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APPENDIX A

SAMPLE OF CALCULATIONS

1. Preparation of 8% Cu/Al_2O_3 Catalyst with Incipient Impregnation Method

Reagent : Copper(II)Nitrate ($Cu(NO_3)_2.3H_2O$) Analar grade ;
Purity 99.5 % ; Molecular weight = 241.6,
manufactured by Merck Co., Ltd.
(Atomic weight of copper = 63.54)

Support : Alumina (Al_2O_3) ; type KNH-3 ; pore volume = 1.0 cc./gm.
from Sumitomo Aluminium Smelting Co., Ltd.

Calculation for prepared 8% Cu/Al_2O_3 catalyst

basis on : 8% Cu/Al_2O_3 catalyst = 10 gm.

Al_2O_3 = 10 * (92/100) gm.

= 9.2 gm.

Cu = 10 * (8/100) gm.

= 0.8 gm.

Pore volume of Al_2O_3 (KNH-3) = 1.0 cc./gm.

Pore volume of Al_2O_3 (KNH-3) 9.2 gm.

= 9.2 * 1.0

= 9.2 cc.

Copper(Cu) prepared from $Cu(NO_3)_2.3H_2O$

Copper(Cu) 0.8 gm. prepared from $Cu(NO_3)_2.3H_2O$

= 0.8 * (241.6/63.54)

* (100/99.5)

= 3.057 gm.

Use $Cu(NO_3)_2.3H_2O$ weight 3.057 gm. made to cupric nitrate solution volume of 9.2 cc. for impregnating on 9.2 gm of Al_2O_3 support.

2. Preparation of 0.3% Pt-8% Cu/Al_2O_3 Catalyst with Incipient Impregnation Method

Reagent : Copper(II)Nitrate ($Cu(NO_3)_2.3H_2O$) Analar grade ; Purity 99.5 % ; Molecular weight = 241.6, manufactured by Merck Co., Ltd.
(Atomic weight of copper = 63.54)
Chloroplatinic acid ($H_2PtCl_6.6H_2O$) ; Molecular weight = 517.92, manufactured by WAKO PURE CHEMICAL INDUSTRIES CO., LTD.
(Atomic weight of Platinum = 195.1)

Support : Alumina (Al_2O_3) ; type KNH-3 ; pore volume = 1.0 cc./gm. from Sumitomo Aluminium Smelting Co., Ltd.

Calculation for prepared 0.3% Pt-8% Cu/Al_2O_3 catalyst

basis on : 0.3% Pt-8% Cu/Al_2O_3 catalyst = 10 gm.

Al_2O_3 = 10 * (91.7/100) gm.

= 9.17 gm.

Cu = 10 * (8/100) gm.

= 0.8 gm.

Pt = 10 * (0.3/100) gm.

= 0.03 gm.

Pore volume of Al_2O_3 (KNH-3) = 1.0 cc./gm.

Pore volume of Al_2O_3 (KNH-3) 9.17 gm.

= 9.17 * 1.0

= 9.17 cc.

Copper(Cu) prepared from $Cu(NO_3)_2.3H_2O$

Copper(Cu) 0.8 gm. prepared from $Cu(NO_3)_2.3H_2O$

= 0.8 * (241.6/63.54)

* (100/99.5)

= 3.057 gm.

In this study, 25 ml. of stock solution of chloroplatinic acid was prepared by dissolving 1 gm. of chloroplatinic acid in distilled and de-ionized water.

Platinum (Pt) prepared from the stock solution of chloroplatinic acid.

Platinum 0.03 gm. prepared from the stock solution of chloroplatinic acid. = 0.03 * (25/0.3767)

= 1.99 cc.

Each of the reagents used, $Cu(NO_3)_2.3H_2O$ 3.057 gm. and chloroplatinic acid from the stock solution 1.99 cc., is made to the impregnating solution volume of 9.17 cc. for impregnating on 9.17 gm. of Al_2O_3 support by using the consecutive impregnation method.

3. The Determination of Copper Active Sites By Reaction with Nitrous Oxide [16]

Copper active sites of catalyst was measured by reaction with nitrous oxide. The methods were based upon the decomposition of a nitrous oxide molecule on a copper active site which was accompanied by the liberation of one nitrogen molecule according to

$$N_2O\ (g) + 2\ Cu_s \longrightarrow N_2\ (g) + (Cu\text{-}O\text{-}Cu)_s$$

where the subscript 's' signified surface atom.

Calculation of Copper Active Site on Copper Catalysts

Example weight of 8% Cu/Al_2O_3 catalyst = 0.252 gm.

- N_2O peak area of nitrous oxide reaction
  = 2688 unit
- N_2O peak area after nitrous oxide reaction
  = 2864 unit

Used N_2O in nitrous oxide reaction = 176 unit

Standard N_2O peak area of 1 cc. = 2864 unit

Volume of N_2O in reaction = (176/2864) * 1 cc.

= $6.145 * 10^{-2}$ cc.

Mole of N_2O in reaction = $6.145 * 10^{-2}/24860$

= $2.473 * 10^{-6}$ mole

(Volume of gas 1 mole at 30 °c = 24860 cc.)

Copper active sites on catalysts = $(mNN_s)/w$

m = moles of nitrous oxide in reaction (mole)

N = Avogadro's number = $6.02 * 10^{23}$

N_s = Surface stoichiometry of Cu_s/O_{ads} = 2

w = Weight of copper catalysts

Copper Active Sites of 8% Cu/Al_2O_3 catalysts

$$= (2 * 2.472 * 10^{-6} * 6.02 * 10^{23})/0.252$$

$$= 7.5 * 10^{17} \text{ sites/gm.}$$

4. BET Surface Area Calculation [26]

From BET equation :

$$\frac{x}{v(1-x)} = \frac{1}{v_m C} + \frac{C-1}{v_m C} * x \qquad (4.1)$$

where : x = ratio of partial pressure P/P_o

P_o = saturated vapour pressure of N_2 (or adsorbed gas)

P = equilibrium vapour pressure of N_2

v = amount of adsorption at the equilibrium, c.c. at the NTP/gm of sample

v_m = amount of adsorption to cover the surface, c.c. at the NTP/gm of sample

$C = \exp(E_1 - E_2/RT)$ (4.2)

where : E_1 = heat of adsorption of the first layer

E_2 = heat of condensation of adsorbed gas

assume $C \longrightarrow \infty$, then

$$\frac{x}{v(1-x)} = \frac{1 * x}{v_m C} \qquad (4.3)$$

let : $v_m = v_m'$

v_m' = mean amount of adsorption to form the N_2 complete monolayer

v = amount of adsorption measuring by G.C.

$x = P/P_o$

$$\frac{P_b V}{273} = \frac{P_t V}{T} \qquad (4.4)$$

where : V = constant volume

P_b = pressure at 0 °C

P_t = pressure at t °C

T = 273.15 + t, K

$P_b = (273.15/T) * P_t = 1$ atm

partial pressure

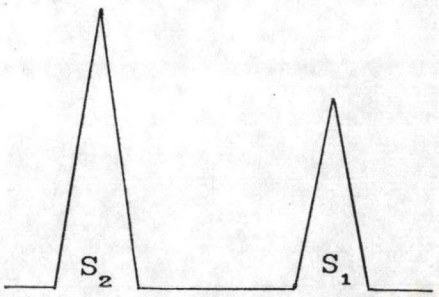
$$P = \frac{[\text{Flow of } (He+N_2) - \text{Flow of } He] * P_b}{\text{Flow of } (He+N_2)} \qquad (4.5)$$

= 0.3 atm

N_2 saturated vapour pressure, P_o = 1.1 atm = 836 mm.Hg

$x = P/P_o = P/1.1$

How to measure v



1 ml/1 atm at room temperature

desorption N_2 calibration

of N_2 area area

$$v = \frac{S_2}{S_1} * \frac{1}{w} * \frac{273.15}{T} \quad \text{c.c./g of catalyst} \qquad (4.6)$$

where : w = weight of sample

$$v_m' = \frac{v[1-(\text{flow of He+}N_2 - \text{flow of He})/1.1]}{\text{flow of He+}N_2} \quad \text{c.c.NTP/g of cat.} \qquad (4.7)$$

$$S_b = S * v_m' \qquad (4.8)$$

where : S = surface area from literature of N_2

= 4.373 m^2/c.c. of N_2

so that : S_b = 4.373 v_m' m^2/g of catalyst

5. Material Balance for CO Oxidation Reaction

For CO oxidation reaction, the chemical equation is expressed as follows:

$$2CO + O_2 \longrightarrow 2CO_2$$

At the reaction temperature of 220 °C;

The amount of CO in feed steam = $3.955 * 10^{-7}$ mole

The amount of CO in effluent = $2.361 * 10^{-7}$ mole

Because 1 mole of CO convert to 1 mole of CO_2.

So, the amount of CO_2 should have been obtained from the reaction

= $1.594 * 10^{-7}$ mole

The actual amount of CO_2 from the reaction

= $1.575 * 10^{-7}$ mole

% error = 1.2 %

APPENDIX B

Physical Properties of Carbon Monoxide

Property	Value
mol. wt.	28.011
m.p.	68.09 K
b.p.	81.65 K
H, fusion (68 K)[a]	0.837 kJ/mol
H, vaporization (81 K)[a]	6.042 kJ/mol
density [273 K, 101.33 kPa(1atm)]	1.2501 g/L
sp. gr., liquid, 79 K[b]	0.814
sp. gr., gas, 298 K[c]	0.968
critical temperature	132.9 K
critical pressure	3.496 MPa(34.5 atm)
critical density	0.3010 g/cm^3
G° formation (298 K)[a]	-137.16 kJ/mol
H° formation (298 K)[a]	-110.53 kJ/mol
S° formation (298 K)[a]	0.1975 kJ/(mol.K)
C_p° (298 K)[a]	29.1 J/(mol.K)
C_v° (298 K)[a]	20.8 J/(mol.K)
autoignition temperature	925 K
flammability limits in air[d]	
upper limit, %	74.2
lower limit, %	12.5

[a] To convert J to cal, divide by 4.184

[b] With respect to water at 277 K.

[c] With respect to air at 298 K.

[d] Saturated with water vapor at 290 K.

Ambient Air Quality Standard of Thailand (1981)

Pollutants	average value (mg/m^3)				methods of measurement
	1 h	8 h	24 h	1 yr	
Carbon Monoxide (CO)	50	20	-	-	Non-Dispersive Infrared Detection
Nitrogen Dioxide (NO_2)	0.32	-	-	-	Gas Phase Chemiluminescence
Sulfur Dioxide (SO_2)	-	-	0.3	0.1*	Pararosanniline
Suspended Particulate Matter (SPM)	-	-	0.33	0.1*	Gravimetric
Photochemical Oxidant (O_3)	0.20	-	-	-	Chemiluminescence
Lead (Pb)	-	-	0.01	-	Wet Ashing

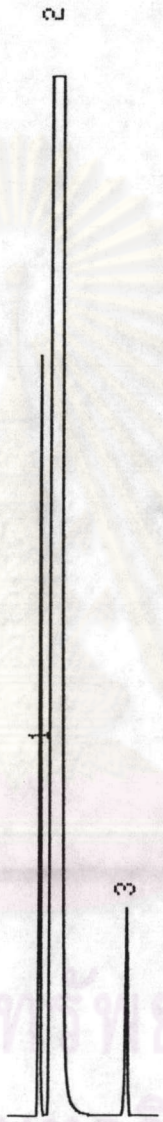
Note : * = Geometric mean

Specification of Alumina Support (Al_2O_3) Type KNH-3 from Sumitomo Aluminium Smelting Co., Ltd.

Chemical Composition (weight percent)		
- Al_2O_3	60-70	%
- SiO_2	30-35	%
- Fe_2O_3	0.3-0.5	%
- TiO_2	0.5-0.7	%
- CaO	0.1-0.2	%
- MgO	0.2-0.4	%
- Na_2O	0.3-0.4	%
- K_2O	0.2-0.3	%
- ZrO_2 + HfO_2	0.03-0.04	%

Physical Properties	
- Bulk Density (g/cc)	1.3-1.5
- Apparent Specific Gravity	3.1-3.3
- Packing Density (lb/ft^3)	20-25
- Pore Volume (cc/g)	1.0-1.3
- Surface Area (m^2/g)	340-350

Sample of Chromatogram



PKNO	TIME	AREA	CONC	NAME
1	1.343	15266	1.1923	OXYGEN
2	1.803	1250138	97.6190	NITROGEN
3	5.218	15226	1.1887	CARBON MONOXIDE
		---	---	
	TOTAL	1280630	100	

VITA

Mr. Thawatchai Majitnapakul was born on January 13, 1968. He received his Bachelor Degree of Science, Department of Chemistry, Faculty of Science, Mahidol University in 1989.