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Appendix A

Samples of Calculation

A.1 Calculation of Concentration of Acetone and Toluene Vapors

The concentration of acetone and toluene is calculated from the vapor pressure and total pressure of the system. At temperature 30 ° C;

- Acetone

Vapor pressure of acetone = 286.90 mmHg
Total pressure = atmospheric pressure + the pressure form the difference level of manometer
= 760 mmHg + 1.58 mmHg
= 761.58 mmHg
Then the mole fraction is $= \left(\frac{286.90}{761.58}\right)$
= 0.377
= 37.7 %

- Toluene

Vapor pressure of toluene = 37.31 mmHg
Total pressure = atmospheric pressure + the pressure form the difference level of manometer
= 760 mmHg + 1.33 mmHg
= 761.33 mmHg
Then the mole fraction is = $\left(\frac{37.31}{761.33}\right)$
= 0.049
= 4.6 %

Estimate the injection concentration in the carrier gas flow

Minimum flowrate 20 ml/min

Amount of injection 100 μl

Time of injection 2 sec

Volume of carrier within 2 sec = 0.67 cm^3
Amount of acetone in 100 μl = 0.37 × 100
= 0.037 cm^3
% by volume of acetone = 0.037/0.67
= 0.055
= 5.5 %
Amount of toluene in 100 μl = 0.049 × 100
= 0.0049 cm^3
% by volume of toluene = 0.0049/0.67
= 0.0073
= 0.73 %

A.2 Calculation of Adsorption Equilibrium Constants

The adsorption equilibrium constant is calculated from equation A.1 by the plot of L/v versus t_R such as illustrated in figure A.1.

$$t_R = \frac{L}{v}\left(1 + (\frac{1-\epsilon}{\epsilon})K_H\right) \qquad (A.1)$$

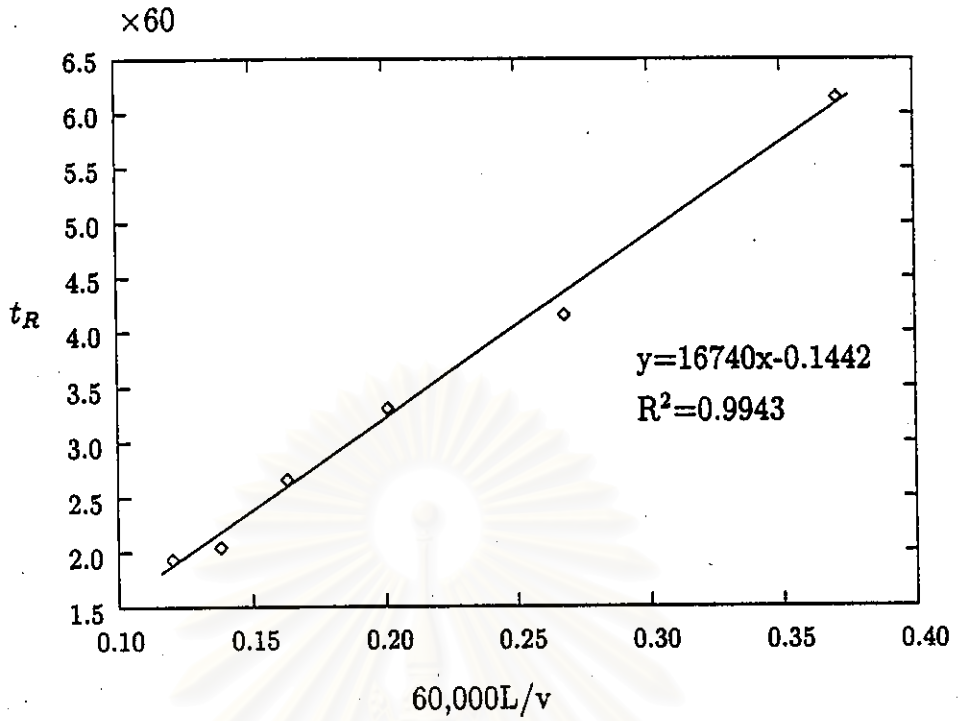

Figure A.1: Retention times of acetone on YAO4/8 at 160° C

The slope of the straight line is equal to $1 + (\frac{1-\epsilon}{\epsilon})K$. The bed porosity is 0.308.

Then,

$$\begin{aligned} K_H &= (\text{slope-1})\left(\tfrac{\epsilon}{(1-\epsilon)}\right) \\ &= (16,740 - 1)(0.308/(1 - 0.308)) \\ &= 7,450.13 \end{aligned}$$

A.3 Calculation of Heat of Adsorptions

From Van't Hoff equation

$$\frac{dlnK}{dT} = \frac{\Delta H}{RT^2} \tag{A.2}$$

The intregral of equation A.2 at constant ΔH ;

$$\int_{K_0}^{k} dlnK = \frac{\Delta H}{R} \int \frac{1}{T^2} dt$$

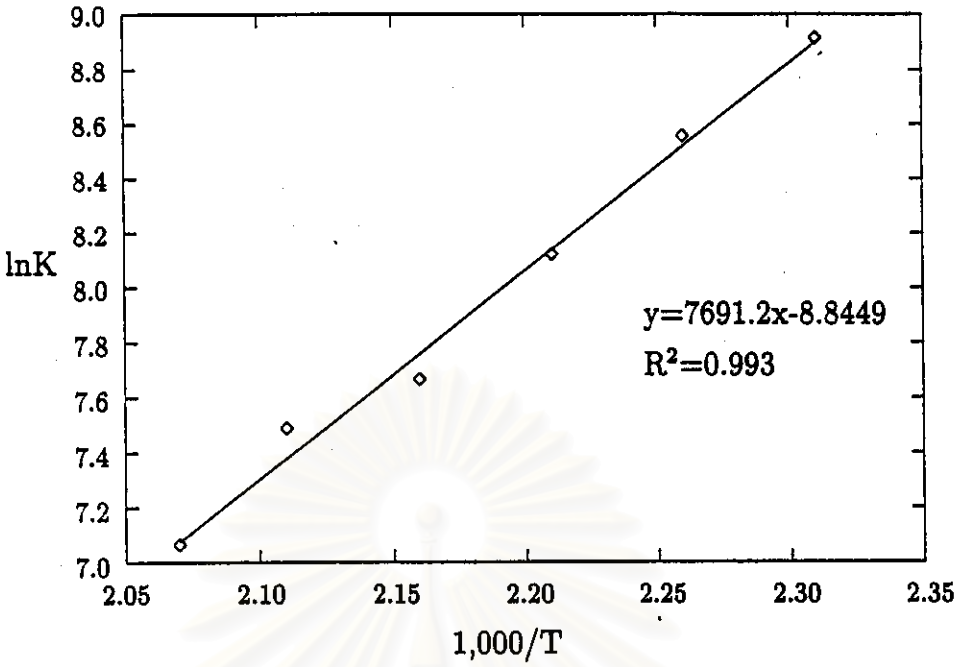

Figure A.2: Adsorption equilibrium constants of acetone on YAO4/8

Then,

$$lnK = lnK_0 + \frac{-\Delta H}{R(T - T_0)} \tag{A.3}$$

The plot of lnK versus $1/T$ is illustrated in figure A.2. The slope of the line used to find the heat of adsorption. Therefore;

$$\begin{aligned} -\Delta H &= \text{slope} \times \text{R} \\ &= 7,619.2 \times 8.314 \quad \text{J/mole} \\ &= 69.94 \quad \text{kJ/mol} \end{aligned}$$

A.4 Calculation of Overall Mass Transfer Coefficients

From equation;

$$\frac{\sigma^2}{2t_R^2} = \frac{D_L}{vL} + \frac{v}{L}\left(\frac{\epsilon}{1-\epsilon}\right)\left(\frac{1}{kK_H}\right)\left(1 + \frac{\epsilon}{(1-\epsilon)K_H}\right)^{-2} \tag{A.4}$$

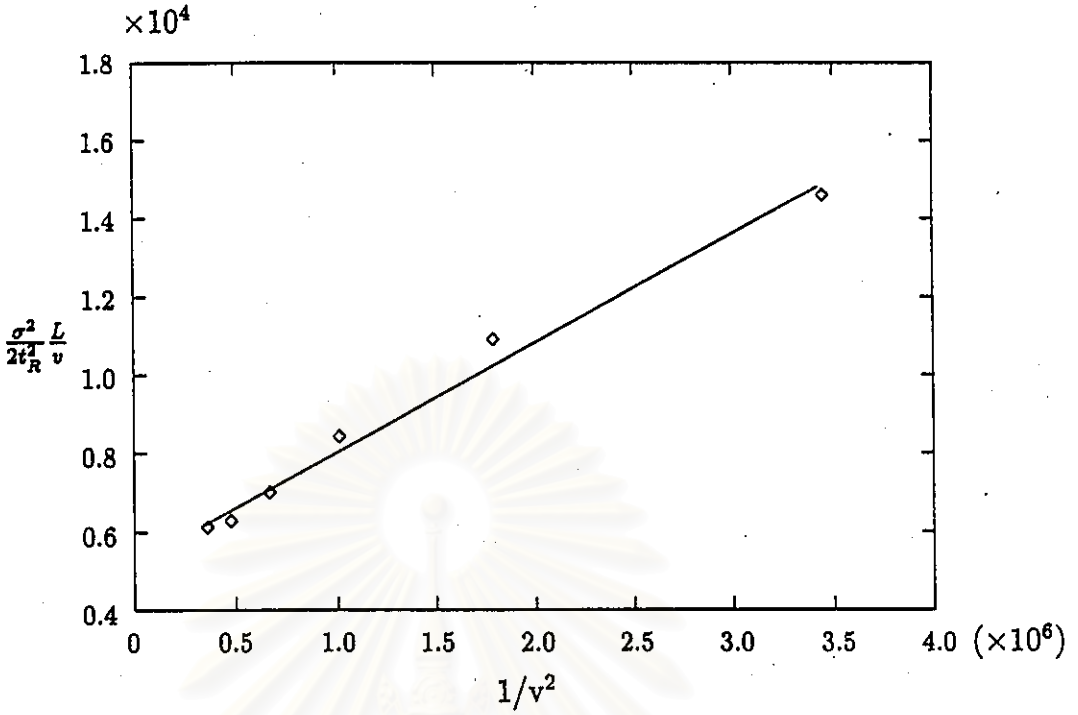

Figure A.3: Overall mass transfer coefficients of acetone on YAO4/8

or

$$\frac{\sigma^2}{2t_R^2}\frac{L}{v} = \frac{D_L}{v^2} + \left(\frac{\epsilon}{1-\epsilon}\right)\left(\frac{1}{kK_H}\right)\left(1+\frac{\epsilon}{(1-\epsilon)K_H}\right)^{-2}$$

The plot of $\frac{\sigma^2}{2t_R^2}\frac{L}{v}$ versus $\frac{D_L}{v^2}$ should be linear shown in figure A.3. The overall mass transfer coefficient is calculated from the intercept of the line and the slope is corresponding to axial dispersion coefficient.

$$\text{intercept} = \left(\frac{\epsilon}{1-\epsilon}\right)\left(\frac{1}{kK_H}\right)\left(1+\frac{\epsilon}{(1-\epsilon)K_H}\right)^{-2}$$

$$\text{and slope} = D_L$$

Therefore, the overall mass transfer coefficient of adsorption of acetone on activated carbons used for air purification (YAO4/8) at 160 ° C is

$$5X10^{-5} = \left(\frac{\epsilon}{1-\epsilon}\right)\left(\frac{1}{kK}\right)\left(1+\frac{\epsilon}{(1-\epsilon)K}\right)^{-2}$$

$$k = \frac{1}{5x10^{-5}}\left(\frac{0.308}{1-0.308}\right)\left(\frac{1}{7450.31}\right)\left(1+\frac{0.308}{(1-0.308)7450.31}\right)^{-2}$$

$$k = 1.20 \ (\text{min}^{-1})$$
$$= 0.02 \ (\text{sec}^{-1})$$

And the axial dispersion is;

$$D_L = \text{slope}$$
$$= 27.83 \ \text{cm}^2/\text{min}$$
$$= 0.464 \ \text{cm}^2/\text{sec}$$

A.5 Calculation of activation energy

From Arrhenius's equation;

$$k = k_0 \exp\left(\frac{E_a}{RT}\right) \tag{A.5}$$

or

$$k = K_0 - E_a/RT$$

The plot of lnk versus $1/T$ is illustrated in figure A.4. The slope of the line used to find the activation energy. Therefore;

$$-E_a = \text{slope} \times \text{R}$$
$$= -8,378.4 \times 8.314 \quad \text{J/mole}$$
$$= -69.66 \quad \text{kJ/mol}$$

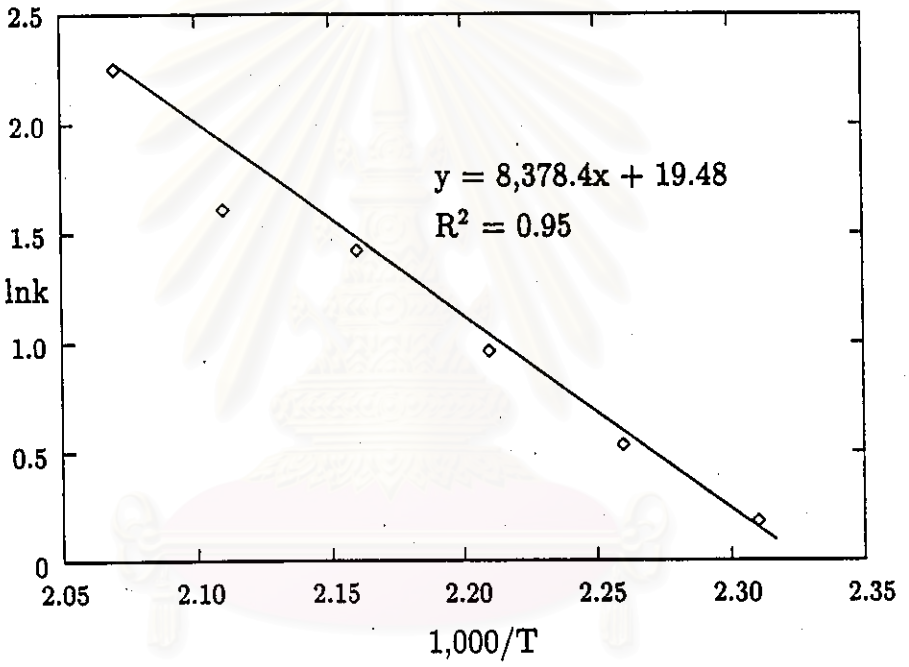

Figure A.4: Activation energy of acetone adsorption on YAO4/8

Appendix B

Determination of Pellet Density

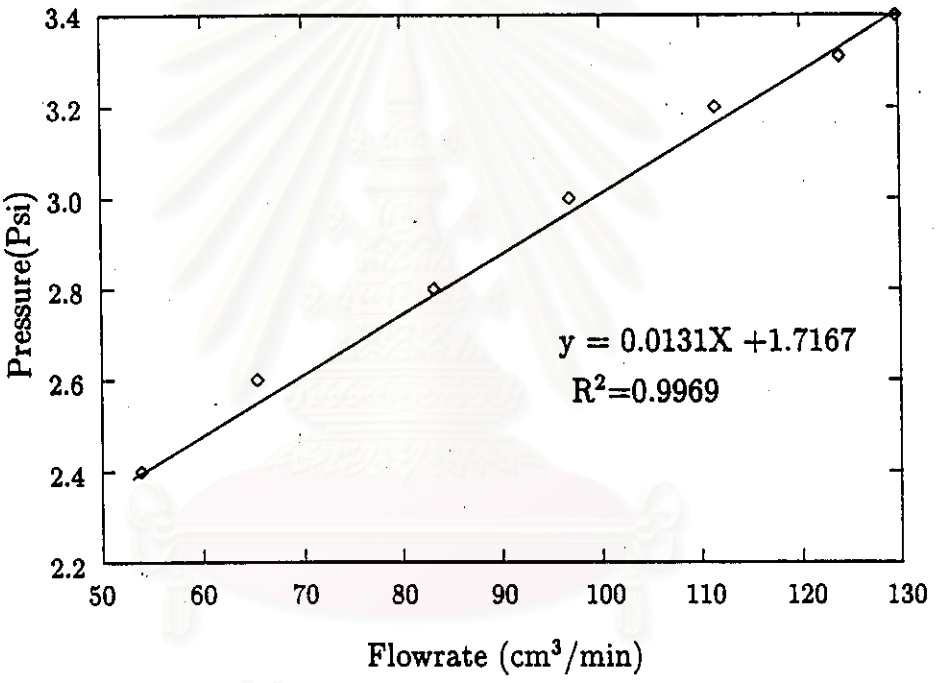

Figure B.1: The plots of pressure drops and carrrier gas velocity for unpacked column

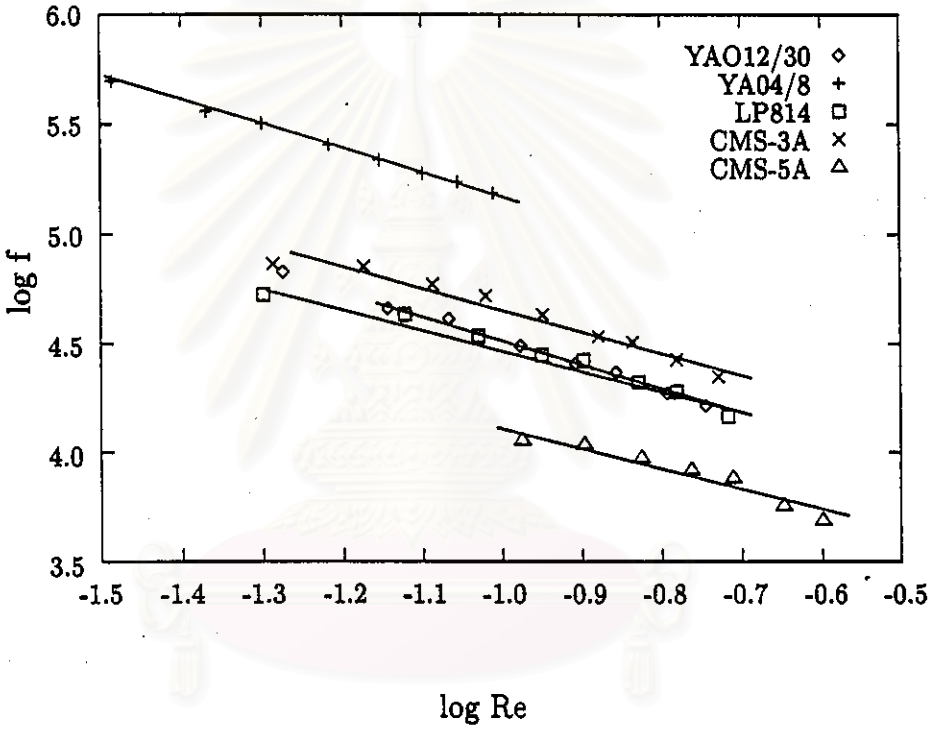

Figure B.2: The plots of friction factor versus Reynold number for flow through packed bed according to Blake-Kozeny equation

Appendix C

Retention Times and Variences

Table C.1: Retention times and variences of acetone on CMS-3A

Temp. (° C)	v (cm/sec)	t_R (sec)	σ^2 ($\times 10^3$) (sec^2)	Temp. (° C)	v (cm/sec)	t_R (sec)	σ^2 ($\times 10^3$)(sec^2)
50	6.940	352.2	87.98	80	6.288	143.7	12.11
	9.297	301.8	74.12		7.948	114.5	8.564
	9.978	288.8	70.24		9.640	101.5	7.153
	13.81	229.3	52.27		12.61	74.22	4.558
	18.33	170.2	34.71		15.94	63.18	3.146
	21.25	152.0	32.05		17.72	48.12	2.059
60	7.305	191.0	22.09	90	6.263	101.7	5.483
	9.230	164.0	16.71		7.543	92.82	4.972
	10.35	162.8	15.71		8.722	79.56	3.582
	13.44	132.7	10.91		10.37	68.28	3.107
	17.72	111.1	11.25		12.64	61.68	2.891
	21.58	76.68	5.256		13.64	60.06	2.668
					17.48	47.88	2.005
70	6.398	173.2	17.94	100	6.073	83.76	4.081
	7.907	137.2	12.01		7.390	72.06	3.027
	9.858	116.5	9.840		9.362	62.52	2.369
	13.44	90.90	7.747		10.20	56.22	1.948
	16.80	77.04	5.897		12.25	47.70	1.616
	18.28	69.12	5.036				

Table C.2: Retention times and variences of acetone on CMS-5A

Temp. (° C)	v (cm/sec)	t_R (sec)	σ^2 ($\times 10^3$)(sec^2)	Temp. (° C)	v (cm/sec)	t_R (sec)	σ^2 ($\times 10^3$)(sec^2)
160	4.618	198.5	38.20	190	3.702	98.40	9.972
	5.075	177.1	28.13		4.362	80.64	6.116
	6.237	143.5	19.83		6.018	61.20	3.740
	7.857	98.52	9.691		7.705	39.48	1.461
	9.447	76.98	7.236		9.152	36.12	1.343
170	4.658	132.6	14.98	200	3.570	78.12	5.782
	5.748	95.10	7.142		4.513	59.16	3.247
	6.662	76.86	5.267		5.372	52.20	2.167
	8.087	58.56	2.977		6.908	39.36	1.281
	10.06	49.26	2.369		8.720	33.00	0.900
180	3.783	132.6	14.98	210	4.277	47.94	1.418
	4.790	95.10	7.142		4.758	44.46	1.281
	5.670	76.86	5.267		5.395	38.70	928.8
	7.218	58.56	2.977		6.648	28.98	453.6
	8.572	49.26	2.369		8.402	22.98	302.4
					9.383	20.58	248.4

Table C.3: Retention times and variences of acetone on LP814

Temp. (° C)	v (cm/sec)	t_R (sec)	σ^2 ($\times 10^3$) (sec^2)	Temp. (° C)	v (cm/sec)	t_R (sec)	σ^2 ($\times 10^3$)(sec^2)
120	4.905	121.7	18.57	150	4.317	61.26	2.192
	6.830	122.6	13.14		5.218	47.70	1.422
	8.352	100.9	9.090		6.603	41.22	1.108
	10.08	81.06	7.214		7.157	40.52	1.047
	11.18	71.01	5.465		7.217	36.66	0.810
	14.00	52.62	3.409		9.070	30.06	0.659
130	4.383	121.7	13.63	160	4.602	44.38	0.828
	5.867	133.7	9.763		5.367	40.92	0.720
	6.717	82.26	6.671		6.510	31.56	0.454
	7.533	79.20	6.059		7.832	28.50	0.403
	9.037	63.90	4.122		9.415	24.72	0.328
	10.07	64.08	3.917		10.12	23.58	0.207
140	4.877	86.70	5.454	170	4.035	38.16	0.850
	5.718	86.88	3.676		6.158	28.92	0.382
	6.477	62.70	3.103		7.345	24.30	0.245
	7.637	52.44	2.437		8.388	23.44	0.223
	8.373	45.24	1.796		9.142	21.00	0.166
	10.56	40.20	1.472				
180 C	3.023	40.20	0.562				
	3.728	34.80	0.396				

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Temp. (° C)	v (cm/sec)	t_R (sec)	σ^2 ($\times 10^3$)(sec^2)	Temp. (° C)	v (cm/sec)	t_R (sec)	σ^2 ($\times 10^3$)(sec^2)
	5.507	26.88	0.209				
	6.118	23.70	0.162				
	7.468	24.24	0.173				
	9.047	20.52	0.108				

Table C.4: Retention times and variences of acetone on YAO4/8

Temp. (° C)	v (cm/sec)	t_R (sec)	σ^2 ($\times 10^3$)(sec^2)	Temp. (° C)	v (cm/sec)	t_R (sec)	σ^2 ($\times 10^3$)(sec^2)
160	8.977	368.9	106.7	190	7.878	132.6	14.71
	12.45	249.3	50.50		11.01	102.9	8.215
	16.59	198.6	33.07		14.90	111.0	10.45
	20.42	159.7	21.92		17.60	69.66	4.043
	24.17	122.6	13.71		22.25	55.47	2.394
	44.50	155.9	13.73		26.07	46.26	2.045
170	8.545	272.8	53.57	200	8.482	106.1	8.590
	11.49	214.4	32.71		10.45	86.70	5.821
	15.75	136.9	14.89		14.79	71.22	3.924
	19.33	113.3	11.09		17.87	56.16	2.563
	23.17	98.52	8.661		20.70	49.08	2.135
	27.00	99.60	8.265		25.90	41.58	1.487
180	8.320	194.0	30.60	210	8.083	69.06	2.4337
	11.28	136.4	15.26		11.70	51.00	1.336
	14.90	111.0	10.45		14.42	38.76	0.810
	19.33	88.08	6.50		17.90	32.46	0.608
	22.68	72.60	4.658		22.07	27.96	0.436
	27.38	66.84	3.898		25.80	24.78	0.403

Table C.5: Retention times and variences of acetone on YAO12/30

Temp. (° C)	v (cm/sec)	t_R (sec)	σ^2 ($\times 10^3$) (sec^2)	Temp. (° C)	v (cm/sec)	t_R (sec)	σ^2 ($\times 10^3$)(sec^2)
110	3.755	1050	1089	170	3.988	104.3	8.539
	5.900	796.2	619.6		4.970	88.37	5.224
	7.427	575.5	311.7		6.233	76.74	4.122
	9.043	542.5	289.7		7.630	67.80	2.966
	9.783	513.3	257.7		9.567	48.48	1.580
	11.13	466.9	220.9				
120	3.587	589.4	280.5	180	3.732	75.06	4.334
	4.977	479.9	192.9		4.060	68.94	3.211
	6.883	396.5	139.5		4.323	64.86	2.945

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Temp. (° C)	v (cm/sec)	t_R (sec)	σ^2 ($\times 10^3$) (sec^2)	Temp. (° C)	v (cm/sec)	t_R (sec)	σ^2 ($\times 10^3$)(sec^2)
	8.655	339.1	104.6		5.788	51.42	1.804
	9.837	301.5	90.94		6.973	48.48	1.714
	10.77	271.0	67.54		8.760	42.66	1.012
130	4.385	290.0	67.46	190	3.170	61.86	2.887
	5.717	260.8	56.88		3.817	55.92	1.980
	7.217	213.5	40.28		4.627	46.44	1.231
	9.122	194.2	34.60		6.452	36.72	0.691
	9.838	166.3	26.04		8.135	27.30	0.435
	11.02	152.3	22.46		10.26	25.92	0.353
140	3.292	278.8	67.28	200	2.638	68.82	2.452
	4.763	197.3	33.95		3.845	56.70	1.426
	6.573	157.5	24.06		4.943	44.16	0.752
	8.355	132.8	19.44		6.273	36.72	0.482
	11.05	105.6	12.46		8.013	28.50	0.259
					9.998	23.82	0.162
150	4.742	170.6	31.45	210	3.722	33.06	0.378
	6.543	126.2	15.42		3.970	30.54	0.295
	8.283	103.9	10.86		4.880	27.42	0.238
	10.15	89.34	8.284		5.790	21.42	0.155
	12.17	78.18	7.560		6.442	20.88	0.137
					7.332	7.920	0.115
160	4.443	164.0	29.48	220	3.420	26.16	284.4
	6.398	122.9	13.28		3.670	24.48	241.2
	7.658	98.82	8.359		4.530	20.16	154.8
	8.942	92.52	8.002		5.573	18.30	126.0
	11.29	67.68	4.525		6.307	20.88	108.0

Table C.6: Retention times and variences of toluene on CMS-3A

Temp. (° C)	v (cm/sec)	t_R (sec)	σ^2 ($\times 10^3$)(sec^2)	Temp. (° C)	v (cm/sec)	t_R (sec)	σ^2 ($\times 10^3$)(sec^2)
60	7.832	591.4	335.8	90	10.10	100.7	11.56
	13.62	417.5	173.5		12.76	87.24	7.293
	14.17	358.1	154.9		14.19	78.66	6.523
	16.23	359.4	153.1		18.32	59.88	3.207
	17.02	278.0	102.1		20.75	57.60	3.031
	20.18	264.7	80.14				
	21.90	227.3	79.27				
70	10.04	278.0	71.86	120	5.108	41.16	1.298
	11.89	242.9	63.79		7.180	31.62	0.691
	12.41	242.1	55.08		10.40	28.38	0.562
	13.92	217.4	46.33		12.35	26.16	0.353

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Temp. (° C)	v (cm/sec)	t_R (sec)	σ^2 ($\times 10^3$)(sec^2)	Temp. (° C)	v (cm/sec)	t_R (sec)	σ^2 ($\times 10^3$)(min^2)
	18.53	178.2	39.38		18.93	24.66	0.335
	20.62	167.3	28.90				
	21.57	156.7	26.67				
80	4.992	296.64	63.07				
	8.047	221.64	36.32				
	11.96	174.48	31.31				
	17.23	110.16	14.58				
	22.37	83.64	9.435				

Table C.7: Retention times and variences of toluene on LP814

Temp. (° C)	v (cm/sec)	t_R (sec)	σ^2 ($\times 10^3$)(sec^2)	Temp. (° C)	v (cm/sec)	t_R (sec)	σ^2 ($\times 10^3$)(sec^2)
210	6.578	857.4	367.9	240	10.193	242.5	44.68
	8.857	613.8	201.1		11.87	200.9	27.18
	10.42	490.8	127.5		14.88	167.0	19.10
	11.38	451.3	87.16		16.52	141.1	11.81
	12.72	390.7	64.94		18.68	132.8	10.68
	16.75	221.2	23.22				
	18.93	165.7	13.95				
220	7.125	406.9	118.9	250	7.708	241.3	38.70
	8.727	356.0	71.75		9.640	189.4	21.60
	11.48	271.2	50.65		11.77	153.5	12.21
	13.63	228.1	36.32		11.22	130.2	7.938
	16.23	184.8	27.05		15.33	125.5	8.402
	18.20	154.2	17.50				
230	8.707	455.9	123.4				
	10.64	382.9	82.91				
	13.48	335.3	65.84				
	16.10	291.2	48.35				
	18.08	254.8	33.92				

Table C.8: Retention times and variences of toluene on YAO 4/8

Temp. (° C)	v (cm/sec)	t_R (sec)	σ^2 ($\times 10^3$) (sec^2)	Temp. (° C)	v (cm/sec)	t_R (sec)	σ^2 ($\times 10^3$)(sec^2)
200	12.09	998.4	771.6	220	10.74	578.6	191.5
	14.96	1,015	778.2		14.27	510.8	153.6
	18.00	937.8	770.1		17.82	438.2	128.6
	26.05	818.4	704.9		21.92	373.0	101.3
	29.88	777.6	696.2		254.65	361.4	100.0

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Temp. (° C)	v (cm/sec)	t_R (sec)	σ^2 ($\times 10^3$)(sec^2)	Temp. (° C)	v (cm/sec)	t_R (sec)	σ^2 ($\times 10^3$)(sec^2)
210	10.63	697.2	353.4	240	9.405	439.4	126.36
	15.15	592.3	288.5		12.87	325.3	70.02
	19.75	548.7	263.3		17.02	266.5	52.34
	22.68	506.6	223.7		20.77	209.0	33.26
	25.33	428.8	206.8		24.83	169.9	22.15
	29.12	404.5	191.0		28.48	159.5	21.28

Table C.9: Retention times and variences of toluene on YAO 12/30

Temp. (° C)	v (cm/sec)	t_R (sec)	σ^2 ($\times 10^3$)(sec^2)	Temp. (° C)	v (cm/sec)	t_R (sec)	σ^2 ($\times 10^3$)(sec^2)
200	4.240	1,196	974.5	230	4.900	377.5	83.53
	6.188	913.8	451.4		6.070	311.4	50.26
	8.153	754.8	396.4		7.835	245.6	33.36
	9.582	631.8	211.3		9.845	206.8	22.09
	12.01	533.8	168.2		11.30	183.1	18.67
210	6.038	711.0	254.3	240	5.860	288.5	28.62
	6.693	630.0	204.3		7.673	191.2	28.62
	8.270	533.8	152.6		8.947	159.0	14.02
	9.647	475.9	116.3		10.79	130.6	8.788
	11.34	428.1	85.10				
220	4.438	570.1	174.1				
	6.400	464.2	108.0				
	8.015	359.2	59.65				
	9.723	329.0	56.41				
	11.14	277.3	36.04				

Appendix D

The Plot of the Retention Times of Acetone and Toluene Vapors with the Recipocal Velocity

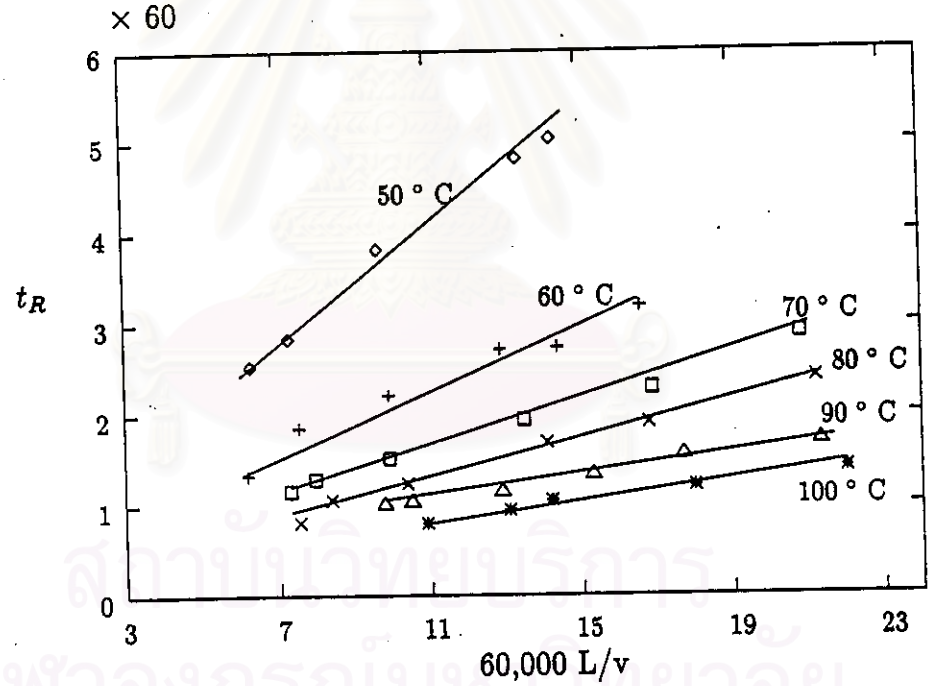

Figure D.1: The retention times of actone on CMS-3A

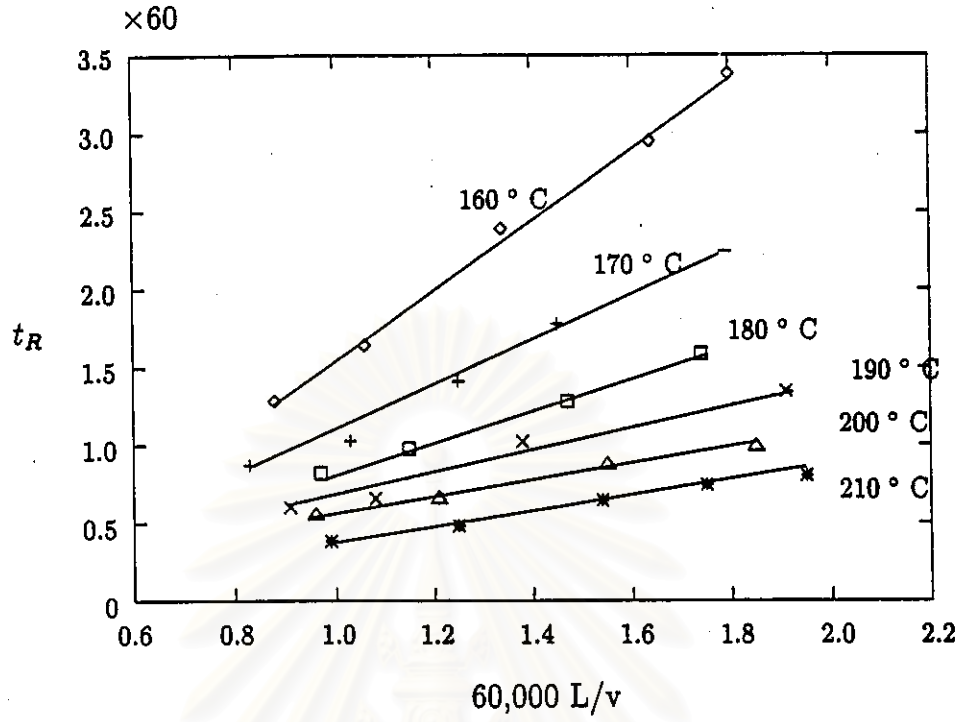

Figure D.2: The retention times of actone on CMS-5A

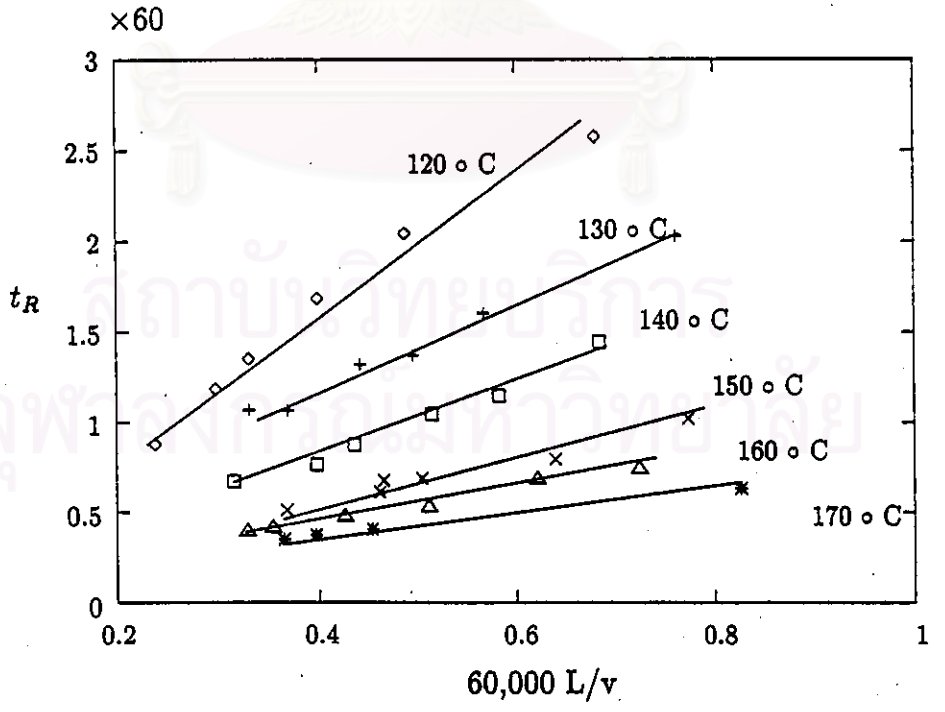

Figure D.3: The retention times of actone on LP814

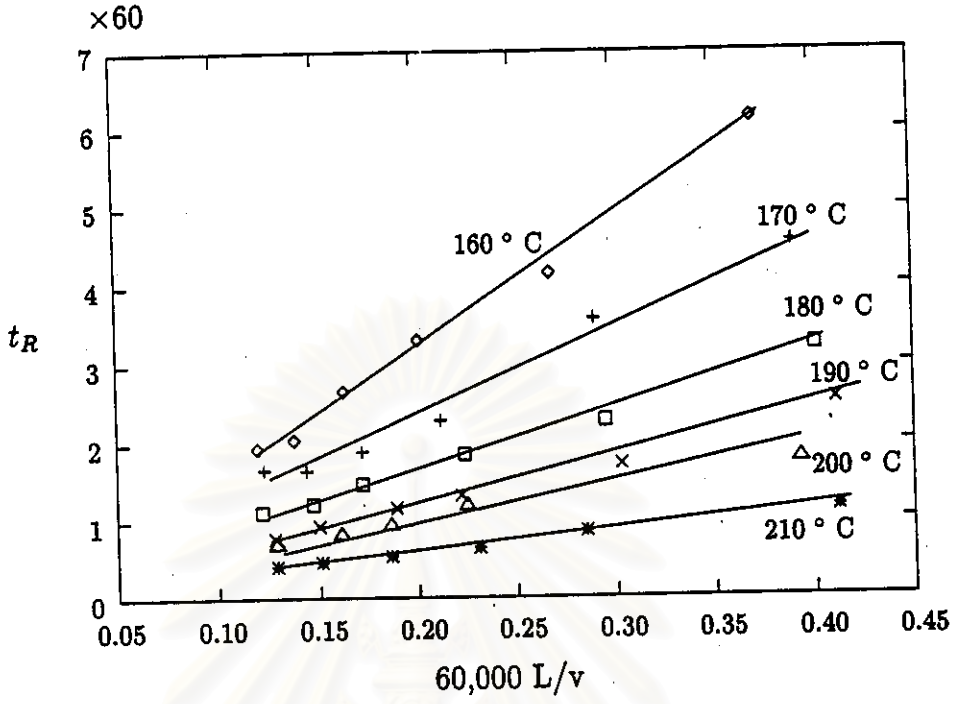

Figure D.4: The retention times of actone on YAO4/8

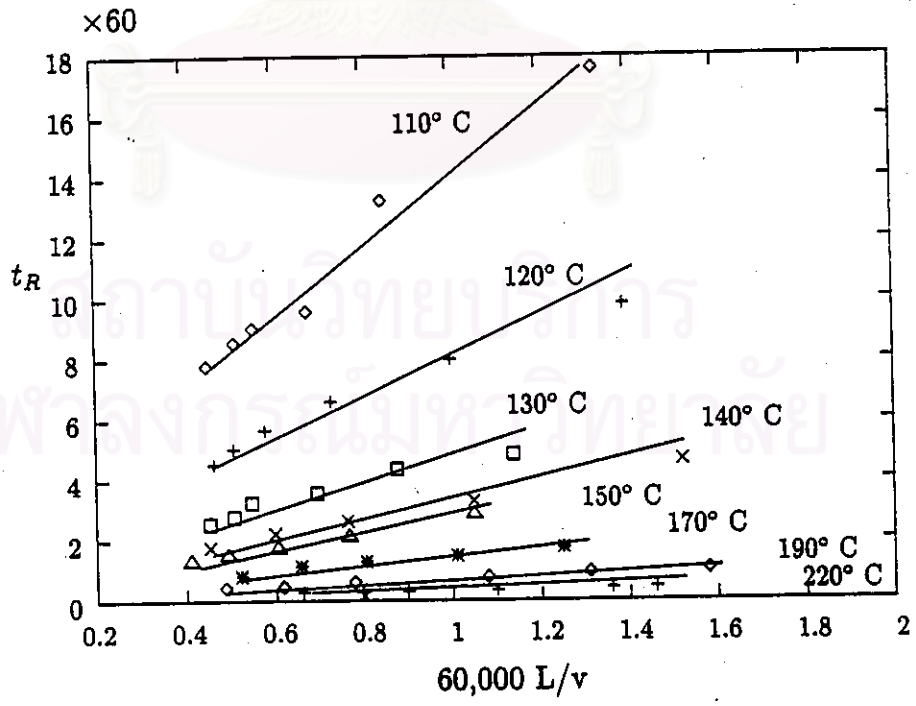

Figure D.5: The retention times of actone on YAO12/30

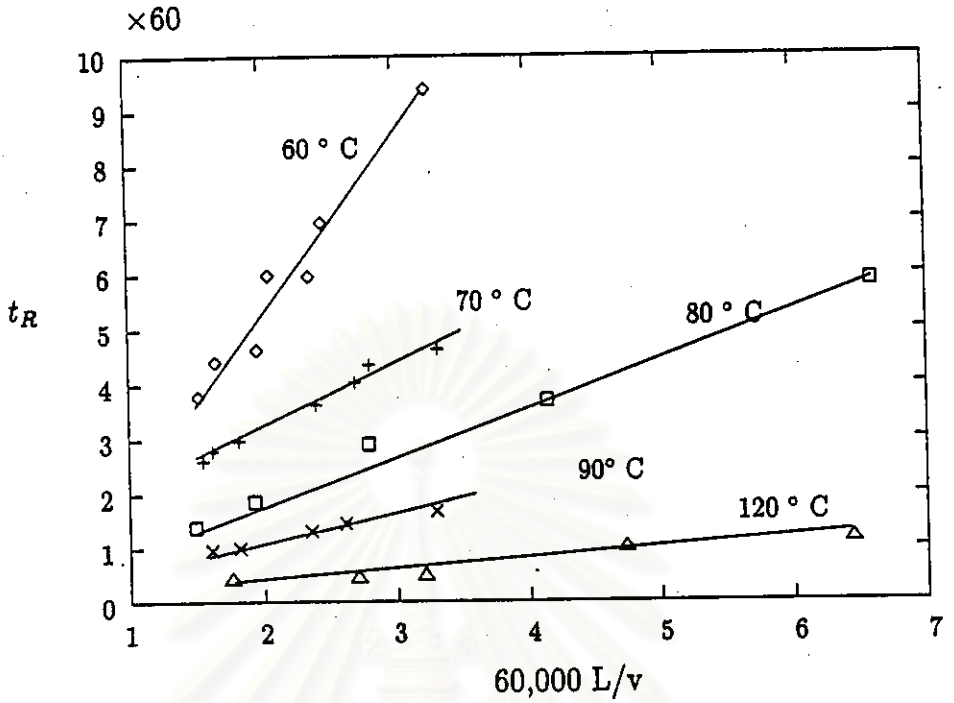

Figure D.6: The retention times of toluene on CMS-3A

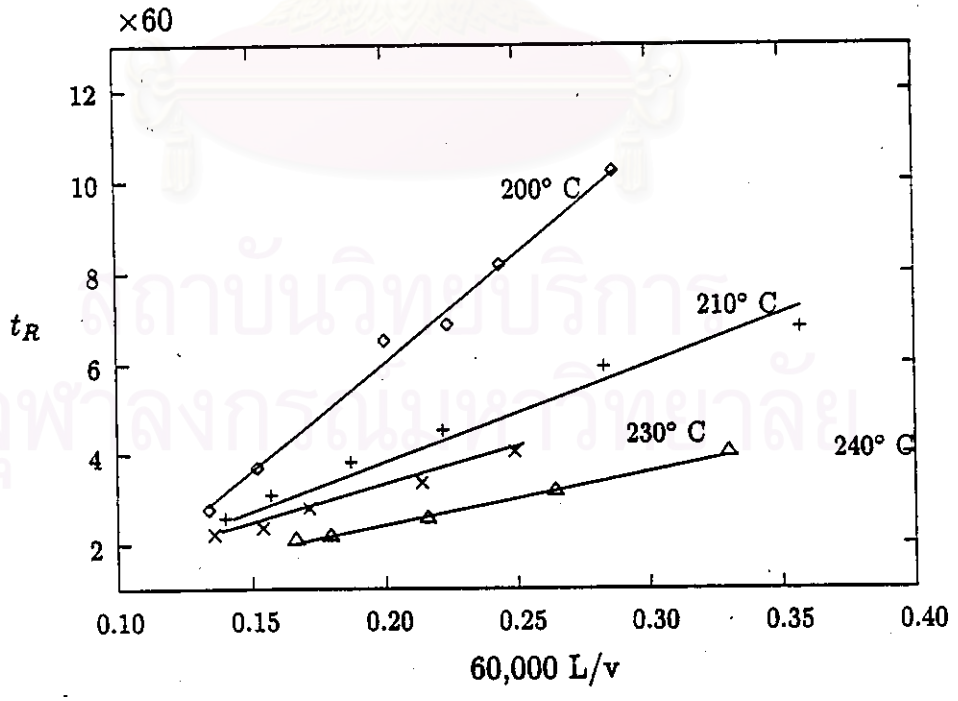

Figure D.7: The retention times of toluene on LP814

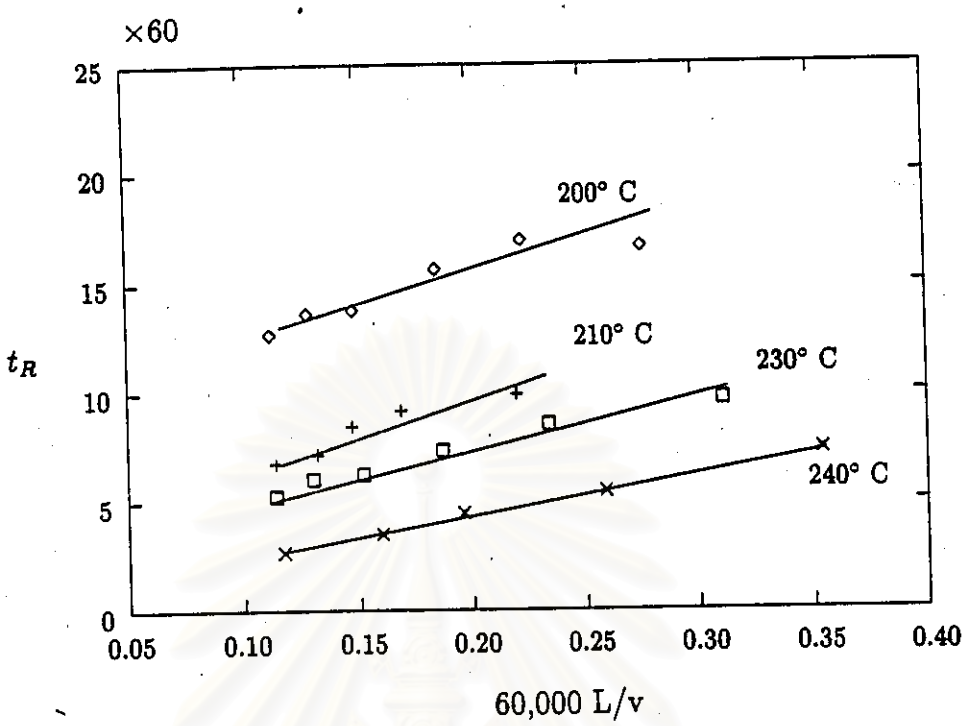

Figure D.8: The retention times of toluene on YAO4/8

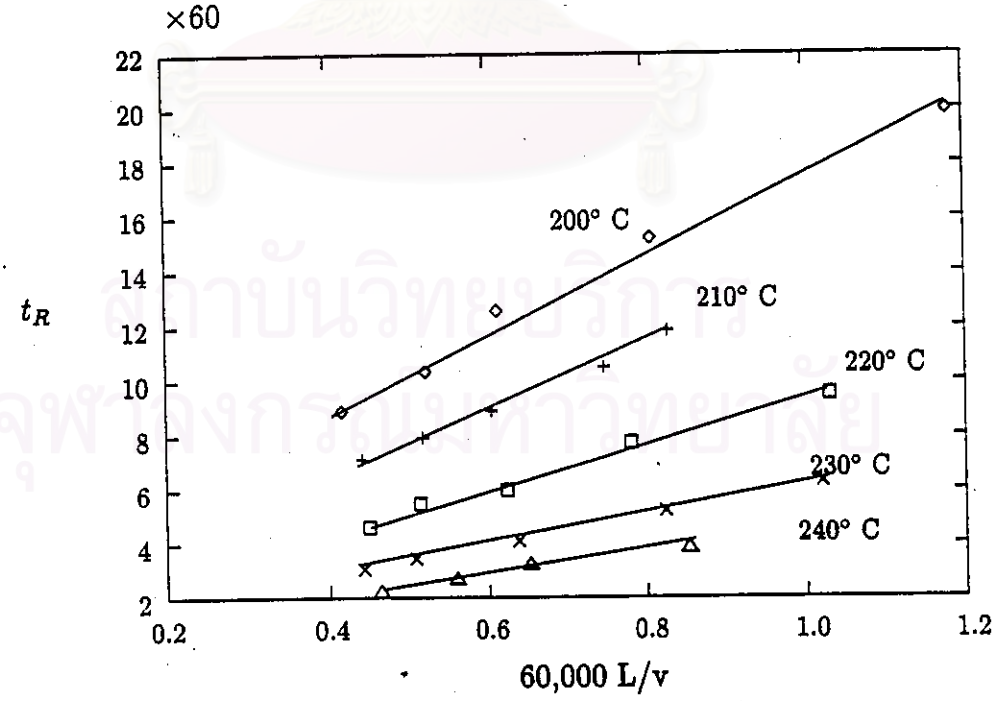

Figure D.9: The retention times of toluene on YAO12/30

Appendix E

Molecular Diffusivities and Axial Dispersions

Table E.1: Axial dispersions of acetone and toluene

Adsorbents	Acetone			Toluene		
	T (° C)	D_m (cm^2/sec)	D_L (cm^2/sec)	T (° C)	D_m (cm^2/sec)	D_L (cm^2/sec)
CMS-3A	50	30.60	498.0	60	28.80	22.20
	60	32.40	600.0	70	30.00	28.20
	70	34.20	377.4	80	31.60	30.00
	80	36.60	474.6	90	33.60	32.40
	90	38.40	361.2			
	100	40.20	460.8			
CMS-5A	160	52.80	31.20			
	170	55.20	28.20			
	180	57.60	29.40			
	190	60.00	40.20			
	200	61.80	39.60			
	210	64.80	30.60			
LP814	120	44.40	10.80	210	56.40	20.40
	130	46.20	15.60	220	58.80	19.80
	140	48.60	10.80	230	61.20	28.80
	150	50.40	8.400	240	63.00	37.80
	160	52.80	6.600	250	65.40	27.60
	170	55.20	12.60			
	180	57.60	5.400			
YAO4/8	160	52.80	27.60	200	54.60	24.00
	170	55.20	24.00	210	56.40	22.80
	180	57.60	29.40	220	58.80	18.60
	190	60.00	28.80	240	63.00	23.40
	200	61.80	26.40			

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Adsorbents	Acetone			Toluene		
	T (° C)	D_m (cm^2/sec)	D_L (cm^2/sec)	T (° C)	D_m (cm^2/sec)	D_L (cm^2/sec)
	210	64.80	16.20			
YAO12/30	110	42.00	24.00	200	54.60	19.80
	120	44.40	17.40	210	56.40	18.60
	130	46.20	19.20	220	58.80	17.40
	140	48.60	16.20	230	61.20	18.60
	150	50.40	31.20	240	63.00	19.20
	160	52.80	33.00			
	170	55.20	21.60			
	180	57.60	18.60			
	190	60.00	18.00			
	200	61.80	11.40			
	210	64.80	7.800			
	220	67.20	9.000			

CURRICULUM VITAE

Miss Ratchada Rattanamung was born in January,1972 in Ratchaburi. She graduated high school from Satit Prasanmitr School in 1991. She recieved Bachelor's Degree of Chemical Technology in the faculty of Science from Chulalongkorn University in 1995. Subsequently, she completed the requirement for Master's degree in Chemical Engineering at the Department of Chemical Engineering, Faculty of Engineering, Chulalongkorn University in 1997.