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APPENDICES

APPENDIX A
SAMPLE OF CALCULATIONS

A-1 Calculation of Si/Al Atomic Ratio for Beta Zeolite Preparation

The calculatioin is based on weight of Sodium Aluminate (Al/NaOH = 0.78) in gel preparation.

Molecular Weight of Al = 26.9815

Molecular Weight of $NaAlO_2$ = 81. 97

Using Sodium Aluminate ($NaAlO_2$) 0.702 g as gel preparation.

$$\text{Mole of Al used} = \text{wt.} \times \frac{(\%)}{100} \times \frac{(\text{M.W. of Al})}{(\text{M.W. of } NaAlO_2)} \times \frac{(1\,\text{mole})}{(\text{M.W. of Al})}$$

$$= (0.702)(0.78)\left(\frac{1}{81.97}\right)$$

$$= 6.680 \times 10^{-3} \text{ mole}$$

For example, to prepare Beta zeolite at Si/Al atomic ratio of 80 by using cataloid (SiO_2 30% wt in water) for silicon source.

Molecular Weight of Si = 28.0855

Molecular Weight of SiO_2 = 60.0843

Si/Al atomic ratio of 80

Mole of SiO_2 required = $(6.680 \times 10^{-3})(80)$

= 0.5344 mole

Amount of SiO_2 = (0.5344)(60.0843)

= 32.1090 g

Amount of Cataloid = $\left(\frac{100}{30}\right)(32.1090)$

= 107.0301 g

This is the amount of $NaAlO_2$ and SiO_2 used in gel preparation.

A-2 Calculation of Reactant Flow Rate

The catalyst used = 0.3000 g

packed catalyst into quartz reactor (inside diameter = 0.6 cm)

determine the average high of catalyst bed = H cm. So that,

Volume of bed= $\pi(0.3)^2 \times h$ ml-cat.

Used Gas Hourly Space Velocity (GHSV) = 3000 h^{-1}

$$\text{GHSV} = \frac{\text{Volumetric flow rate}^1}{\text{Volume of bed}}$$

$$\text{Volumetric flow rate}^1 = 3000 \times \text{Volume of bed}$$

$$= 3000\pi \times (0.3)^2 \times H \quad \text{ml/h}$$

$$= \left(\frac{3000\pi \times (0.3)^2 \times H}{60}\right) \text{ml/min}$$

at STP condition:

$$\text{Volumetric flow rate} = \text{Volumetric flow rate}^1 \times \frac{(273.15 + T)}{273.15}$$

Where T = room temperature, °C

A-3 Calculation benzene/isopropanol mole ratio, conversion and selectivity

The alkylation of benzene and isopropanol activity and selectivity was evaluated as follow:

$$\text{Benzene/Isopropanol mole ratio} = \left(\frac{\text{Mole Benzene}}{\text{Mole Isopropanol}}\right)$$

$$\text{Conversion (\%)} = \left(\frac{\text{Feed in - Feed out}}{\text{Feed in}}\right) \times 100$$

For example: H-Beta (Si/Al = 50).

Reaction condition: Temperature = 200°C, GHSV = 3000 h^{-1}, 40 min on stream.

Area of Feed in Benzene = 820821

Area of Feed in Isopropanol = 134560

Area of Feed out Benzene = 578361

Area of Feed out Isopropanol = 3089

From Appendix B: calibration curve of Benzene and Isopropanol

Mole of Feed Benzene = 3.14×10^{-6} mole

Mole of Feed Isopropanol = 1.12×10^{-6} mole

Therefore,

Benzene/Isopropanol mole ratio = 2.79

Conversion of Isopropanol = 97.7 %

Conversion of Benzene = 29.54 %

For example: H-Beta (Si/Al = 50).

Reaction condition: Temperature = 200°C, GHSV = 3000 h^{-1}, 40 min on stream.

Product	Area	Correction factor	Fixed Area	Selectivity (C-wt%)
C_1-C_4	25038	1.0000	25038	6.42
Toluene	4150	1.1111	4611	1.18
Xylene	10089	1.0733	10829	2.78
Cumene	268953	1.1087	298179	76.48
n-Propylbenzene	4664	1.0909	5088	1.31
1,3 DIPB	21378	1.1139	23812	6.11
1,4 DIPB	8457	1.0065	8512	2.18
Other	13809	1.0000	13809	3.54
		Total product area	389879	100.00

Correction factor is obtained from Appendix C

Fixed Area = Area×Correction factor

$$\text{Selectivity (C-wt\%)} = \left(\frac{\text{Fixed area}}{\text{Total product area}}\right) \times 100$$

APPENDIX B

CALIBRATION CURVE

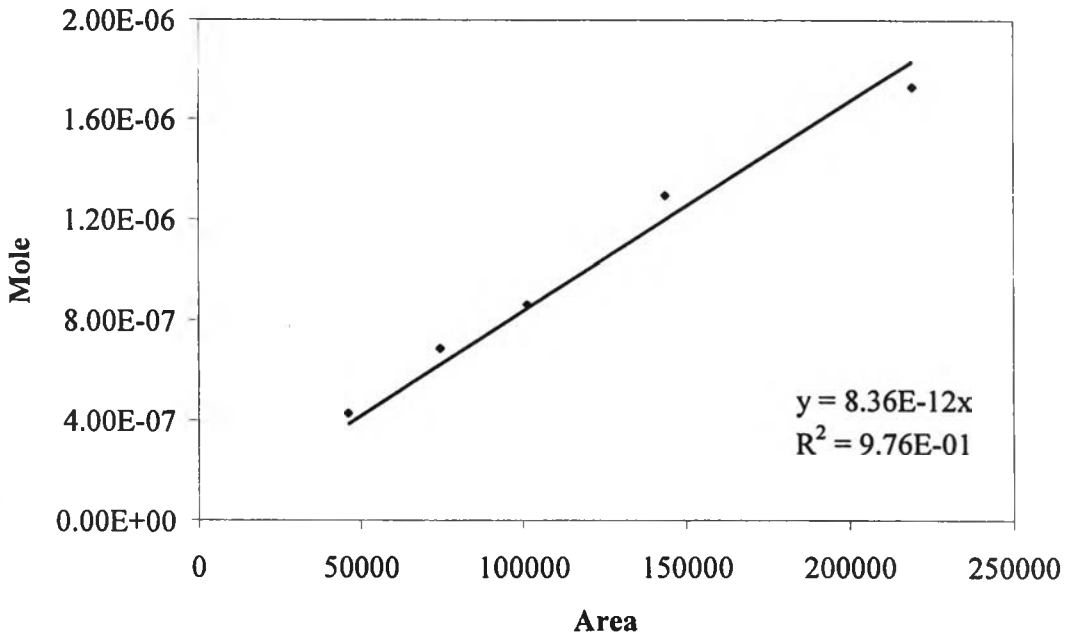

Figure C-1 Calibration curve of Isopropanol

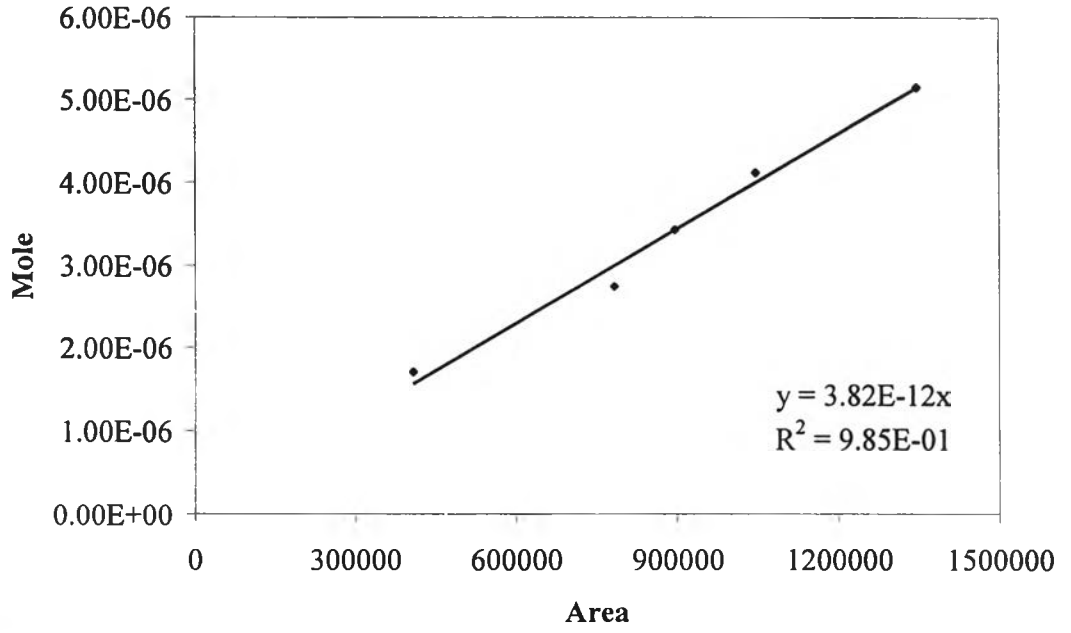

Figure C-2 Calibration curve of Benzene

APPENDIX C
CORRECTION FACTOR

Correction factor for GC with column DB-1

Correction factor, $F = \frac{A/W_{component}}{A/W_{standard}}$ [40]

Give n-heptane is standard component (F = 1)

Reactant	Weight (W)	Area (A)	A/W	Correction factor (F)
C_1-C_4				1.0000
n-Hexane	6.56E-08	206333	3.15×10^{12}	0.9912
n-Heptane	6.82E-08	216505	3.17×10^{12}	1.0000
Isopropanol	7.85E-08	147672	1.88×10^{12}	0.5925
Benzene	8.75E-08	333989	3.82×10^{12}	1.2028
Toluene	8.66E-08	305364	3.53×10^{12}	1.1111
Xylene	8.76E-08	298368	3.41×10^{12}	1.0733
Cumene	8.60E-08	302590	3.52×10^{12}	1.1087
n-Propylbenzene	8.58E-08	297052	3.46×10^{12}	1.0909
1,3 DIPB	8.12E-08	287239	3.54×10^{12}	1.1139
1,4 DIPB	8.53E-08	272489	3.20×10^{12}	1.0065
Other				1.0000

APPENDIX D

DATA OF EXPERIMENT

Table D1 Data of Figure 5.10

Conversion (%)

Temperature (°C)	100	150	200	250	300
Isopropanol	21.56	98.22	97.70	97.90	97.90
Benzene	4.57	25.51	29.54	21.73	13.95

Selectivity (C-wt%)

Cumene	7.81	44.29	76.48	62.93	47.12

Table D2 Data of Figure 5.11

Product distribution (%wt)

Temperature (°C)	100	150	200	250	300
C_1-C_4	88.02	6.53	6.42	16.41	38.15
Toluene	0.00	0.00	1.18	2.53	1.02
Xylene	0.00	0.00	2.78	3.81	2.00
Cumene	7.81	44.29	76.48	62.93	47.12
n-Propylbenzene	0.00	0.00	1.31	3.17	2.15
1,3 DIPB	4.17	28.00	6.11	2.77	0.85
1,4 DIPB	0.00	12.06	2.18	1.06	0.31
Other	0.00	9.12	3.54	7.33	8.39
Total	100.00	100.00	100.00	100.00	100.00

Table D3 Data of Figure 5.12

Conversion (%)

GHSV (h^{-1})	1000	2000	3000	4000	5000
Isopropanol	96.82	97.43	97.70	98.14	98.34
Benzene	29.40	28.69	29.54	28.18	27.76

Selectivity (C-wt%)

Cumene	65.96	72.54	76.48	72.85	63.57

Table D4 Data of Figure 5.13

Product distribution (%wt)

GHSV (h^{-1})	1000	2000	3000	4000	5000
C_1-C_4	12.46	7.98	6.42	7.58	8.00
Toluene	4.56	2.03	1.18	0.58	0.32
Xylene	7.24	3.94	2.78	1.74	1.11
Cumene	65.96	72.54	76.48	72.85	63.57
n-Propylbenzene	2.46	1.89	1.31	0.76	0.55
1,3 DIPB	2.16	5.41	6.11	9.43	15.56
1,4 DIPB	0.79	2.01	2.18	3.42	6.03
Other	4.37	4.20	3.54	3.64	4.87
Total	100.00	100.00	100.00	100.00	100.00

Table D5 Data of Figure 5.14

Conversion (%)

TOS (min)	10	20	40	60	80	100	120	180	240	300	360
Isopropanol	96.34	97.55	97.70	98.53	98.36	97.99	98.24	98.64	98.93	99.04	99.20
Benzene	17.39	32.27	29.54	30.31	29.87	27.30	27.32	26.53	25.55	20.77	19.88

Selectivity (C-wt%)

Cumene	66.93	75.15	76.48	72.37	70.84	69.92	68.00	66.64	60.27	52.81	47.58
1,3+1,4 DIPB	2.51	6.67	8.29	17.43	17.55	17.03	19.77	22.58	24.42	29.72	30.66

Table D6 Data of Figure 5.15

Conversion (%)

Form	Na-form	NH_4-form	H-form
Isopropanol	97.67	97.55	97.70
Benzene	18.17	18.96	29.54

Selectivity (C-wt%)

Cumene	57.92	59.51	76.48

Table D7 Data of Figure 5.16

Product distribution (%wt)

Form	Na-form	NH_4-form	H-form
C_1-C_4	9.19	9.43	6.42
Toluene	0.00	0.00	1.18
Xylene	0.34	0.21	2.78
Cumene	57.92	59.51	76.48
n-Propylbenzene	0.21	0.00	1.31
1,3 DIPB	20.31	19.46	6.11
1,4 DIPB	8.02	7.53	2.18
Other	4.02	3.86	3.54
Total	100.00	100.00	100.00

Table D8 Data of Figure 5.17

Conversion (%)

Si/Al	30	50	80
Isopropanol	97.84	97.70	97.94
Benzene	32.79	29.54	27.18

Selectivity (C-wt%)

Cumene	79.92	76.48	61.96

Table D9 Data of Figure 5.18

Product distribution (%wt)

Si/Al	30	50	80
C_1-C_4	5.62	6.42	6.44
Toluene	1.68	1.18	0.00
Xylene	3.39	2.78	0.75
Cumene	79.92	76.48	61.96
n-Propylbenzene	2.00	1.31	0.43
1,3 DIPB	3.79	6.11	17.87
1,4 DIPB	1.21	2.18	6.72
Other	2.39	3.54	5.83
Total	100.00	100.00	100.00

Table D10 Data of Figure 5.19

Conversion (%)

Si/Al	26			41			70		
TOS (min)	40	80	120	40	80	120	40	80	120
Isopropanol	97.84	97.11	96.46	97.70	98.36	98.24	97.94	97.88	97.54
Benzene	32.79	30.58	28.04	29.54	29.87	27.32	27.18	26.98	26.17

Selectivity (C-wt%)

Cumene	79.92	72.86	67.54	79.48	70.84	68.00	61.96	60.59	59.95

Table D11 Data of Figure 5.20

Conversion (%)

Catalyst	H-Beta*		H-Y*		H-ZSM-5**	
TOS (min)	40 min	120 min	40 min	120 min	40min	120min
Isopropanol	97.70	98.24	98.53	98.75	96.38	97.30
Benzene	29.54	27.32	1.28	12.28	18.72	16.82

Selectivity (C-wt%)

Cumene	76.48	68.00	47.49	20.12	34.58	27.53
n-Propylbenzene	1.31	0.49	0.61	0.00	7.69	5.57

Table D12 Data of Figure 5.21

Conversion (%)

Catalyst	Fresh	Regen1	Regen2
Isopropanol	97.70	97.83	97.20
Benzene	29.54	28.34	29.41

Selectivity (C-wt%)

Cumene	76.48	75.78	74.36

Table D13 Data of Figure 5.22

Product distribution (%wt)

Catalyst	Fresh	Regen1	Regen2
C_1-C_4	6.42	6.22	7.02
Toluene	1.18	1.24	1.28
Xylene	2.78	2.88	2.59
Cumene	76.48	75.78	74.36
n-Propylbenzene	1.31	1.42	1.38
1,3 DIPB	6.11	6.18	6.51
1,4 DIPB	2.18	2.20	2.73
Other	3.54	4.09	4.12
Total	100	100	100

Table D14 Data of Figure 5.23

Conversion (%)

Alkylating agent	Isopropanol		Propylene	
TOS	40 min	180 min	40 min	180 min
Isopropanol	97.70	98.64	98.18	96.73
Benzene	29.54	26.53	27.96	18.43

Selectivity (C-wt%)

Cumene	76.48	66.64	70.29	49.71

VITA

Mr. Somchai Panichsarn was born in Bangkok, Thailand on March 3, 1977. He received Bachelor's Degree of Science from Department of Chemical Technology, Faculty of Science, Chulalongkorn University in 1998.