\right)\frac{1}{K}\left(1+\frac{\varepsilon}{(1-\varepsilon)K}\right)^{-2}$$

Therefore, the overall mass transfer coefficient of adsorption of o-xylene on synthesized 4A is

$$k = \frac{1}{0.0377}\left(\frac{0.461}{1-0.461}\right)\frac{1}{713.34}\left(1+\frac{0.461}{(1-0.461)713.34}\right)^{-2}$$

$$k = 3.17 \times 10^{-2} \ \text{sec}^{-1}$$

The axial dispersion coefficient is

$$D_L = slope$$

$$= 3.44 \times 10^{-1} \ \text{cm}^2/\text{sec}$$

APPENDIX B

EXPERIMENT DATA

Table B-1 The retention times and variances of toluene on commercial 4A

Temperature	v (cm/sec)	t_R (sec)	σ^2 (sec^2)
80 °C	2.36	681.14	230,064.36
	5.38	281.29	42,415.98
	8.39	198.40	24,991.05
	11.45	190.15	26,195.01
	14.58	196.53	30,843.94
100 °C	1.39	364.16	68,213.64
	3.02	216.87	22,130.84
	5.81	138.51	12,987.71
	9.07	113.38	8,642.35
	12.24	112.44	12,637.39
	16.15	99.32	9,266.97

Table B-1 (continued)

Temperature	v (cm/sec)	t_R (sec)	σ^2 (sec^2)
120 °C	2.18	138.49	9,187.23
	5.40	59.53	2,318.48
	8.44	45.40	1,918.57
	11.45	37.96	1,294.25
	14.77	36.53	1,014.05
150 °C	2.17	96.35	3,649.18
	4.09	56.87	1,444.45
	6.28	41.852	795.68
	9.01	28.77	507.45
	12.00	24.73	326.15

Table B-2 The retention times and variances of toluene on synthesized 4A

Temperature	v (cm/sec)	t_R (sec)	σ^2 (sec^2)
80 °C	2.14	385.23	50,361.97
	3.78	258.29	32,153.99
	6.17	184.17	21,557.07
	9.30	140.34	13,235.89
	12.99	97.63	6,199.45

Table B-2 (continued)

Temperature	v (cm/sec)	t_R (sec)	σ^2 (sec^2)
100 °C	2.22	214.36	27,571.80
	3.51	161.10	15,933.85
	5.49	101.46	9,978.23
	7.92	81.13	8,608.46
	11.48	55.67	3,915.77
120 °C	1.82	98.97	6,065.98
	3.78	51.17	2,484.25
	5.63	37.37	1,363.22
	8.77	23.84	524.39
	11.93	19.77	342.80
150 °C	2.04	36.85	508.32
	3.79	24.16	247.69
	5.88	15.47	109.86
	8.26	8.21	50.809
	11.88	7.10	22.425

Table B-3 The retention times and variances of toluene on NaZSM-5

Temperature	v (cm/sec)	t_R (sec)	σ^2 (sec^2)
80 °C	5.33	505.68	282,574.75
	6.61	404.65	203,478.24
	8.12	298.05	111,250.43
	9.91	226.04	80,433.92
100 °C	4.30	492.41	228,263.06
	5.20	393.22	175,260.39
	6.91	285.20	119,710.19
	9.23	213.18	85,809.82
120 °C	5.06	242.94	79,688.05
	6.31	228.21	75,540.15
	8.16	196.23	72,897.31
	9.60	185.66	56,332.42

Table B-4 The retention times and variances of toluene on NH_4ZSM-5

Temperature	v (cm/sec)	t_R (sec)	σ^2 (sec^2)
150 °C	7.74	726.35	486,442.83
	11.81	572.17	318,489.37
	15.26	498.29	252,463.913
	17.64	430.54	188,143.63
	21.80	391.87	151,000.26
175 °C	8.69	412.68	167,670.64
	10.95	341.43	139,148.94
	13.29	312.49	113,123.15
	16.25	260.50	90,654.97
	19.79	224.61	75,170.57
200 °C	7.57	247.35	92,820.68
	11.55	182.51	63,171.09
	13.84	168.76	56,733.43
	17.87	123.48	32,310.11
	21.04	109.57	25,870.85

Table B-5 The retention times and variances of toluene on HZSM-5

Temperature	v (cm/sec)	t_R (sec)	σ^2 (sec^2)
150 °C	9.99	591.90	271,505.59
	13.30	440.01	209,854.01
	19.72	370.97	149,158.86
	23.07	316.37	118,123.55
175 °C	6.59	386.83	208,913.78
	8.85	366.26	168,417.77
	11.57	284.18	110,991.07
	15.95	235.83	79,058.95
	19.16	191.86	50,436.558
200 °C	7.45	167.12	53,124.22
	9.74	125.73	33,613.86
	12.88	99.09	19,001.32
	16.65	87.20	12,805.99
	19.85	66.97	7,980.59

Table B-6 The retention times and variances of toluene on 13X

Temperature	v (cm/sec)	t_R (sec)	σ^2 (sec^2)
175 °C	7.09	1,696.14	1,215,206.11
	10.43	1,296.16	685,255.68
	12.46	1,220.72	620,280.44
	18.45	1,010.00	452,791.17
200 °C	7.16	1,201.06	758,345.68
	9.60	1,119.11	513,001.02
	13.41	889.99	356,781.79
	17.85	781.78	280,578.65
225 °C	5.77	778.74	306,295.06
	9.77	580.93	173,766.42
	13.48	453.60	110,726.87
	17.66	353.11	70,777.99

Table B-7 The retention times and variances of o-xylene on commercial 4A

Temperature	v (cm/sec)	t_R (sec)	σ^2 (sec^2)
80 °C	5.94	1,462.34	775,944.94
	6.89	1,343.30	629,820.24
	9.21	1,010.43	370,782.82
	12.08	791.70	287,571.44
100 °C	5.09	600.31	170,393.70
	7.44	453.47	105,847.65
	9.29	355.16	68,108.48
	12.33	312.77	62,581.91
120 °C	5.02	312.69	61,397.68
	6.57	272.78	49,887.79
	8.68	208.72	31,828.12
	11.83	177.51	26,956.88
150 °C	2.64	84.11	3,817.25
	3.99	56.53	2,117.95
	6.07	42.66	1,474.20
	8.00	32.63	968.45
	10.70	23.48	488.14

Table B-7 (continued)

Temperature	v (cm/sec)	t_R (sec)	σ^2 (sec^2)
175 °C	2.50	60.78	2,062.06
	4.13	39.35	1,042.60
	6.28	27.32	526.19
	8.35	23.42	346.96
	11.26	14.56	196.67

Table B-8 The retention times and variances of o-xylene on synthesized 4A

Temperature	v (cm/sec)	t_R (sec)	σ^2 (sec^2)
80 °C	2.63	1,114.81	189,190.02
	4.69	710.19	86,009.31
	6.82	555.23	63,517.61
	9.16	462.59	60,053.78
	12.63	333.15	32,452.66
100 °C	2.78	429.69	45,348.95
	4.69	296.48	26,584.22
	6.87	220.20	17,983.87
	9.43	172.33	12,219.91
	12.46	131.29	8,699.86

Table B-8 (continued)

Temperature	v (cm/sec)	t_R (sec)	σ^2 (sec^2)
120 °C	3.10	147.29	13,660.23
	4.32	105.42	7,701.30
	6.58	77.61	5,529.08
	8.57	68.46	4,786.56
	11.86	48.04	2,806.02
150 °C	2.79	64.12	3,817.25
	4.65	40.41	2,117.95
	6.31	29.56	1,474.20
	8.46	24.90	968.45
	10.68	14.46	488.14

Table B-9 The retention times and variances of o-xylene on NaZSM-5

Temperature	v (cm/sec)	t_R (sec)	σ^2 (sec^2)
80 °C	6.80	326.33	177,0833.40
	9.44	229.16	108,428.70
	11.42	182.90	83,820.05
	12.99	166.896	61,313.80
100 °C	4.17	294.60	147,264.60
	6.64	233.38	106,986.30
	11.08	138.02	56,343.72
	12.26	129.58	42,035.98
120 °C	2.56	307.49	126,111.30
	5.20	167.40	57,647.79
	8.68	123.61	37,851.09
	12.30	62.34	13,682.73

Table B-10 The retention times and variances of o-xylene on NH_4ZSM-5

Temperature	v (cm/sec)	t_R (sec)	σ^2 (sec^2)
120 °C	6.25	763.11	614,267.04
	7.75	586.28	407,369.31
	9.95	439.28	251,637.43
	13.51	309.93	140,558.57
	16.51	257.67	98,697.96
150 °C	5.72	639.40	399,522.78
	7.51	558.76	359,278.16
	9.76	416.99	211,119.60
	11.42	340.67	150,687.01
	14.30	274.56	101,032.11
175 °C	5.66	468.72	213,212.23
	7.16	312.12	120,637.38
	9.66	316.61	140,299.02
	11.88	231.63	93,100.02
	14.55	201.46	57,654.33
200 °C	4.84	227.53	67,012.91
	6.78	187.54	50,727.65
	8.51	128.20	31,667.04
	10.53	101.87	20,106.78
	12.97	65.13	9,099.88

Table B-11 The retention times and variances of o-xylene on HZSM-5

Temperature	v (cm/sec)	t_R (sec)	σ^2 (sec^2)
120 °C	6.95	594.38	313,504.14
	10.20	411.56	161,958.70
	12.76	336.00	127,276.77
	16.08	222.45	64,082.47
150 °C	7.16	495.21	218,720.63
	10.70	378.89	157,826.65
	14.16	275.73	99,903.82
	17.57	203.01	63,838.37
175 °C	5.46	346.24	132,581.85
	9.01	201.20	60,254.81
	12.53	156.79	43,274.15
	14.94	113.51	25,488.55
	19.21	82.59	14,786.03
200 °C	6.29	187.82	60,469.29
	7.92	134.87	38,100.69
	10.02	91.95	21,017.10
	13.50	60.57	11,232.48
	17.33	38.93	5,238.44

Table B-12 The retention times and variances of o-xylene on 13X

Temperature	v (cm/sec)	t_R (sec)	σ^2 (sec^2)
100 °C	1.99	212.32	50,156.67
	3.43	142.97	24,042.62
	5.97	81.28	9,589.41
	8.14	59.18	6,047.41
	11.39	43.03	2,542.82
120 °C	1.65	150.70	23,803.87
	3.75	80.50	7,800.31
	5.80	50.66	2,744.81
	7.66	34.02	1,595.45
	11.01	23.92	672.53
150 °C	2.06	80.94	8,926.55
	3.46	51.05	4,028.11
	5.74	33.04	2,083.12
	7.18	27.36	1,414.21
	9.44	23.21	1,047.26
175 °C	2.35	56.11	2,957.65
	3.77	35.54	1,227.241
	5.67	23.07	709.95
	7.52	20.13	553.17
	10.31	16.87	347.81

Table B-12 (continued)

Temperature	v (cm/sec)	t_R (sec)	σ^2 (sec^2)
200 °C	2.66	33.98	1,005.01
	4.17	23.86	493.90
	6.20	16.46	296.73
	7.73	14.31	199.27
	9.78	11.56	103.47

VITA

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