

## REFERENCES

- Barthomeuf, D., and Mallmann, A. (1990). Adsorption of aromatics in NaY and  $\text{AlPO}_4.5$  correlation with the desorbent properties in separation. Industrial Engineering Research, 29, 1435-1438.
- Barthomeuf, D. (1991). Acidity and basicity in zeolites. Catalysis and Adsorption by Zeolites (pp.157-169). Amsterdam C: Elsevier Science Publisher B. V.
- Barthomeuf, D. (1996). Basic Zeolites: Characterization and Uses in Adsorption and Catalysis. (pp.541-572). Marcel Dekker Inc.
- Bellat, J. P., Pilverdierr, E., Simonot-Grange, M. H., and Julian, S. (1997). Microporous volume and external surface of Y zeolite accessible to *p*-xylene and *m*-xylene. Microporous Materias, 9, 213-220.
- Bellat, J. P., Simonot-Grange, M. H., and Julian, S. (1995). Adsorption of gaseous *p*-xylene and *m*-xylene on NaY, KY, and BaY zeolites: Part 1, adsorption equilibria of pure xylene. Zeolite, 15, 124-130.
- Choi, S.Y., Park, Y.S., Hong, S.B., and Yoon, K.B. (1996). Iodine as a visible probe for the evaluation of zeolite donor strenght. Journal of American Chemical Sociaty, 118, 9377-9386.
- Cottier, V., Bellet, J. P., and Simonot-Grange, M. H. (1997). Adsorption of *p*-xylene/*m*-xylene gas mixture on BaY and NaY zeolite. Coadsorption equilibria and selectivities. Journal of Physical Chemistry, 101, 4798-4802.
- Douglas, M. (1984). Principles of adsorption and adsorption process. New Brunswick: Wiley.
- Furlan, L.T., Chaves, B.C., and Santana, C.G. (1992). Separation of liquid mixtures of *p*-Xylene/ *o*-Xylene in X zeolites: the role of water content on the adsorbent selectivity. Industrial & Engineering Chemistry Research, 31, 1780-1784.
- Geankoplis, J.C. (1993). Transport Process and Unit Operation. 3th ed. (pp. 697-702). New York: Printice Hall International.
- Heider, R., Janssens, G.A., Mortior, W.J., and Schoonheydt, R.A. (1996). Charge sensitivity analysis of intrinsic basicity of faujasite-type zeolites using the

- electronegativity equalization method (EEM). The Journal of Physical Chemistry, 100, 19728-19734.
- Hulme, R., Ronald, E., Weig, R., and Ruthven, D. M. (1991). Binary and ternary equilibria for C<sub>8</sub> aromatics on KY faujasite. Engineering Chemical Research, 30, 752-760.
- Kitagawa, T., Tsunekawa, T., and Iwayama, K. (1996). Monte Carlo simulation on adsorptions of benzene and xylenes in sodium Y zeolites. Microporous Materials, 7, 227-233.
- Lachet, V., Boutin, A., Tavitiyan, B., and Fuchs, A.H. (1999). Molecular simulation of *p*-xylene/ *m*-xylene adsorption in Y zeolites single components with binary mixtures study. Langmuir, 15, 8678-8685.
- Lachet, V., Boutin, A., Tavitiyan, B., and Fuchs, A.H. (1998). Computation study of *p*-xylene/ *m*-xylene mixtures adsorbed in NaY zeolite. The Journal of Physical Chemistry B, 102, 9224-9233.
- Ngamkitidachakul, T. (2000). Fundamentals of Xylene Adsorptives Separation. M.S. Thesis in Petrochemical Technology, The petroleum and Petrochemical College, Chulalongkorn University.
- Pichon, C., Methivier, A.A., Simonot-Grange, M. H., and Baerlocher, C. (1999). Location of water and xylene molecules adsorbed on prehydrated zeolite BaX. A low-temperature neutron powder diffraction study. The Journal of Physical Chemistry B, 103, 10197-10203.
- Pichon, C., Methivier, A. and Simonot-Grange, M. H. (2000). Adsorption of *m*-xylene on prehydrated zeolite BaX: Correlation between T-program desorption and low-temperature neutron powder diffraction studies. Langmuir, 16, 1931-1936.
- Sanderson, R.T. (1976). Chemical Bonds and Bond Energy. Academic Press, New York.
- Sanderson, R.T. (1983). Electronegativity and bond energy. American Chemical Society, 105, 8, 2259-2261.
- Seko, M., Miyake, T., and Inada, K. (1980). Sieves for Mixed Xylenes Separation. Hydrocarbon Processing, Jan, 133-138.

- Suntornpun, R. (2002). Acid-Base Interaction between C<sub>8</sub> Aromatics and X and Y Zeolites. M.S. Thesis in Petrochemical Technology, The petroleum and Petrochemical College, Chulalongkorn University.
- Tournier, H., Barreau, A., Tavitian, B., Roux, D.L., Sulger, C., and Beaument, V. (2000). Two experimental methods to study adsorption equilibria of xylene isomers in the liquid phase on a Y zeolites. Microporous and Mesoporous Materials, 39, 537-547.
- Tournier, H. , Barreau, A., Tavitian, B., Roux, D.L., Moise, J.C., Bellat, J.P., and Paulin, C. (2001). Adsorption equilibrium of xylene isomer and p-diethylbenzene on a prehydrated BaX zeolite. Industrial & Engineering Chemistry Research, 40, 5983-5990.
- Tsoug, D. (1989). Separation of *p*-xylene and ethylbenzene from C<sub>8</sub> aromatics using medium-pore zeolite. Engineering Chemical Research, 28, 572-576.
- Tsoug, Y. (1988). Effects of moisture in separation of C<sub>8</sub> aromatics using medium-pore zeolites. Industrial & Engineering Chemistry Research, 27, 1665-1668.
- Varayanond, V. (2001). Fundamentals of xylene adsorptives separation. M.S. Thesis in Petrochemical Technology, The petroleum and Petrochemical College, Chulalongkorn University.
- Yang, R. T. (1997). Gas Separation By Adsorption Process (pp. 19-23). London: Imperial college Press.

## APPENDIX

### A1. Sample preparation

#### A1.1 Multi-component Pulse Test

**Table A.1** Sample preparation for the Multi-component Pulse Test

component	wt., g.	Density, g/ml.	Volume, ml.
<i>p</i> -xylene	20	0.8610	23.229
<i>m</i> -xylene	20	0.8684	23.031
<i>o</i> -xylene	20	0.8970	22.297
ethylbenzene	20	0.8670	23.068
n-C <sub>9</sub>	20	0.7217	27.712

The 120 ml, approximately, of stock solution for using in the Dynamic Adsorption Multi-component Pulse Test was prepared followed Table A.1 above.

**Table A.2** Zeolite used in the Multi-component Pulse Test

zeolites	Amount, g.
<i>Mg2.0X</i>	43.4
<i>Ca2.0X</i>	45.9
<i>Sr2.0X</i>	48.0
<i>Ba2.0X</i>	55.1
<i>Mg2.5X</i>	52.3
<i>Ca2.5X</i>	46.4
<i>Sr2.5X</i>	50.9
<i>Ba2.5X</i>	51.6
<i>MgY</i>	43.9
<i>CaY</i>	43.6
<i>SrY</i>	47.0
<i>BaY</i>	51.6

## A1.2 Multi-component Breakthrough Test

**Table A.3** Sample preparation for the Multi-component Breakthrough Test

component	wt., g.	Density, g/ml.	Volume, ml.
<i>p</i> -xylene	20	0.8610	23.229
<i>m</i> -xylene	40	0.8684	46.062
<i>o</i> -xylene	20	0.8970	22.297
ethylbenzene	13	0.8670	15.379
n-C <sub>9</sub>	7	0.7217	9.237

The 120 ml, approximately, of stock solution for using in the Dynamic Adsorption Multi-component Breakthrough Test was prepared followed Table A.1 above.

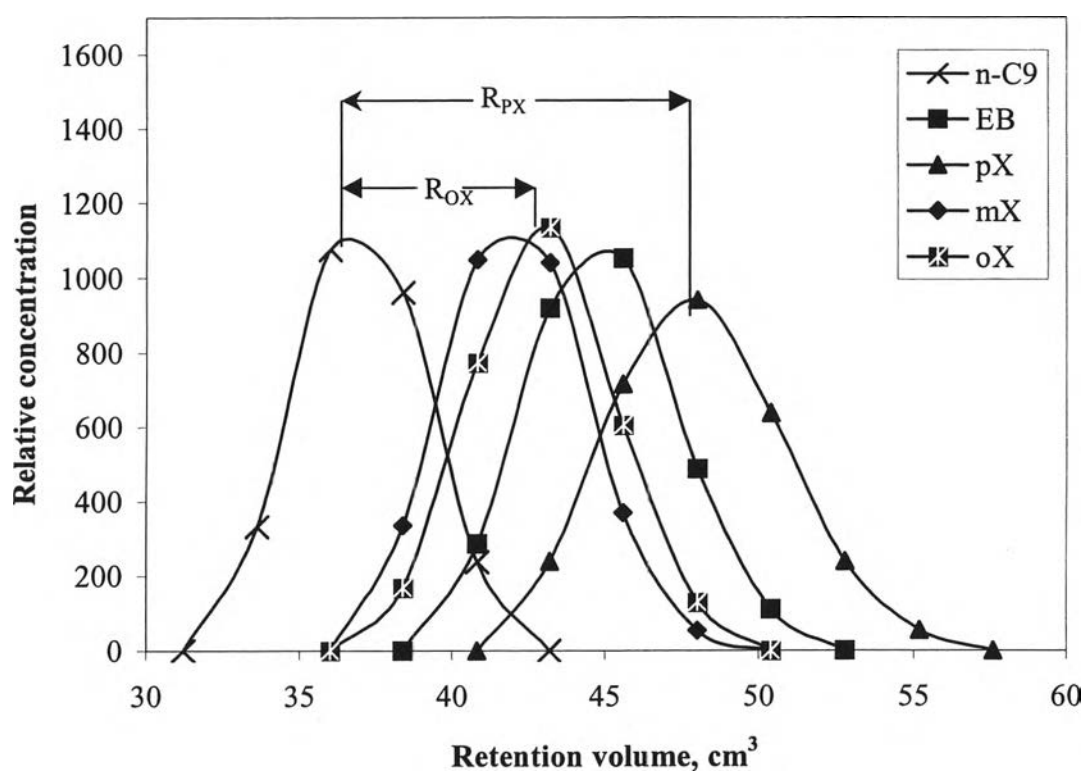
**Table A.4** Zeolite used in the Multi-component Breakthrough Test

zeolites	Amount, g.
<i>Mg2.0X</i>	43.4
<i>Ca2.0X</i>	45.9
<i>Sr2.0X</i>	48.0
<i>Ba2.0X</i>	55.1
<i>Mg2.5X</i>	52.3
<i>Ca2.5X</i>	46.4
<i>Sr2.5X</i>	50.9
<i>Ba2.5X</i>	51.6
<i>MgY</i>	43.9
<i>CaY</i>	43.6
<i>SrY</i>	47.0
<i>BaY</i>	51.6

## A2. Selectivity calculation

### A2.1 Multi-component Pulse Test

Data obtained from experiment was relative effluent concentration of each component. The relative concentration were plotted versus effluent volume as showed in Figure A.1.



**Figure A.1** A schematic of Multi-component pulse test.

Selectivity is a ratio of net retention volume. For example, the *p*-xylene selectivity with respect *o*-xylene can be calculated from the ratio of net retention volumes of *p*-xylene,  $R_{PX}$ , to *o*-xylene,  $R_{OX}$ .

$$\alpha_{PX/OX} = \frac{R_{PX}}{R_{OX}} \quad (A1)$$

The net retention volume of each component was measured by using the index of the tracer peak as the zero origin. As showed in Figure A.1,  $R_{px}$  is a distance from center of tracer, nonane, peak to a center of *p*-xylene peak.

The *p*-xylene selectivity with respect to the other components, ethylbenzene and *m*-xylene, can be calculated in the same way.

The selectivity can be calculated from the net retention volume. Because the net retention volume of any component is ideally proportional to its distribution coefficient, i.e., its concentration in the adsorbed phase divided by its concentration in the unadsorbed phase, the calculated quantity is essentially equivalent to selectivity as defined separations carried out in a liquid system (Kulprathipanja, 2001)

In this work, Sorbex Database was used for calculating selectivity from Pulse Test technique. It is a soft ware that was developed and provided by UOP, LLC.

## A2.2 Multi-component Breakthrough test

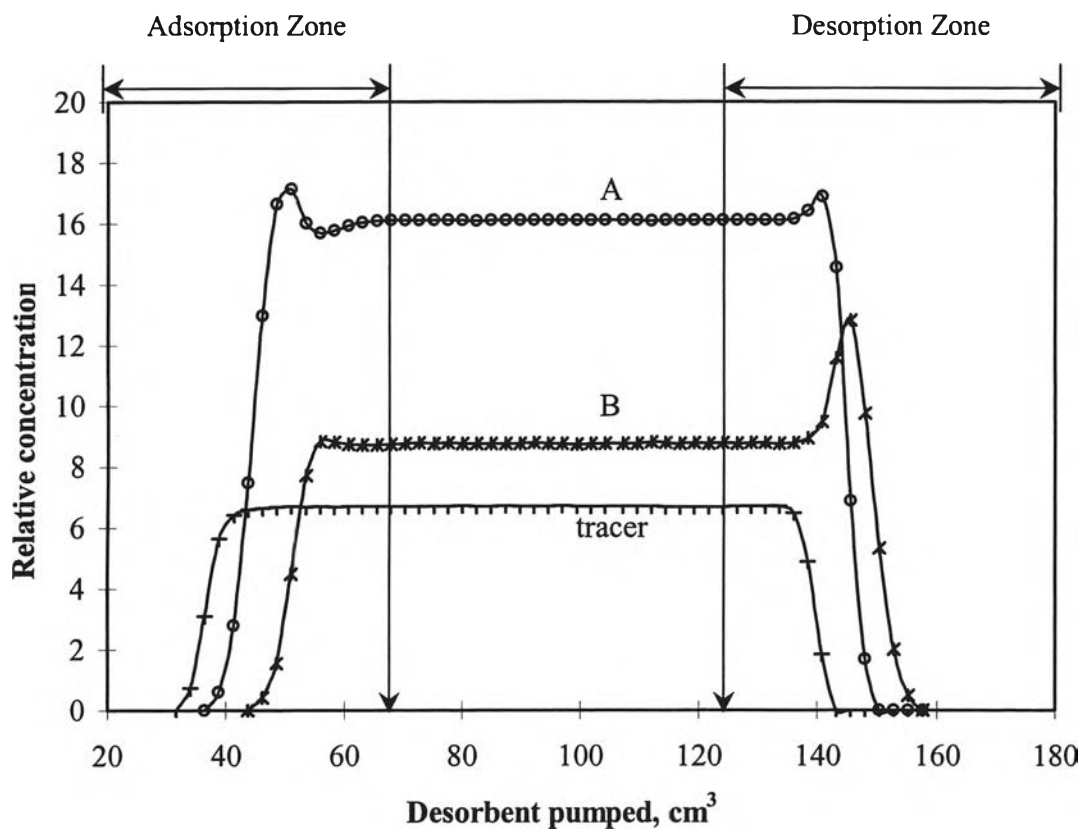
From Breakthrough curve, there are adsorption zone and desorption zone as showed in Figure A.2. Selectivity can be calculated both in these 2 zones. All selectivities reported in this work were calculated from adsorption zone. Selectivity can be calculated by using the same principal as in Pulse Test technique. By finding the ratio of net retention volume of two components. Firstly, the area under adsorption curve of the components  $A_{tracer}$ ,  $A_A$  and  $A_B$  were calculated. The constant height in breakthrough region of each curve,  $H_{tracer}$ ,  $H_A$  and  $H_B$  was measured. Consequently, the adsorbed volume of each component was calculated as

$$L_A = \frac{A_A}{H_A} \quad (A3)$$

By subtracting  $L_{tracer}$  from  $L$  of component, the adsorbed volume of each component was obtained. The selectivity of component *B* with respect to component *A* was defined as the ratio of adsorbed volume *A* to adsorbed volume *B*

$$\alpha_{B/A} = \frac{L_{tracer} - L_R}{L_{tracer} - L_A} \quad (A4)$$

By using the same method, the *p*-xylene selectivity with respect to the others, *m*-xylene, *o*-xylene and ethylbenzene, was calculated.



**Figure A.2** A schematic of Multi-component Breakthrough Test.



### A3. Heat of adsorption calculation

According to equation (4.2), parameters of adsorption model were calculated by using a solver function in Microsoft Excel. The calculation of each component was based on a set of temperature: 100, 120, 150, 177 °C. Ethylbenzene, *o*-xylene and *m*-xylene, subscript 2, were calculated by comparing with *p*-xylene, subscript 1.

**Table A.5** Adsorption parameters of *p*-xylene and ethylbenzene

Temperature	$k_1$	$k_2$	$K_{01}$	$H_1$	$K_{02}$	$H_2$	Selectivity
373	0.2388	0.1519	1.8809	1.199	1.2129	0.970	1.572488
393	0.2973	0.1817	1.8809	1.199	1.2129	0.970	1.636708
423	0.3876	0.204	1.8809	1.199	1.2129	0.970	1.900194
450	0.3162	0.204	1.8809	1.199	1.2129	0.970	1.550387

**Table A.6** Adsorption parameters of *p*-xylene and *m*-xylene

Temperature	$k_1$	$k_2$	$K_{01}$	$H_1$	$K_{02}$	$H_2$	Selectivity
373	0.3591	0.1519	2.0589	1.199	0.8991	0.842	2.364343
393	0.4158	0.1817	2.0589	1.199	0.8991	0.842	2.288982
423	0.5115	0.204	2.0589	1.199	0.8991	0.842	2.507917
450	0.4073	0.204	2.0589	1.199	0.8991	0.842	1.996713

**Table A.7** Adsorption parameters of *p*-xylene and *o*-xylene

Temperature	$k_1$	$k_2$	$K_{01}$	$H_1$	$K_{02}$	$H_2$	Selectivity
373	0.3776	0.1519	2.0841	1.199	0.8408	0.814	2.486089
393	0.4501	0.1817	2.0841	1.199	0.8408	0.814	2.477554
423	0.5451	0.204	2.0841	1.199	0.8408	0.814	2.672646
450	0.4152	0.204	2.0841	1.199	0.8408	0.814	2.035549

## CURRICURUM VITAE

**Name:** Ms. Suwanna Limsamutchaikul

**Date of Birth:** Jun 4, 1979

**Nationality:** Thai

**University Education:**

1997-2000 Bachelor Degree of Science in Chemical Technology, Faculty of Science, Chulalongkorn University, Bangkok, Thailand.

