

## REFERENCES

- Armaroli, T., Finocchio, E., Busca, G., Rossini, S. (1999) A FT-IR study of the adsorption of C5 olefinic compounds on NaX zeolite. Vibretional Spectroscopy, 20, 85-94.
- Auerbach, S. M., Carrado, K.A., and Dutta, P.K. (2003) Handbook of Zeolite Science and Technology. New York: Marcel Dekker.
- Chempath, S., Denayer, J.F.M., De Meyer, K., Baron, G.V. and Snurr, R.Q. (2004) Adsorption of liquid-phase mixtures in silicalite: Simulations and experiment. Langmuir, 20, 150-156.
- Choudhary, V.R. and Mayadevi, S. (1996) Adsorption of methane, ethane, ethylene, and carbon dioxide on silicalite-I. Zeolites, 17(5-6),501-507.
- De Meyer, K., Chempath, S., Denayer, J.F.M., Martens, J.A., Snurr, R.Q., and Baron, G.V. (2003) Packing effects in the liquid-phase adsorption of C5-C22 n-alkanes on ZSM-5. The Journal of Physical Chemistry B, 107, 10760-10766.
- Denayer, J.F.M., De Meyer, K., Martens, J.A. and Baron, G.V. (2003) Molecular competition effects in liquid-phase adsorption of long-chain n-alkane mixtures in ZSM-5 zeolite pores. Angewandte Chemie International Edition, 115(42), 2880-2883.
- Huften, J.R. and Danner, R.P. (1993) Chromatographic study of alkanes in silicalite: Equilibrium properties. American Institute of Chemical Engineers Journal, 39(6), 954-961.
- Huften, J.R. and Danner, R.P. (1993) Chromatographic study of alkanes in silicalite: Transport properties. American Institute of Chemical Engineers Journal, 39(6), 962-973.
- Kulprathipanja, S. and Johnson, A.J. (2001) Handbook of Porous Solids Chapter 6.4, Liquid Separations.
- Olson, D.H., Kokotallo, G.T., and Lawton, S.L. (1981) Crystal structure and structure-related properties of ZSM-5. The Journal of Physical Chemistry, 85, 2238-2243

- Pascual, P., Ungerer, P., Tavitian, B., and Boutin, A. (2004) Development of a transferable guest-host force field for adsorption of hydrocarbons in zeolite. II. Prediction of alkane/alkene selectivity in silicalite. The Journal of Physical Chemistry B, 108, 393-398.
- Richards, R.E. and Rees, L.V.C. (1986) Sorption and packing of n-alkane molecules in ZSM-5. Langmuir, 3, 335-340.
- Ruthven, D.M. (1984). Principles of Adsorption and Adsorption Processes. New York: Wiley.
- Sun, M.S., Talu, O., and Shah, D.B. (1996) Adsorption equilibrium of C<sub>5</sub>-C<sub>10</sub> normal alkanes in silicalite crystals. The Journal of Physical Chemistry, 100, 17276-17280.
- Talu, O., Sun, M.S., and Shah, D.B. (1998) Diffusivities of n-alkanes in silicalite by steady-state single-crystal membrane technique. American Institute of Chemical Engineers Journal, 44(3), 681-694.
- Zhu, W., Van de Graaf, J.M., Van den Broeke, L. J. P., Kapteijn, F., and Moulijn, J. A. (1998) TEOM: A unique technique for measuring adsorption properties. Light alkanes in silicalite-1. Industrial & Engineering Chemistry Research, 37, 1934-1942.

## APPENDIX

### A.1. Selectivity Calculation

#### A.1.1 Binary Competitive Equilibrium Adsorption Isotherm

The n-paraffin selectivity with respect to n-olefin was determined as

$$\alpha_{P/O} = \frac{X_P / X_O}{Y_P / Y_O} \quad (\text{A.1})$$

where  $X_P$  is the mole fraction of n-paraffin in adsorbed phase.

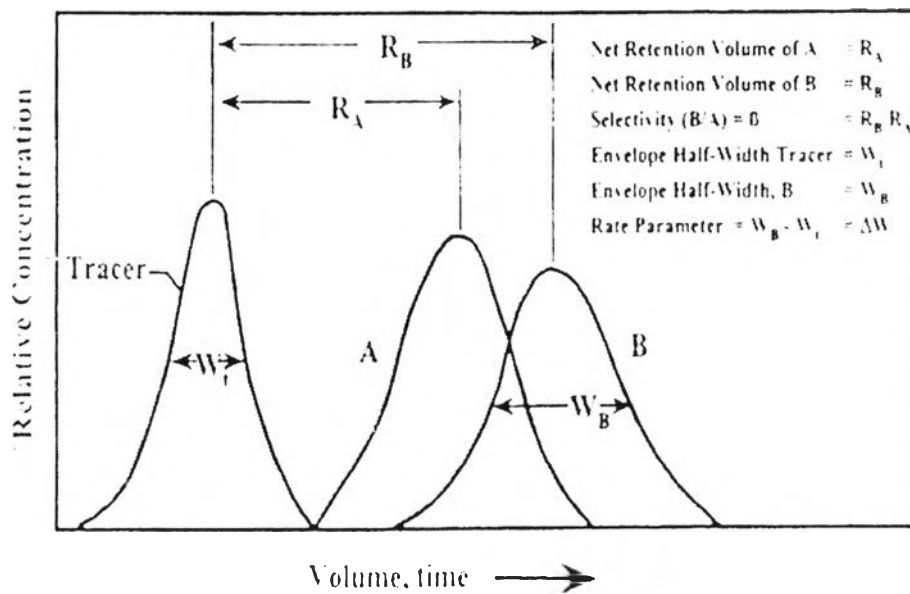
$X_O$  is the mole fraction of n-olefin in adsorbed phase.

$Y_P$  is the mole fraction of n-paraffin in liquid phase.

$Y_O$  is the mole fraction of n-olefin in liquid phase.

#### A.1.2 Dynamic Adsorption: Multi-Component Pulse Test

A schematic pulse test is shown in Figure A.1. In this example, the feed contains components A and B along with a tracer. The tracer is selected so that it will not be adsorbed by the system being studied. Each peak is indexed on the volume scale at the midpoint of the cord at 50% peak height. The net retention volume of each component is measured using the index of the tracer peak as the zero origin. The adsorbent selectivity for a more strongly adsorbed component B over a less strongly adsorbed component A can be calculated from the ratio of net retention volume of component B to component A. (Kulprathipanja and Johnson, 2001)



**Figure A.1** Schematic pulse test: 2 components and tracer.

## A.2. Sample Preparation

### A.2.1 Single Component Adsorption Isotherm

**Table A.1** Sample preparation for single component adsorption isotherms

wt., g.	Hydrocarbon, g	iso-Octane, g
0.5	0.05	9.95
1	0.1	9.90
1.5	0.15	9.85
2	0.2	9.80
3	0.3	9.70
5	0.5	9.50

### A.2.2 Binary Competitive Adsorption Isotherm

**Table A.2** Sample preparation for binary competitive adsorption isotherms

Wt., g.	n-Paraffin, g	n-Olefin, g	iso-Octane, g
0.5	0.025	0.025	9.95
1	0.050	0.050	9.90
1.5	0.075	0.075	9.85
2	0.10	0.10	9.80
3	0.15	0.15	9.70
5	0.25	0.25	9.50

### A.3. Double Site Langmuir Parameters.

#### A.3.1 Single Component Adsorption Isotherm

**Table A.3** Double site Langmuir parameters for n-paraffin and n-olefin adsorbed on silicalite at 25 °C in single adsorption isotherms

Hydrocarbons	$Q_{max, C}$	$Kd_C$	$Q_{max, I}$	$Kd_I$	R
C <sub>6</sub>	3.4720	0.0259	3.5866	0.0259	0.9809
1-C <sub>6</sub>	2.1646	0.0006	4.7173	0.0237	0.9999
C <sub>8</sub>	3.4873	0	0.3378	0.0011	0.9952
1-C <sub>8</sub>	3.2070	0	0.6264	0.0798	0.9994
C <sub>10</sub>	1.9751	0.0074	1.9516	0.0073	0.9941
1-C <sub>10</sub>	3.7463	0.0064	0.1419	1.0339	0.9999
C <sub>12</sub>	1.9018	0.0012	1.8615	0.0012	0.9999
1-C <sub>12</sub>	1.9466	0.0013	1.9028	0.0012	0.9983
C <sub>14</sub>	1.7581	0.0009	1.6991	0.0009	0.9999
1-C <sub>14</sub>	1.7906	0.0011	1.7577	0.0011	0.9986
C <sub>16</sub>	1.4629	0.0012	1.4342	0.0012	0.9981

Hydrocarbons	$Q_{\max, C}$	$Kd_C$	$Q_{\max, I}$	$Kd_I$	R
1- C <sub>16</sub>	1.5241	0.0097	1.5117	0.0097	0.9995
C <sub>18</sub>	1.4224	0.1424	1.3881	0.1425	0.9921
1- C <sub>18</sub>	1.2398	0.0295	1.2094	0.0295	0.9995
C <sub>20</sub>	1.1907	0.0072	1.1267	0.0072	0.9960
1-C <sub>20</sub>	1.2365	0.0117	1.1992	0.0117	0.9999

### A3.2 Binary Competitive Adsorption Isotherm

**Table A.4** Double site Langmuir parameters for n-paraffin and n-olefin adsorbed on silicalite at 25 °C in binary adsorption isotherms

Mixtures	Hydrocarbons	$Q_{\max, C}$	$Kd_C$	$Q_{\max, I}$	$Kd_I$	R
C <sub>6</sub> /1-C <sub>6</sub>	C <sub>6</sub>	0.8207	3.26E-11	2.6262	0.0204	0.9614
	1- C <sub>6</sub>	0.7151	5.88E-11	2.6541	0.0155	0.9482
	Total C-6	1.5666	4.24E-11	5.2782	0.0172	0.9510
C <sub>8</sub> /1-C <sub>8</sub>	C <sub>8</sub>	1.7458	0.0012	0.4610	0.1771	0.9996
	1- C <sub>8</sub>	0.9024	0.0013	0.9006	0.0013	0.9995
	Total C-8	3.5957	0.0012	0.4059	0.1958	0.9996
C <sub>16</sub> /1-C <sub>16</sub>	C <sub>16</sub>	1.0788	5.18E-11	0.2218	0.0312	0.9966
	1- C <sub>16</sub>	1.2493	4.07E-12	0.1179	0.1776	0.9971
	Total C-16	2.4115	2.69E-12	0.2544	0.0996	0.9969
C <sub>18</sub> /1-C <sub>18</sub>	C <sub>18</sub>	0.6440	0.0388	0.6234	0.0384	0.9918
	1- C <sub>18</sub>	0.5967	0.0384	0.5714	0.0384	0.9905
	Total C-18	1.2382	0.0355	1.1927	0.0355	0.9914
C <sub>20</sub> /1-C <sub>20</sub>	C <sub>20</sub>	1.1444	0.0058	0.1110	0.3402	0.9986
	1- C <sub>20</sub>	0.5496	0.0005	0.5317	0.0006	0.9977
	Total C-20	1.1718	0.0061	1.1392	0.0061	0.9980

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