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APPENDICES

APPENDIX A

SAMPLE OF CALCULATIONS

A-1. Calculation of Si/Al Atomic Ratio for ZSM-5

The calculations base on weight of sodium silicate ($Na_2O.SiO_2.H_2O$) in B1 and B2 solution.

Molecular weight of Si	=	28.0855
Molecular weight of SiO_2	=	60.0843
Weight percent of SiO_2 in sodium silicate	=	28.5
Molecular weight of Al	=	26.9815
Molecular weight of $AlCl_3$	=	133.3405
Weight percent purity of $AlCl_3$	=	97

For example, to prepare MFI at Si/Al atomic ratio of 80
Using sodium silicate 69 g with 45 ml of water as B1 and B2 solution.

$$\text{Mole of Si used} = \frac{\text{wt(\%)}}{100} \times \frac{\text{(M.W. of Si)}}{\text{(M.W. of SiO2)}} \times \frac{\text{(1 mole)}}{\text{(M.W. of Si)}}$$

$$= 69 \times (28.5/100) \times (1/60.0843)$$

$$= 0.3273$$

Si/Al atomic ratio = 80

Mole of $AlCl_3$ required	=	0.3273/80
	=	4.09125×10^{-2} mole
Amount of $AlCl_3$	=	$4.09125 \times 10^{-2} \times 133.34 (100/97)$
	=	0.5625 g

Which used in A1 and A2 solutions.

A-2 Calculation of the amount of cobalt loaded to ZSM-5 catalyst

Determine the amount of cobalt are used loading to catalyst by incipient impanation method.

The catalyst use = 0.1 g

For example, to prepare Co/ZSM-5 at 1% wt cobalt loading.

The cobalt use = X

So that

$$\frac{X}{1+X} = \frac{1}{100}$$

$$99X = 1$$

$$X = 1/99 = 0.010$$

Use $Co(NO_3)_2.6H_2O$ (M.W. 291.03)

Weight of $Co(NO_3)_2.6H_2O$ $= 0.01 \times \frac{291.03}{58.93}$

$= 0.04938$ g

A-3 Calculation of particle size from SEM photograph

Diameter sizes measured from SEM photograph of the as-synthesized product of the H/ZSM-5 catalysts were calculated as follow,

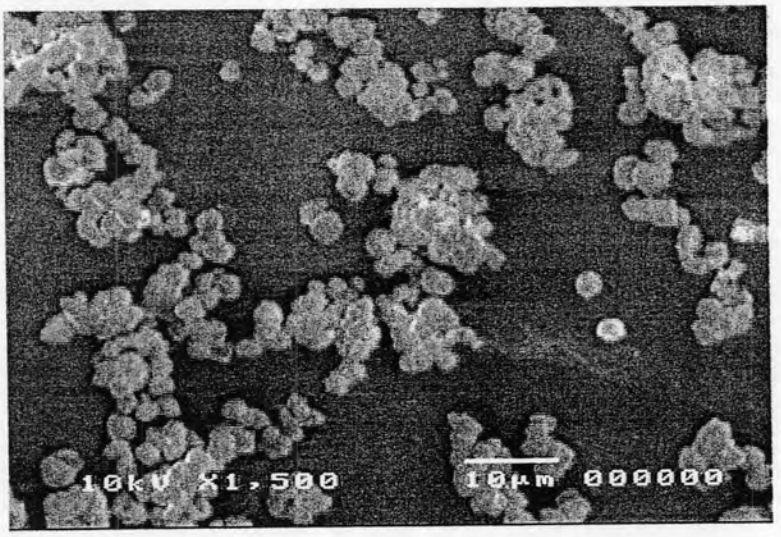

Figure A1 Scanning electron micrograph of H/ZSM-5 (3.4µm) catalyst.

At x 1500 magnification, the scale is

1.6 cm = 10µm

From SEM photograph, it was found that the diameter size of particle was 0.5 cm. Therefore, the diameter size observed by SEM is

$$\text{Diameter size} = \frac{10\mu m \times 0.5\ cm}{1.6\ cm}$$

$$\text{Diameter size} = 3.2\ \mu m$$

The measure diameter sizes from SEM photograph were cm. The average particle size was

$$\text{Particle size} = \frac{3.4 + 3.2 + 3.8 + 4.0 + 3.4 + 3 + 3.2 + 3.4 + 3.5 + 3.1}{10}$$

$$= 3.4\ \mu m$$

A-4 Calculation the vapor pressure of methanol

Set the partial pressure of methanol to the requirement by adjusting the temperature of saturator according to the Antoine equation

$$\log P = A - \frac{B}{(T+C)}$$

When P = Pressure, mm Hg

T = temperature, °C

A, B and C is constants

A = 7.89750 B = 1474.08 C = 229.13

A-5 Calculation of percent crystallinity

$$\% \text{ Crystallinity} = \frac{\text{Area under XRD pattern of sample X 100}}{\text{Area under XRD pattern of reference}}$$

APPENDIX B

CALCULATIONS OF REACTION FLOW RATE

Sample of calculation

The used catalyst = 0.050 g

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

Determine the average high of catalyst bed = 0.5 cm, so that

Volume of bed = ¶$(0.3)^2$ x 0.5 = 0.1413 ml

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

$$GHSV = \frac{60 \text{ (ml/min)}}{0.1413 \text{ ml}}$$

$$GHSV = 424.6285 \text{ min}^{-1}$$

$$GHSV = 424.6285 * 60 = 25477 \text{ h}^{-1}$$

At STP condition :

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

Where T = room temperature

APPENDIX C

DATA OF EXPERIMENT

Calculation of conversion and hydrocarbon distribution of methanol conversion reaction

Methanol conversion activity was evaluated in term of conversion of methanol into other hydrocarbon

$$\text{Methanol conversion (\%)} = \frac{(\text{methanol conversion}_{in} - \text{methanol conversion}_{out}) \times 100}{\text{methanol conversion}_{in}}$$

Selectivity of product is defined as mole of product (B) from with respect to mole of methanol converted:

$$\text{Selectivity B (\%)} = \frac{\text{mole of B form} \times 100}{\text{mole of methanol converted}}$$

Where B is product, mole of B can be measure employing the calibration curve of products.

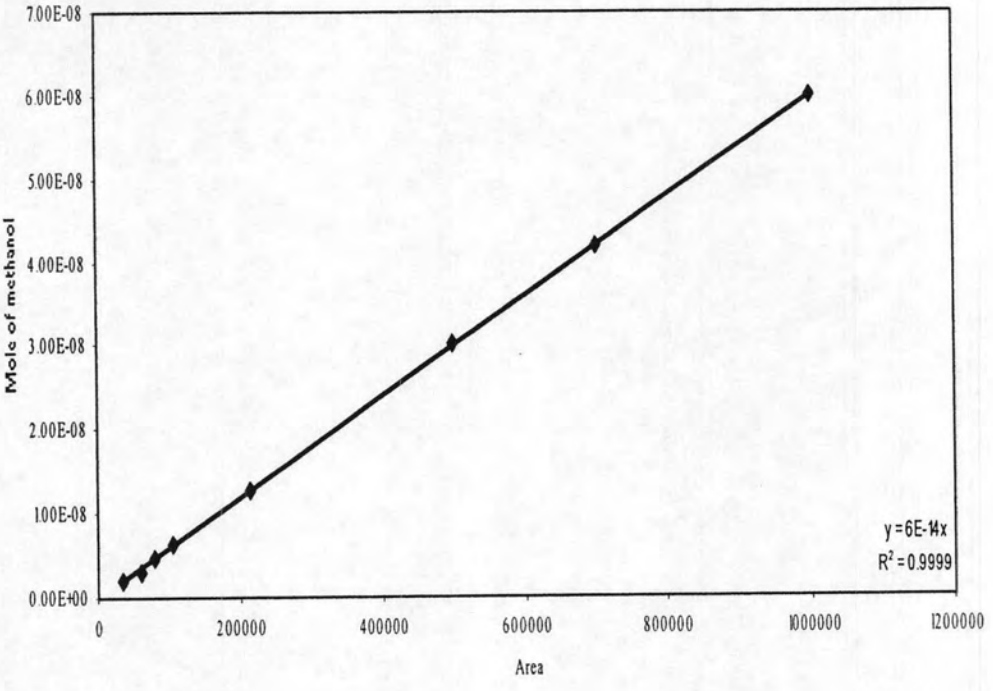

Figure C.1 The calibration curve of methanol.

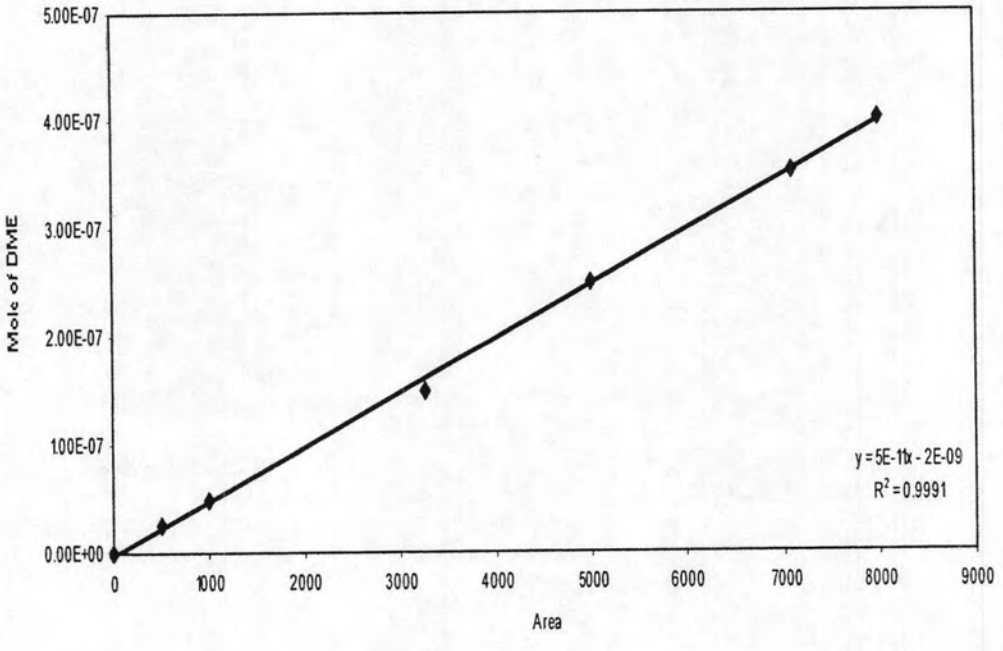

Figure C.2 The calibration curve of DME.

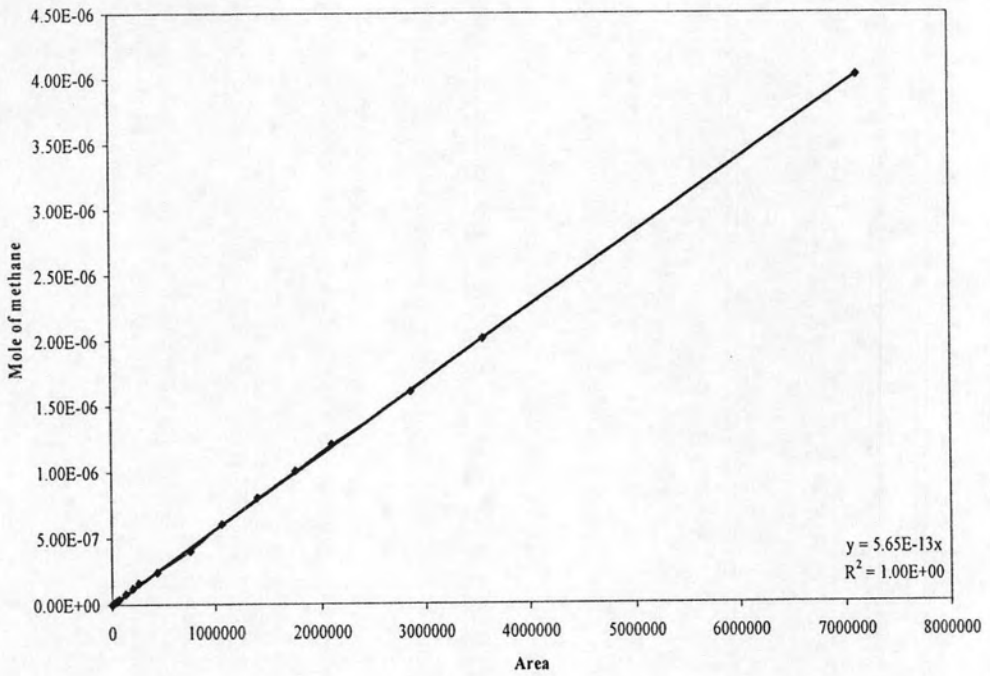

Figure C.3 The calibration curve of methane.

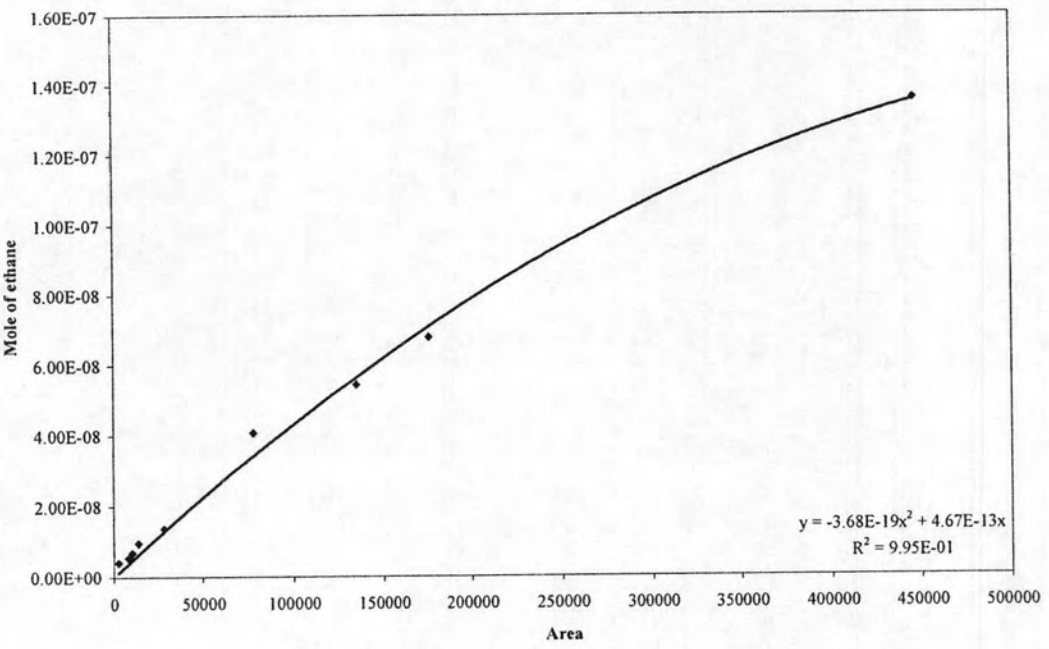

Figure C.4 The calibration curve of ethane.

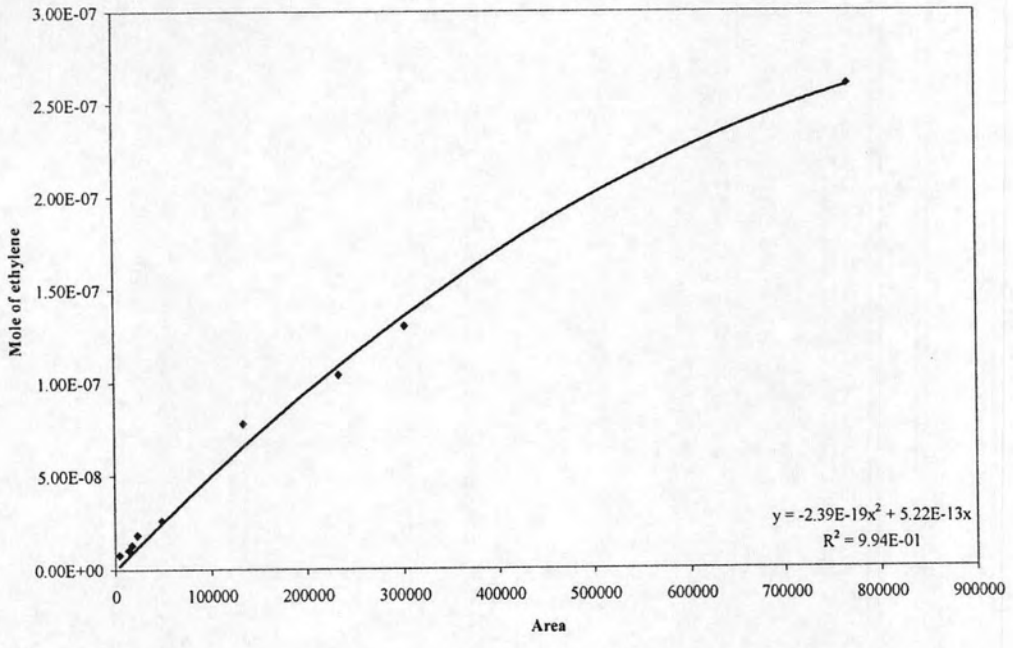

Figure C.5 The calibration curve of ethylene.

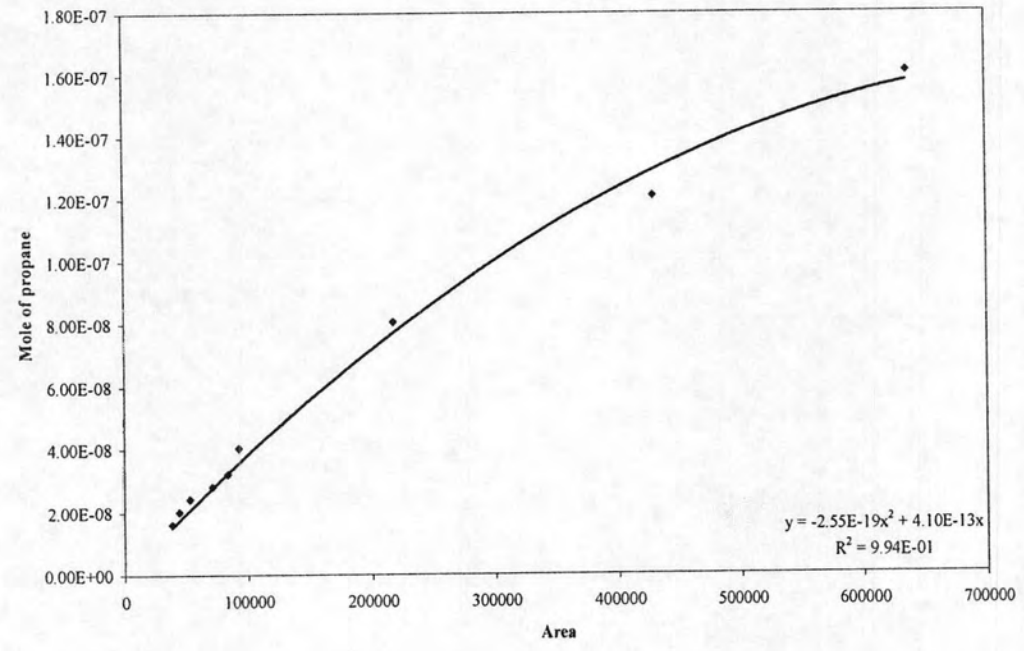

Figure C.6 The calibration curve of propane.

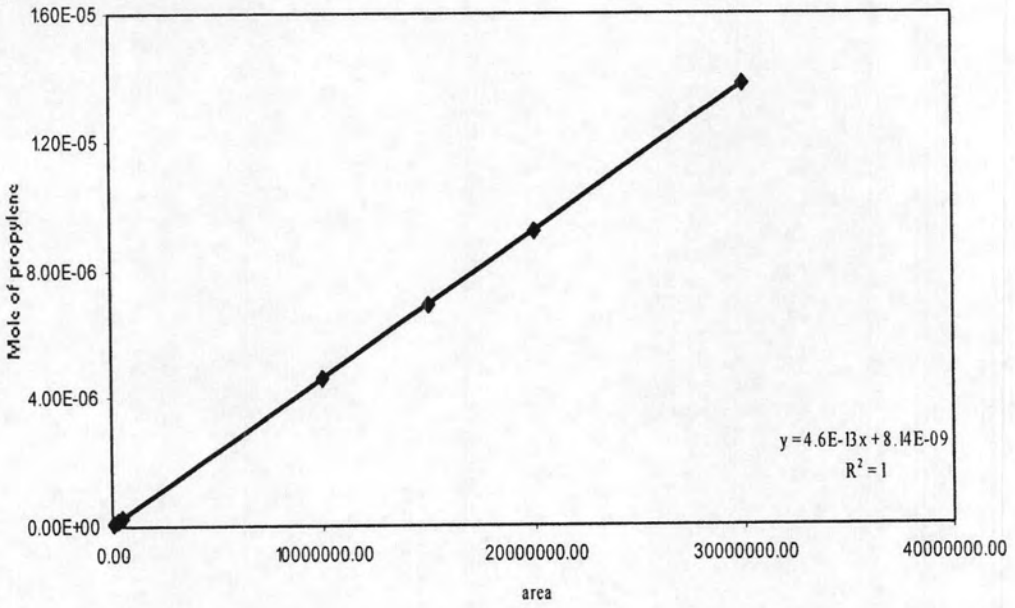

Figure C.7 The calibration curve of propylene.

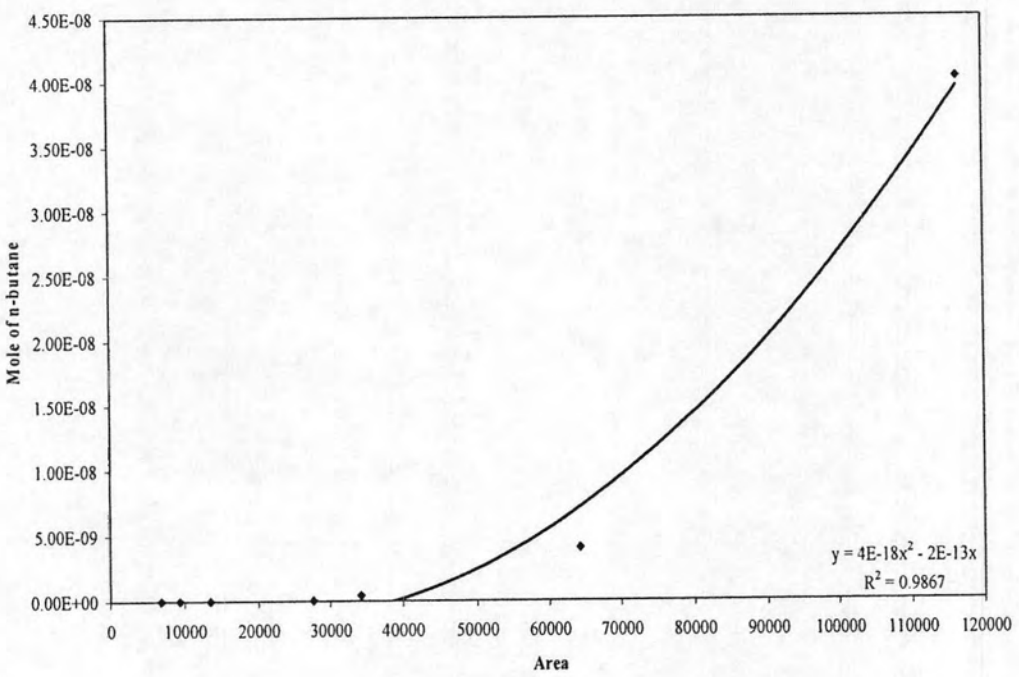

Figure C.8 The calibration curve of n-butane.

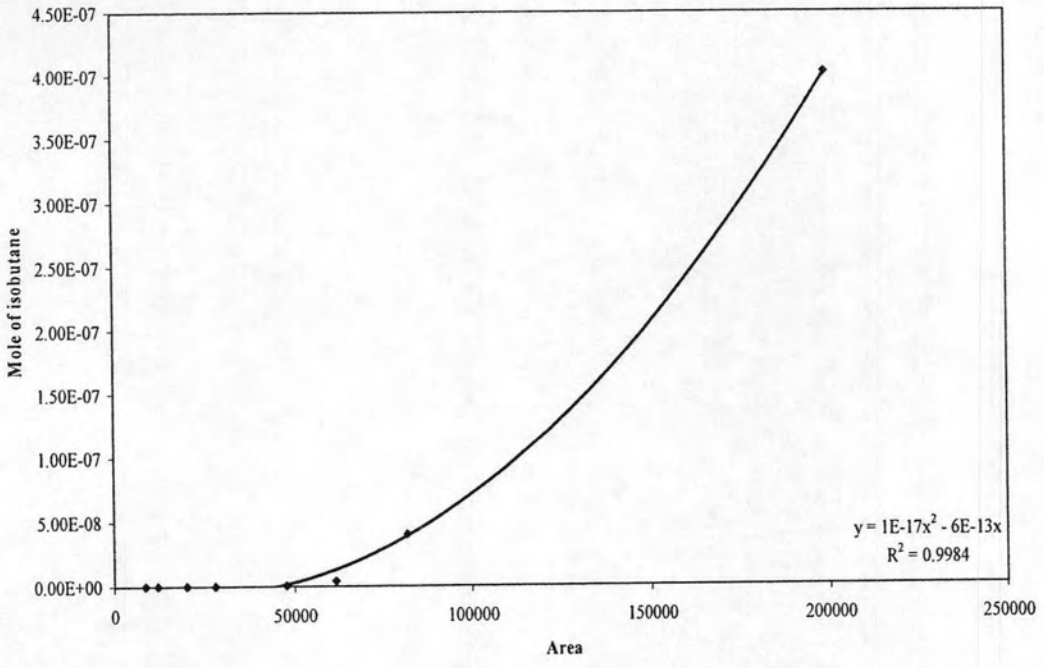

Figure C.9 The calibration curve of isobutane.

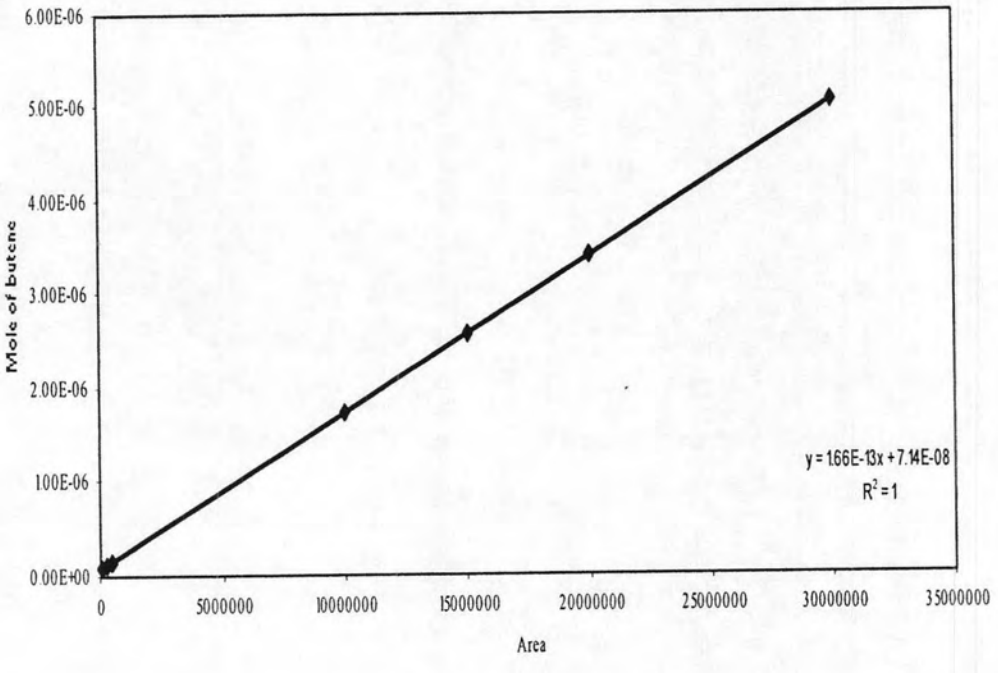

Figure C.10 The calibration curve of isobutene.

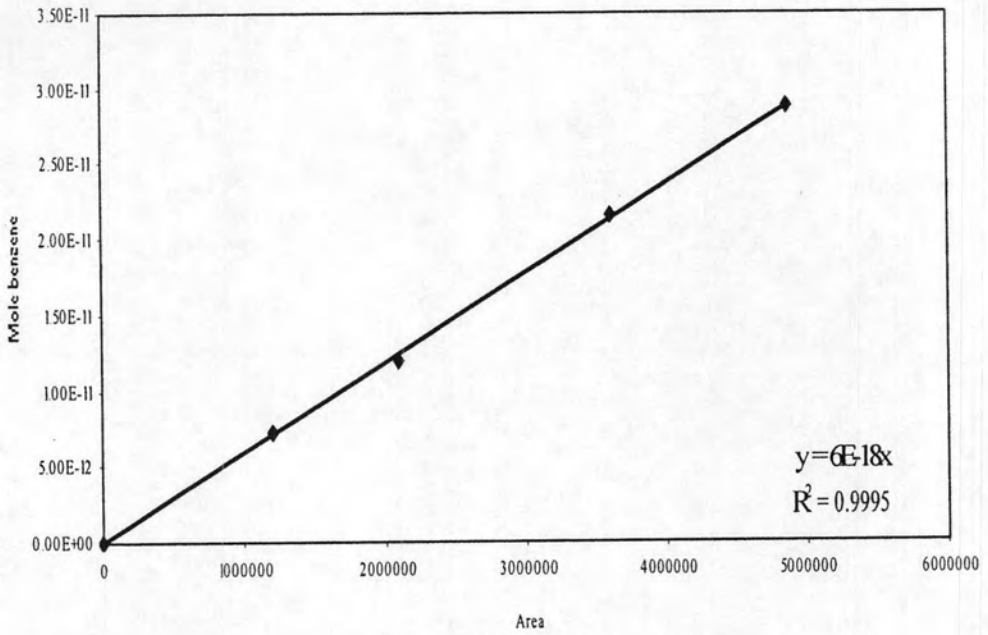

Figure C.11 The calibration curve of benzene

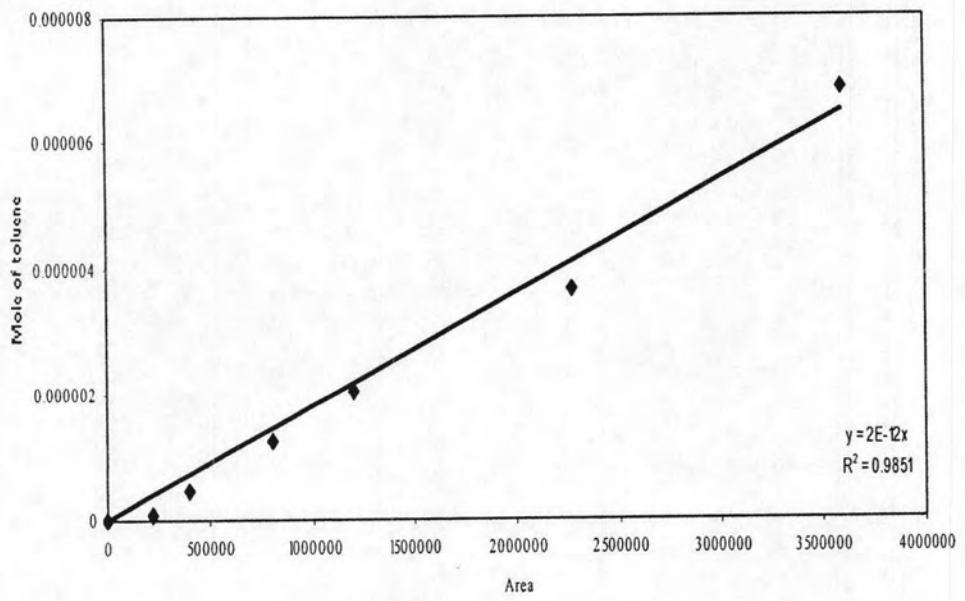

Figure C.12 The calibration curve of toluene

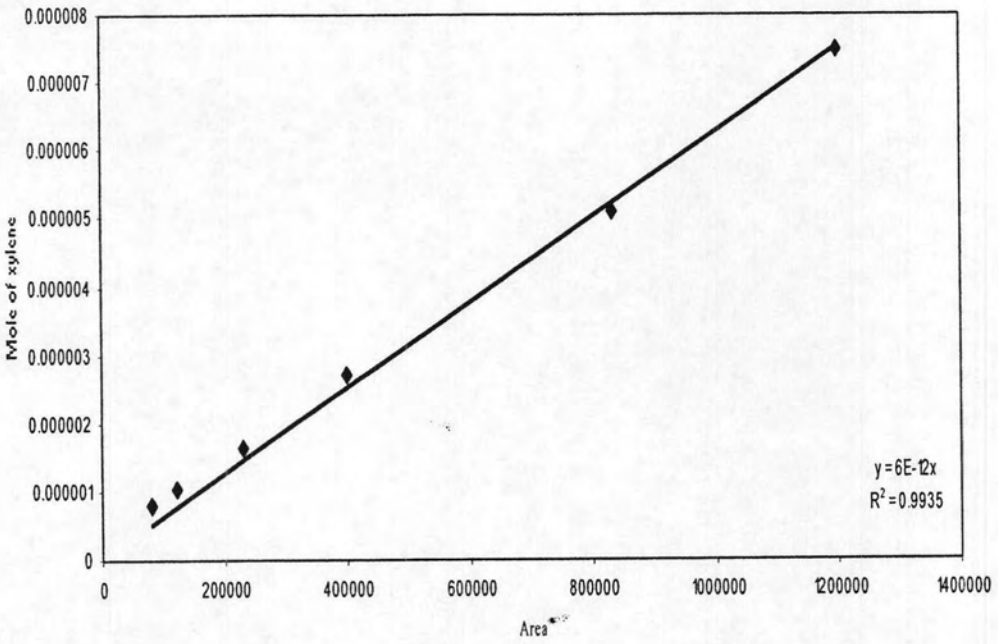

Figure C.13 The calibration curve of xylene

APPENDIX D

DATA AND CALCULATION OF ACID SITE

Calculation of total acid sites

For example, H/ZSM-5 (4.7μm), total acid site is calculated from the following step.

1. Conversion of total peak area to total peak volume

Conversion factor from Micromeritrics Chemisorb 2750 is equal to 77.57016 ml/area unit. Therefore, total peak volume is derived from

$$\begin{aligned}\text{Total peak volume} &= 77.57016 \times \text{total peak area} \\ &= 77.57016 \times 0.0748559 \\ &= 5.8089 \text{ ml}\end{aligned}$$

2. Calculation for adsorbed volume of 15% NH_3

$$\begin{aligned}\text{Adsorbed volume of 15\% } NH_3 &= 0.15 \times \text{total peak volume} \\ &= 0.15 \times 5.8089 \text{ ml} \\ &= 0.8713 \text{ ml}\end{aligned}$$

3. Total acid sties are calculated from the following equation

$$\text{Total acid sites} = \frac{(\text{Adsorbed volume, ml}) \times 101.325 \text{ Pa}}{\left(8.314 \times 10^{-3} \dfrac{\text{Pa} \cdot \text{ml}}{\text{K} \cdot \mu\text{mol}}\right) \times 298 \text{ K} \times (\text{weight of catalyst, g})}$$

For H/ZSM-5 (4.7μm) sample, 0.1000 g of this one was measured, therefore

$$\text{Total acid sites} = \frac{0.8713\ \text{ml} \times 101.325\ \text{Pa}}{\left(8.314 \times 10^{-3}\ \frac{\text{Pa} \cdot \text{ml}}{\text{K} \cdot \mu\text{mol}}\right) \times 298\ \text{K} \times (0.1031\ \text{g})}$$

$$= 356\ \mu\text{mol}\ H^{+}/\text{g}$$

APPENDIX E

LIST OF PUBLICATION

1. Pleawtein Jirakansuvan, Suphot Phatanasri and Piyasarn Praserthdam, "Synthesis of light olefins from methanol on Co/ZSM-5 catalyst", Proceeding of the Thai Institute of Chemical Engineering and Applied Chemical Conference 17th, Chiang Mai, Thailand, Oct.,29-30, 2007.

VITA

Miss. Pleawtein Jirakansuvan was born on 5th October 1983, in Suratthani, Thailand. She received her Bachelor degree of Engineering with Chemical Engineering from Prince of Songkla University, Thailand in March 2006. Since June 1, 2006, she has been studying for his Master degree of Engineering from the department of Chemical Engineering, Chulalongkorn University.