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APPENDICES

APPENDIX A

CALCULATION OF CATALYST PREPARATION

Preparation of Co-Mg-O/Al_2O_3 catalysts by the Wet Impregnation Method is shown as follow:

Reagent: - Cobalt acetate tetrahydrate [$Co(CH_3COO)_2 \cdot 4H_2O$]
Molecular weight = 249 g.
- Magnesium nitrate [$Mg(NO_3)_2$]
Molecular weight = 256.41 g.
Support - Alumina [Al_2O_3]

Calculation for the preparation of the Co_3O_4/Al_2O_3 catalyst

The Co_3O_4/Al_2O_3 aqueous solution used in catalyst preparation consists of Co 8wt% and Al_2O_3 92wt%. The amount of cobalt in Co_3O_4/Al_2O_3 catalyst is calculated as follows:

Basis: Al_2O_3 1 g.
If the weight of catalyst was 100 gram, Co_3O_4/Al_2O_3 would compose of cobalt 8 g. and Al_2O_3 92 g. Therefore, in this system,

the amount of Co = $8/92 \times 1$
= 0.0869 g.

Cobalt (Co) 0.0869 g. was prepared from $Co(CH_3COO)_2 \cdot 4H_2O$ 99% and molecular weight of Co = 59, then

the $Co(CH_3COO)_2 \cdot 4H_2O$ content = $(249 \times 0.0869 \times 100)/(59 \times 99)$
= 0.3712 g.

Calculation for the preparation of the 8Co-0.5Mg-O/Al_2O_3 catalyst

The 8Co-0.5Mg-O/Al_2O_3 aqueous solution used in catalyst preparation consists of Co 8wt% and Al_2O_3 92wt%. The amount of cobalt in 8Co-0.5Mg-O/Al_2O_3 catalyst is calculated as follows:

Basis: Al_2O_3 1 g.

If the weight of catalyst was 100 gram, 8Co-0.5Mg-O/Al_2O_3 would compose of cobalt 8 g. and Al_2O_3 92 g. Therefore, in this system,

the amount of Co $= 8/92 \times 1$

$= 0.0869$ g.

Cobalt (Co) 0.0869 g. was prepared from $Co(CH_3COO)_2 \cdot 4H_2O$ 99% and molecular weight of Co = 59, then

the $Co(CH_3COO)_2 \cdot 4H_2O$ content $= (249 \times 0.0869 \times 100)/(59 \times 99)$

$= 0.3712$ g.

Then, Mg 0.5% was loaded on 8Co/Al_2O_3 catalyst 100 gram.

The amount of Mg $= (0.0869+0.5)/100$

$= 0.0059$ g.

Magnesium (Mg) 0.0059 g. was impregnated from $Mg(NO_3)_2$ solution 99% and molecular weight of Mg = 24.305 g.

Thus, the amount of $Mg(NO_3)_2$ used $= (0.0059 \times 256.41)/24.305$

$= 0.0622$ g.

Calculation for the preparation of the 8Co-1Mg-O/Al_2O_3 catalyst

The 8Co-Mg-O/Al_2O_3 aqueous solution used in catalyst preparation consists of Co 8wt% and Al_2O_3 92wt%. The amount of cobalt in 8Co-Mg-O/Al_2O_3 catalyst is calculated as follows:

Basis: Al_2O_3 1 g.

If the weight of catalyst was 100 gram, 8Co-Mg-O/Al_2O_3 would compose of cobalt 8 g. and Al_2O_3 92 g. Therefore, in this system,

the amount of Co = 8/92 × 1
= 0.0869 g.

Cobalt (Co) 0.0869 g. was prepared from $Co(CH_3COO)_2 \cdot 4H_2O$ 99% and molecular weight of Co = 59, then

the $Co(CH_3COO)_2 \cdot 4H_2O$ content = (249×0.0869×100)/(59×99)
= 0.3712 g.

Then, Mg 1% was loaded on 8Co/Al_2O_3 catalyst 100 gram.

The amount of Mg = (0.0869+1)/100
= 0.010869 g.

Magnesium (Mg) 0.010869 g. was impregnated from $Mg(NO_3)_2$ solution 99% and molecular weight of Mg = 24.305 g.

Thus, the amount of $Mg(NO_3)_2$ used = (0.010869×256.41)/24.305
= 0.1157 g.

Calculation for the preparation of the 8Co-2Mg-O/Al_2O_3 catalyst

The 8Co-2Mg-O/Al_2O_3 aqueous solution used in catalyst preparation consists of Co 8wt% and Al_2O_3 92wt%. The amount of cobalt in 8Co-2Mg-O/Al_2O_3 catalyst is calculated as follows:

Basis: Al_2O_3 1 g.

If the weight of catalyst was 100 gram, 8Co-2Mg-O/Al_2O_3 would compose of cobalt 8 g. and Al_2O_3 92 g. Therefore, in this system,

the amount of Co = 8/92 × 1
= 0.0869 g.

Cobalt (Co) 0.0869 g. was prepared from $Co(CH_3COO)_2 \cdot 4H_2O$ 99% and molecular weight of Co = 59, then

the $Co(CH_3COO)_2 \cdot 4H_2O$ content = (249×0.0869×100)/(59×99)
= 0.3712 g.

Then. Mg 2% was loaded on $8Co/Al_2O_3$ catalyst 100 gram.

The amount of Mg = (0.0869+2)/100
= 0.0209 g.

Magnesium (Mg) 0.0209 g. was impregnated from $Mg(NO_3)_2$ solution 99% and molecular weight of Mg = 24.305 g.

Thus. the amount of $Mg(NO_3)_2$ used = (0.0209×256.41)/24.305
= 0.2205 g.

Calculation for the preparation of the $8Co\text{-}3Mg\text{-}O/Al_2O_3$ catalyst

The $8Co\text{-}3Mg\text{-}O/Al_2O_3$ aqueous solution used in catalyst preparation consists of Co 8wt% and Al_2O_3 92wt%. The amount of cobalt in $8Co\text{-}3Mg\text{-}O/Al_2O_3$ catalyst is calculated as follows:

Basis: Al_2O_3 1 g.

If the weight of catalyst was 100 gram. $8Co\text{-}3Mg\text{-}O/Al_2O_3$ would compose of cobalt 8 g. and Al_2O_3 92 g. Therefore. in this system.

the amount of Co = 8/92 × 1
= 0.0869 g.

Cobalt (Co) 0.0869 g. was prepared from $Co(CH_3COO)_2 \cdot 4H_2O$ 99% and molecular weight of Co = 59, then

the $Co(CH_3COO)_2 \cdot 4H_2O$ content = (249×0.0869×100)/(59×99)
= 0.3712 g.

Then. Mg 3% was loaded on $8Co/Al_2O_3$ catalyst 100 gram.

The amount of Mg = (0.0869+3)/100
= 0.0309 g.

Magnesium (Mg) 0.0309 g. was impregnated from $Mg(NO_3)_2$ solution 99% and molecular weight of Mg = 24.305 g.

Thus, the amount of $Mg(NO_3)_2$ used = $(0.0309 \times 256.41)/24.305$

= 0.3257 g.

Calculation for the preparation of the MgO/Al_2O_3 catalyst

The MgO/Al_2O_3 aqueous solution used in catalyst preparation consists of Mg 1wt% and Al_2O_3 99wt%. The amount of cobalt in MgO/Al_2O_3 catalyst is calculated as follows:

Basis: Al_2O_3 1 g.

If the weight of catalyst was 100 gram, MgO/Al_2O_3 would compose of magnesium 1 g. and Al_2O_3 99 g. Therefore, in this system,

the amount of Mg = 1/99

= 0.0101 g.

Magnesium (Mg) 0.0101 g. was impregnated from $Mg(NO_3)_2$ solution 99% and molecular weight of Mg = 24.305 g.

Thus, the amount of $Mg(NO_3)_2$ used = $(0.0101 \times 256.41)/24.305$

= 0.1066 g.

Calculation for the preparation of the $6Co\text{-}1Mg\text{-}O/Al_2O_3$ catalyst

The $6Co\text{-}1Mg\text{-}O/Al_2O_3$ aqueous solution used in catalyst preparation consists of Co 6wt% and Al_2O_3 94wt%. The amount of cobalt in $6Co\text{-}1Mg\text{-}O/Al_2O_3$ catalyst is calculated as follows:

Basis: Al_2O_3 1 g.

If the weight of catalyst was 100 gram, $6Co\text{-}1Mg\text{-}O/Al_2O_3$ would compose of cobalt 6 g. and Al_2O_3 94 g. Therefore, in this system,

the amount of Co = $6/94 \times 1$

= 0.0638 g.

Cobalt (Co) 0.0638 g. was prepared from $Co(CH_3COO)_2 \cdot 4H_2O$ 99% and molecular weight of Co = 59, then

the $Co(CH_3COO)_2 \cdot 4H_2O$ content $= (249 \times 0.0638 \times 100)/(59 \times 99)$

$= 0.2719$ g.

Then. Mg 1% was loaded on $6Co/Al_2O_3$ catalyst 100 gram.

The amount of Mg $= (0.2719+1)/100$

$= 0.0127$ g.

Magnesium (Mg) 0.0127 g. was impregnated from $Mg(NO_3)_2$ solution 99% and molecular weight of Mg = 24.305 g.

Thus. the amount of $Mg(NO_3)_2$ used $= (0.0127 \times 256.41)/24.305$

$= 0.1339$ g.

Calculation for the preparation of the $7Co\text{-}1Mg\text{-}O/Al_2O_3$ catalyst

The $7Co\text{-}1Mg\text{-}O/Al_2O_3$ aqueous solution used in catalyst preparation consists of Co 7wt% and Al_2O_3 93wt%. The amount of cobalt in $7Co\text{-}1Mg\text{-}O/Al_2O_3$ catalyst is calculated as follows:

Basis: Al_2O_3 1 g.

If the weight of catalyst was 100 gram. $7Co\text{-}1Mg\text{-}O/Al_2O_3$ would compose of cobalt 7 g. and Al_2O_3 93 g. Therefore. in this system,

the amount of Co $= 7/93 \times 1$

$= 0.0753$ g.

Cobalt (Co) 0.0753 g. was prepared from $Co(CH_3COO)_2 \cdot 4H_2O$ 99% and molecular weight of Co = 59, then

the $Co(CH_3COO)_2 \cdot 4H_2O$ content $= (249 \times 0.0753 \times 100)/(59 \times 99)$

$= 0.321$ g.

Then. Mg 1% was loaded on $7Co/Al_2O_3$ catalyst 100 gram.

The amount of Mg $= (0.321+1)/100$

= 0.0132 g.

Magnesium (Mg) 0.0132 g. was impregnated from $Mg(NO_3)_2$ solution 99% and molecular weight of Mg = 24.305 g.

Thus, the amount of $Mg(NO_3)_2$ used = $(0.0132\times256.41)/24.305$

= 0.1393 g.

Calculation for the preparation of the 9Co-1Mg-O/Al_2O_3 catalyst

The 9Co-1Mg-O/Al_2O_3 aqueous solution used in catalyst preparation consists of Co 9wt% and Al_2O_3 91wt%. The amount of cobalt in 9Co-1Mg-O/Al_2O_3 catalyst is calculated as follows:

Basis: Al_2O_3 1 g.

If the weight of catalyst was 100 gram, 9Co-1Mg-O/Al_2O_3 would compose of cobalt 9 g. and Al_2O_3 91 g. Therefore, in this system,

the amount of Co = $9/91 \times 1$

= 0.0989 g.

Cobalt (Co) 0.0989 g. was prepared from $Co(CH_3COO)_2\cdot4H_2O$ 99% and molecular weight of Co = 59, then

the $Co(CH_3COO)_2\cdot4H_2O$ content = $(249\times0.0989\times100)/(59\times99)$

= 0.4216 g.

Then, Mg 1% was loaded on 9Co/Al_2O_3 catalyst 100 gram.

The amount of Mg = $(0.4216+1)/100$

= 0.0142 g.

Magnesium (Mg) 0.0142 g. was impregnated from $Mg(NO_3)_2$ solution 99% and molecular weight of Mg = 24.305 g.

Thus, the amount of $Mg(NO_3)_2$ used = $(0.0142\times256.41)/24.305$

= 0.1498 g.

Calculation for the preparation of the 10Co-1Mg-O/Al_2O_3 catalyst

The 10Co-1Mg-O/Al_2O_3 aqueous solution used in catalyst preparation consists of Co 10wt% and Al_2O_3 90wt%. The amount of cobalt in 10Co-1Mg-O/Al_2O_3 catalyst is calculated as follows:

Basis: Al_2O_3 1 g.
If the weight of catalyst was 100 gram, 10Co-1Mg-O/Al_2O_3 would compose of cobalt 10 g. and Al_2O_3 90 g. Therefore, in this system,

the amount of Co = 10/90 × 1
= 0.1111 g.

Cobalt (Co) 0.1111 g. was prepared from $Co(CH_3COO)_2{\cdot}4H_2O$ 99% and molecular weight of Co = 59, then

the $Co(CH_3COO)_2{\cdot}4H_2O$ content = $(249\times0.1111\times100)/(59\times99)$
= 0.4736 g.

Then, Mg 1% was loaded on 10Co/Al_2O_3 catalyst 100 gram.

The amount of Mg = (0.4736+1)/100
= 0.0147 g.

Magnesium (Mg) 0.0147 g. was impregnated from $Mg(NO_3)_2$ solution 99% and molecular weight of Mg = 24.305 g.

Thus, the amount of $Mg(NO_3)_2$ used = $(0.0147\times256.41)/24.305$
= 0.1551 g.

APPENDIX B

CALCULATION OF DIFFUSIONAL LIMITATION EFFECT

In the present work there are doubt whether the external and internal diffusion limitations interfere with the propane reaction. Hence, the kinetic parameters were calculated based on the experimental data so as to prove the controlled system. The calculation is divided into two parts; one of which is the external diffusion limitation, and the other is the internal diffusion limitation.

1. External diffusion limitation

The phthalic anhydride combustion reaction is considered to be an irreversible first order reaction occurred on the interior pore surface of catalyst particles in a fixed bed reactor. Assume isothermal operation for the reaction.

In the experiment, 0.05% phthalic anhydride, 21% O_2 was used as the unique reactant in the system. Because percentage of phthalic anhydride was rather small compared to the oxygen that it can be neglected. Molecular weight of nitrogen and oxygen are 28.02 and 31.98, respectively. Thus, the average molecular weight of the gas mixture was calculated as follows:

$$M_{AB} = 0.72\times28.02 + 0.21\times31.98$$
$$= 26.890 \text{ g/mol}$$

Calculation of reactant gas density

Consider the phthalic anhydride combustion is operated at low pressure and high temperature. We assume that the gases are respect to ideal gas law. The density of such gas mixture reactant at various temperatures is calculated in the following.

$$\rho = \frac{PM}{RT} = \frac{1.0\times10^{5}\times26.890\times10^{-3}}{8.314T}$$

We obtained : $\rho = 0.684\ \text{kg/m}^3$ at T = 200°C

$\rho = 0.618\ \text{kg/m}^3$ at T = 250°C

$\rho = 0.564\ \text{kg/m}^3$ at T = 300°C

$\rho = 0.519\ \text{kg/m}^3$ at T = 350°C

<u>Calculation of the gas mixture viscosity</u>

The simplified methods for determining the viscosity of low pressure binary are described anywhere (Reid, 1988). The method of Wilke is chosen to estimate the gas mixture viscosity.

For a binary system of 1 and 2,

$$\mu_m = \frac{y_1 \mu_1}{y_1 + y_2 \Phi_{12}} + \frac{y_2 \mu_2}{y_2 + y_1 \Phi_{21}}$$

where μ_m = viscosity of the mixture

μ_1, μ_2 = pure component viscosity

y_1, y_2 = mole fractions

$$\phi_{12} = \frac{\left[1 + \left(\frac{\mu_1}{\mu_2}\right)^{1/2} \left(\frac{M_1}{M_2}\right)^{1/4}\right]^2}{\left[8\left(1 + \frac{M_1}{M_2}\right)\right]^{1/2}}$$

$$\phi_{21} = \phi_{12} \left(\frac{\mu_2}{\mu_1}\right)\left(\frac{M_1}{M_2}\right)$$

M_1, M_2 = molecular weight

Let 1 refer to nitrogen and 2 to oxygen

$M_1 = 28.02$ and $M_2 = 31.98$

From Perry the viscosity of nitrogen at 200°C, 250°C, 300°C, 350°C, 400°C, 450°C and 500°C are 0.0248, 0.027, 0.0286, 0.0305, 0.032, 0.0338, and 0.0368 cP, respectively. The viscosity of oxygen at 200°C, 250°C, 300°C and 350°C are 0.0281, 0.03, 0.032 and 0.034 cP, respectively.

<u>At 200°C</u> :

$$\phi_{12} = \frac{\left[1+\left(\frac{0.0248}{0.0281}\right)^{1/2}\left(\frac{28.02}{31.98}\right)^{1/4}\right]^2}{\left[8\left(1+\frac{28.02}{31.98}\right)\right]^{1/2}} = 0.940$$

$$\phi_{21} = 0.940\left(\frac{0.0281}{0.0248}\right)\left(\frac{28.02}{31.98}\right) = 0.933$$

$$\mu_m = \frac{0.79\times 0.0248}{0.79+0.02\times 0.940} + \frac{0.21\times 0.0281}{0.21+0.79\times 0.933} = 0.0260\text{cP} = 2.60\times 10^{-5}\text{kg/m}-\text{sec}$$

<u>At 250°C</u> :

$$\phi_{12} = \frac{\left[1+\left(\frac{0.027}{0.03}\right)^{1/2}\left(\frac{28.02}{31.98}\right)^{1/4}\right]^2}{\left[8\left(1+\frac{28.02}{31.98}\right)\right]^{1/2}} = 0.949$$

$$\phi_{21} = 0.949\left(\frac{0.03}{0.027}\right)\left(\frac{28.02}{31.98}\right) = 0.924$$

$$\mu_m = \frac{0.79\times 0.027}{0.79+0.21\times 0.949} + \frac{0.21\times 0.03}{0.21+0.79\times 0.924} = 0.0283\text{cP} = 2.83\times 10^{-5}\text{kg/m}-\text{sec}$$

<u>At 300°C</u> :

$$\phi_{12} = \frac{\left[1+\left(\frac{0.0286}{0.032}\right)^{1/2}\left(\frac{28.02}{31.98}\right)^{1/4}\right]^2}{\left[8\left(1+\frac{28.02}{31.98}\right)\right]^{1/2}} = 0.948$$

$$\phi_{21} = 0.948\left(\frac{0.032}{0.0286}\right)\left(\frac{28.02}{31.98}\right) = 0.929$$

$$\mu_m = \frac{0.79 \times 0.0286}{0.79 + 0.21 \times 0.948} + \frac{0.21 \times 0.032}{0.21 + 0.79 \times 0.929} = 0.0299\text{cP} = 2.99 \times 10^{-5}\,\text{kg/m} - \text{sec}$$

At 350°C :

$$\phi_{12} = \frac{\left[1 + \left(\frac{0.0305}{0.034}\right)^{1/2}\left(\frac{28.02}{31.98}\right)^{1/4}\right]^2}{\left[8\left(1 + \frac{28.02}{31.98}\right)\right]^{1/2}} = 0.945$$

$$\phi_{21} = 0.945\left(\frac{0.034}{0.0305}\right)\left(\frac{28.02}{31.98}\right) = 0.923$$

$$\mu_m = \frac{0.79 \times 0.0305}{0.79 + 0.21 \times 0.945} + \frac{0.21 \times 0.034}{0.21 + 0.79 \times 0.923} = 0.0320\text{cP} = 3.20 \times 10^{-5}\,\text{kg/m} - \text{sec}$$

Calculation of diffusion coefficients

Diffusion coefficients for binary gas system at low pressure calculated by empirical correlation are proposed by Reid (1988). Wilke and Lee method is chosen to estimate the value of D_{AB} due to the general and reliable method. The empirical correlation is

$$D_{AB} = \frac{\left(3.03 - \frac{0.98}{M_{AB}^{1/2}}\right)\left(10^{-3}\right)T^{3/2}}{PM_{AB}^{1/2}\sigma_{AB}^{2}\Omega_D}$$

where D_{AB} = binary diffusion coefficient,cm^2/s

T = temperature,K

M_A ,M_B = molecular weights of A and B ,g/mol

$$M_{AB} = 2\left[\left(\frac{1}{M_A}\right) + \left(\frac{1}{M_B}\right)\right]^{-1}$$

P = pressure,bar

σ = characteristic length,^{0}A

Ω_D = diffusion collision integral, dimensionless

The characteristic Lennard-Jones energy and Length, ε and σ , of nitrogen and propane are as follows: (Reid,1988)

For O_2 : $\sigma = 3.467\ {}^{0}A$, $\varepsilon/k = 106.7$
For N_2 : $\sigma = 3.798\ {}^{0}A$, $\varepsilon/k = 71.4$

The sample rules are usually employed.

$$\sigma_{AB} = \frac{\sigma_A + \sigma_B}{2} = \frac{3.798 + 3.467}{2} = 3.63$$

$$\varepsilon_{AB}/k = \left(\frac{\varepsilon_A \varepsilon_B}{k^2}\right)^{1/2} = (71.4 \times 106.7)^{1/2} = 87.28$$

Ω_D is tabulated as a function of kT/ε for the Lennard-Jones potential. The accurate relation is

$$\Omega_D = \frac{A}{(T^*)^B} + \frac{C}{\exp(DT^*)} + \frac{E}{\exp(FT^*)} + \frac{G}{\exp(HT^*)}$$

where $T^* = \frac{kT}{\varepsilon_{AB}}$, A = 1.06036 , B = 0.15610 , C = 0.19300 , D = 0.47635 , E = 1.03587 , F = 1.52996 , G = 1.76474 , H = 3.89411

Then $T^* = \frac{473}{87.28} = 5.419$ at 200°C

$T^* = \frac{523}{87.28} = 5.992$ at 250°C

$T^* = \frac{573}{87.28} = 6.565$ at 300°C

$T^* = \frac{623}{87.28} = 7.138$ at 350°C

$$\Omega_D = \frac{1.06036}{(T^*)^{0.15610}} + \frac{0.19300}{\exp(0.47635T^*)} + \frac{1.03587}{\exp(1.52996T^*)} + \frac{1.76474}{\exp(3.89411T^*)}$$

Ω_D = 0.928 ; 200°C

Ω_D = 0.813 ; 250°C

Ω_D = 0.799 ; 300°C

Ω_D = 0.787 ; 350°C

With Equation of D_{AB},

<u>At 200°C</u> : $D(N_2\text{-}O_2) = \dfrac{\left(3.03 - \dfrac{0.98}{29.869^{0.5}}\right)(10^{-3})473^{3/2}}{1 \times 29.869^{0.5} \times 3.63^2 \times 0.829}$

$= \quad 0.491 \quad m^2/s$

<u>At 250°C</u> : $D(N_2\text{-}O_2) = \dfrac{\left(3.03 - \dfrac{0.98}{29.869^{0.5}}\right)(10^{-3})523^{3/2}}{1 \times 29.869^{0.5} \times 3.63^2 \times 0.813}$

$= \quad 0.582 \quad m^2/s$

<u>At 300°C</u> : $D(N_2\text{-}O_2) = \dfrac{\left(3.03 - \dfrac{0.98}{29.869^{0.5}}\right)(10^{-3})573^{3/2}}{1 \times 29.869^{0.5} \times 3.63^2 \times 0.799}$

$= \quad 0.679 \quad m^2/s$

<u>At 350°C</u> : $D(N_2\text{-}O_2) = \dfrac{\left(3.03 - \dfrac{0.98}{29.869^{0.5}}\right)(10^{-3})623^{3/2}}{1 \times 29.869^{0.5} \times 3.63^2 \times 0.799}$

$= \quad 0.899 \quad m^2/s$

Reactant gas mixture was supplied at 100 ml/min. in tubular microreactor used in the phthalic anhydride oxidation system at 30°C

oxygen flow rate through reactor = 100 ml/min. at 30°C

The density of oxygen , $\rho = \dfrac{1.0 \times 10^5 \times 26.890 \times 10^{-3}}{8.314(273+30)} = 1.067$ kg/s

Mass flow rate = $1.067\left(\frac{100\times10^{-6}}{60}\right) = 1.78\times10^{-6}$ kg/s

Diameter of stainless steel tube reactor = 9.5 mm

Cross-sectional area of tube reactor = $\frac{\pi(9.5\times10^{-3})^2}{4} = 7.09\times10^{-5}$ m^2

Mass Velocity , G = $\frac{1.78\times10^{-6}}{7.09\times10^{-5}} = 0.025$ kg/m^2-s

Catalyst size = 40-60 mesh = 0.178-0.126 mm

Average catalyst size = (0.126+0.178)/2 = 0.152 mm

Find Reynolds number, Re_p, which is well known as follows:

$$Re_p = \frac{d_pG}{\mu}$$

We obtained

At 200°C : $Re_p = \frac{(0.152\times10^{-3}\times0.025)}{2.60\times10^{-5}} = 0.146$

At 250°C : $Re_p = \frac{(0.152\times10^{-3}\times0.0025)}{2.83\times10^{-5}} = 0.134$

At 300°C : $Re_p = \frac{(0.152\times10^{-3}\times0.025)}{2.99\times10^{-5}} = 0.127$

At 350°C : $Re_p = \frac{(0.152\times10^{-3}\times0.025)}{3.20\times10^{-5}} = 0.119$

Average transport coefficient between the bulk stream and particles surface could be correlated in terms of dimensionless groups, which characterize the flow conditions. For mass transfer the Sherwood number, $k_m\rho/G$, is an empirical function of the Reynolds number, d_pG/μ, and the Schmit number, $\mu/\rho D$. The j-factors are defined as the following functions of the Schmidt number and Sherwood numbers:

$$j_D = \frac{k_m \rho}{G}\left(\frac{a_m}{a_t}\right)(\mu / \rho D)^{2/3}$$

The ratio (a_m/a_t) allows for the possibility that the effective mass-transfer area a_m, may be less than the total external area, a_t, of the particles. For Reynolds number greater than 10, the following relationship between j_D and the Reynolds number well represents available data.

$$j_D = \frac{0.458}{\varepsilon_B}\left(\frac{d_p G}{\mu}\right)^{-0.407}$$

where G = mass velocity(superficial) based upon cross-sectional area of empty reactor

($G = u\rho$)

d_p = diameter of catalyst particle for spheres

μ = viscosity of fluid

ρ = density of fluid

ε_B = void fraction of the interparticle space (void fraction of the bed)

D = molecular diffusivity of component being transferred

Assume $\varepsilon_B = 0.5$

<u>At 200°C</u> ; $j_D = \frac{0.458}{0.5}(0.146)^{-0.407} = 2.004$

<u>At 250°C</u> ; $j_D = \frac{0.458}{0.5}(0.134)^{-0.407} = 2.076$

<u>At 300°C</u> ; $j_D = \frac{0.458}{0.5}(0.127)^{-0.407} = 2.122$

<u>At 350°C</u> ; $j_D = \frac{0.458}{0.5}(0.119)^{-0.407} = 2.178$

A variation of the fixed bed reactor is an assembly of screens or gauze of catalytic solid over which the reacting fluid flows. Data on mass transfer from single screens has been reported by Gay and Maughan. Their correlation is of the form

$$\mathrm{j_D} = \left(\frac{\mathrm{j_D G}}{\mu}\right)(\mu/\rho \mathrm{D})^{2/3}$$

Where ε is the porosity of the single screen.

$$\text{Hence, } \mathrm{k_m} = \left(\frac{\mathrm{j_D G}}{\mu}\right)(\mu/\rho \mathrm{D})^{2/3}$$

$$\mathrm{k_m} = \left(\frac{0.458\mathrm{G}}{\varepsilon_{\mathrm{B}}\rho}\right)\mathrm{Re}^{-0.407}\,\mathrm{Sc}^{-2/3}$$

Find Schmidt number, Sc : $\mathrm{Sc} = \dfrac{\mu}{\rho \mathrm{D}}$

<u>At 200°C</u> : $\mathrm{Sc} = \dfrac{2.60\times10^{-5}}{0.684\times0.491} = 7.74\times10^{-5}$

<u>At 250°C</u> : $\mathrm{Sc} = \dfrac{2.83\times10^{-5}}{0.618\times0.582} = 7.87\times10^{-5}$

<u>At 300°C</u> : $\mathrm{Sc} = \dfrac{2.99\times10^{-5}}{0.564\times0.679} = 7.81\times10^{-5}$

<u>At 350°C</u> : $\mathrm{Sc} = \dfrac{3.20\times10^{-5}}{0.519\times0.899} = 6.86\times10^{-5}$

Find $\mathrm{k_m}$: <u>At 200°C</u>, $\mathrm{k_m} = \left(\dfrac{2.004\times0.025}{0.684}\right)(7.74\times10^{-5})^{-2/3} = 42.57\ \mathrm{m/s}$

<u>At 250°C</u>, $\mathrm{k_m} = \left(\dfrac{2.076\times0.025}{0.618}\right)(7.87\times10^{-5})^{-2/3} = 45.73\ \mathrm{m/s}$

$$\underline{\text{At } 300^{\circ}\text{C}},\ k_m = \left(\frac{2.122\times 0.025}{0.564}\right)(7.81\times 10^{-5})^{-2/3} = 51.48 \text{ m/s}$$

$$\underline{\text{At } 350^{\circ}\text{C}},\ k_m = \left(\frac{2.178\times 0.025}{0.519}\right)(6.86\times 10^{-5})^{-2/3} = 62.61 \text{ m/s}$$

Properties of catalyst

Density = 0.375 g/ml catalyst

Diameter of 40-60 mesh catalyst particle = 0.152 mm

Weight per catalyst particle $= \dfrac{\pi(0.152\times 10^{-1})^3 \times 0.375}{6} = 6.895\times 10^{-7}$ g/particle

External surface area per particle $= \pi(0.152\times 10^{-3})^2 = 7.26\times 10^{-7}$ m^2/particle

$a_m = \dfrac{7.26\times 10^{-7}}{6.895\times 10^{-7}} = 1.052$ m^2/gram catalyst

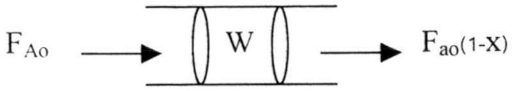
Volumetric flow rate of gaseous feed stream = 100 ml/min

Molar flow rate of gaseous feed stream $= \dfrac{(1\times 10^{5})\left(\dfrac{100\times 10^{-6}}{60}\right)}{8.314(273+30)} = 6.62\times 10^{-5}$ mol/s

oxygen molar feed rate = $0.21\times 6.62\times 10^{-5} = 1.39\times 10^{-5}$ mol/s

phthalic anhydride conversion (experimental data): 29.10 % at 200°C
51.50 % at 250°C
84.50 % at 300°C
85.00 % at 350°C

The estimated rate of phthalic anhydride oxidation reaction is based on the ideal plug flow reactor which there is no mixing in the direction of flow and complete mixing perpendicular to the direction of flow (i.e., in the radial direction). The rate of reaction will vary with reaction length. Plug flow reactors are normally operated at steady state so that properties at any position are constant with respect to time. The mass balance around plug flow reactor becomes



$\{$rate of i into volume element$\}$ - $\{$rate of i out of volume element$\}$

+ $\{$rate of production of i within the volume element$\}$

= $\{$rate of accumulation of i within the volume elecment $\}$

$$F_{Ao} = F_{Ao}(1\text{-}x) + (r_W W)$$

$$(r_W W) = F_{Ao} - F_{Ao}(1\text{-}x) = F_{Ao} = F_{Ao}x$$

$$r_W = \frac{F_{Ao}x}{W} = \frac{1.39\times10^{-5}\times0.291}{0.1} = 4.045\times10^{-5} \text{ mol/s-gram catalyst at } 200^{\circ}\text{C}$$

$$r_W = \frac{F_{Ao}x}{W} = \frac{1.39\times10^{-5}\times0.515}{0.1} = 7.159\times10^{-5} \text{ mol/s-gram catalyst at } 250^{\circ}\text{C}$$

$$r_W = \frac{F_{Ao}x}{W} = \frac{1.39\times10^{-5}\times0.845}{0.1} = 1.175\times10^{-5} \text{ mol/s-gram catalyst at } 300^{\circ}\text{C}$$

$$r_W = \frac{F_{Ao}x}{W} = \frac{1.39\times10^{-5}\times0.85}{0.1} = 1.582\times10^{-4} \text{ mol/s-gram catalyst at } 350^{\circ}\text{C}$$

At steady state the external transport rate may be written in terms of the diffusion rate from the bulk gas to the surface. The expression is:

$$R_{obs} = k_m a_m (C_b\text{-}C_s)$$

$$= \frac{\text{phthalic anhydride converted (mole)}}{\text{(time)(gram of catalyst)}}$$

where C_b and C_s are the concentrations in the bulk gas and at the surface, respectively.

At 200°C, $(C_b\text{-}C_s) = \frac{r_{obs}}{k_m a_m} = \frac{4.045\times10^{-5}}{42.57\times1.052} = 9.03\times10^{-7}$ mol/m^3

At 250°C, $(C_b\text{-}C_s) = \frac{r_{obs}}{k_m a_m} = \frac{7.459\times10^{-5}}{45.73\times1.052} = 1.49\times10^{-6}$ mol/m^3

At 300°C, $(C_b\text{-}C_s) = \dfrac{r_{obs}}{k_m a_m} = \dfrac{1.175\times10^{-4}}{51.48\times1.052} = 2.17\times10^{-6}\ \text{mol/m}^3$

At 350°C, $(C_b\text{-}C_s) = \dfrac{r_{obs}}{k_m a_m} = \dfrac{1.182\times10^{-4}}{62.61\times1.052} = 1.79\times10^{-6}\ \text{mol/m}^3$

Consider the difference of the bulk and surface concentration is small. It means that the external mass transport has no effect on the phthalic anhydride oxidation reaction rate.

2. Internal diffusion limitation

Next, consider the internal diffusion limitation of the phthalic anhydride reaction. An effectiveness factor, η, was defined in order to express the rate of reaction for the whole catalyst pellet, r_p, in terms of the temperature and concentrations existing at the outer surface as follows:

$$\eta = \frac{\text{actual rate of whole pellet}}{\text{rate evaluated at outer surface conditions}} = \frac{r_p}{r_s}$$

The equation for the local rate (per unit mass of catalyst) may be expected functionally as r = f(C,T).

Where C represents, symbolically, the concentrations of all the involved components

Then, $r_p = \eta r_s = \eta f(C_s,T_s)$

Suppose that the phthalic anhydride oxidation is an irreversible reaction A→B and first order reaction, so that for isothermal conditions $r = f(C_A) = k_1C_A$. Then $r_p = \eta k_1(C_A)_s$.

For a spherical pellet, a mass balance over the spherical-shell volume of thickness Δr. At steady state the rate of diffusion into the element less the rate of diffusion out will equal the rate of disappearance of reactant with in the element. This rate will be $\rho_p k_1 C_A$ per unit volume, where ρ_p is the density of the pellet. Hence, the balance may be written, omitting subscript A on C,

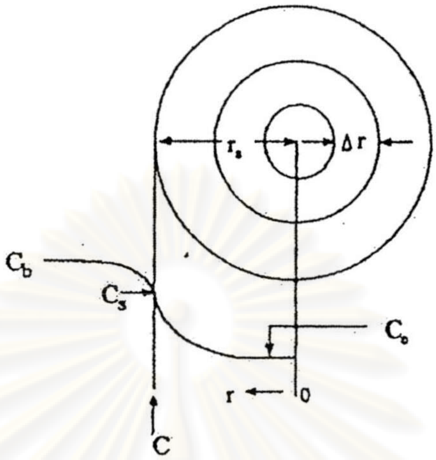


Figure B1. Reactant (A) concentration vs. position for first-order reaction on a spherical catalyst pellet.

$$\left(-4\pi r^2 D_e \frac{dC}{dr}\right)_r - \left(-4\pi r^2 D_e \frac{dC}{dr}\right)_{r+\Delta r} = -4\pi r^2 \Delta r_p k_1 C$$

Take the limit as $\Delta r \rightarrow 0$ and assume that the effective diffusivity is independent of the concentration of reactant. this difference equation becomes

$$\frac{d^2C}{dr^2} + 2\frac{dC}{dr} - \frac{k_1 \rho_p C}{D_e} = 0$$

At the center of the pellet symmetry requires

$$\frac{dC}{dr} = 0 \text{ at } r = 0$$

and at outer surface

$$C = C_s \text{ at } r = r_s$$

Solve linear differential equation by conventional methods to yield

$$\frac{C}{C_s} = \frac{r_s \sinh\left(3\phi_s \frac{r}{r_s}\right)}{r \sinh 3\phi_s}$$

where ϕ_s is Thiele modulus for a spherical pellet defined by $\phi_s = \frac{r_s}{3}\sqrt{\frac{k_1 \rho_p}{D_e}}$

Both D_e and k_1 are necessary to use $r_p = \eta k_1 (C_A)_s$. D_e could be obtained from the reduced pore volume equation in case of no tortuosity factor.

$$D_e = (\varepsilon_s^2 D_{AB})$$

<u>At 200°C</u>, $D_e = (0.5)^2 (0.491) = 0.123$

<u>At 250°C</u>, $D_e = (0.5)^2 (0.582) = 0.146$

<u>At 300°C</u>, $D_e = (0.5)^2 (0.679) = 0.169$

Substitute radius of catalyst pellet, $r_s = 0.107 \times 10^{-3}$ m with ϕ_s equation

$$\phi_s = \frac{0.107 \times 10^{-3}\ \mathrm{m}}{3} \sqrt{\frac{\mathrm{k(m^3/s\text{-}kg\ cat.)} \times 3.75 \times 10^{-4}\mathrm{(kg/m^3)}}{0.123\mathrm{(m^2/s)}}}, \text{at } 200°\text{C}$$

$$\phi_s = 1.97 \times 10^{-6} \sqrt{k} \text{ (dimensionless) at } 200°\text{C}$$

$$\phi_s = 1.81 \times 10^{-6} \sqrt{k} \text{ (dimensionless) at } 250°\text{C}$$

$$\phi_s = 1.68 \times 10^{-6} \sqrt{k} \text{ (dimensionless) at } 300°\text{C}$$

Find k (at 200°C) from the mass balance equation around plug-flow reactor.

$$r_W = \frac{F_{Ao}\, dx}{dW}$$

where $r_W = kC_A$

Thus, $kC_A = \frac{F_{Ao}\,dx}{dW}$

$$kC_{Ao}(1\text{-}x) = \frac{F_{Ao}\,dx}{dW}$$

$$W = \frac{F_{Ao}}{kC_{Ao}} \int_0^{0.3} \frac{1}{1-x}\,dx$$

$$W = \frac{F_{Ao}}{kC_{Ao}} \left[-\ln(1-x)\right]_0^{0.3} = \frac{F_{Ao}}{kC_{Ao}}(-\ln(0.7))$$

$$k = \frac{F_{Ao}}{WC_{Ao}}(-\ln(0.7))$$

$$k = \frac{1.39\times10^{-5}\ (\text{mol/s})}{0.1\times10^{-3}\ (\text{kg})\times6.05(\text{mol/m}^3)}(-\ln(0.7)$$

$$= 8.19\times10^{-3}\ \text{m}^3/\text{s-kg catalyst}$$

Calculate $\phi_s : \phi_s = 1.97\times10^{-6}\sqrt{0.92\times10^{-4}} = 1.78\times10^{-7}$ at 200°C

$$\phi_s = 1.81\times10^{-6}\sqrt{0.92\times10^{-4}} = 2.28\times10^{-7} \text{ at } 250°\text{C}$$

$$\phi_s = 1.68\times10^{-6}\sqrt{0.92\times10^{-4}} = 1.02\times10^{-6} \text{ at } 300°\text{C}$$

For such small values of ϕ_s it was concluded that the internal mass transport has no effect on the rate of phthalic anhydeide oxidation reaction.

APPENDIX C

CALCULATION OF SPECIFIC SURFACE AREA

From Brunauer-Emmett-Teller (BET) equation [Anderson J. R. and co-worker (1985)]

$$\frac{p}{n(1-p)} = \frac{1}{n_m C} + \frac{(C-1)p}{n_m C} \qquad \text{(C1)}$$

Where, p = Relative partial pressure of adsorbed gas, P/P_0

P_0 = Saturated vapor pressure of adsorbed gas in the condensed state at the experimental temperature, atm

P = Equilibrium vapor pressure of adsorbed gas, atm

n = Gas adsorbed at pressure P, ml. at the NTP/g of sample

n_m = Gas adsorbed at monolayer, ml. at the NTP/g of sample

C = $\mathrm{Exp}\,[(H_C - H_l)/RT]$

H_C = Heat of condensation of adsorbed gas on all other layers

H_l = Heat of adsorption into the first layer

Assume $C \rightarrow \infty$, then

$$\frac{p}{n(1-p)} = \frac{p}{n_m}$$

$$n_m = n(1-p) \qquad \text{(C2)}$$

The surface area, S, of the catalyst is given by

$$S = S_b \times n_m \qquad \text{(C3)}$$

From the gas law

$$\frac{P_b V}{T_b} = \frac{P_t V}{T_t} \qquad \text{(C4)}$$

Where, P_b = Pressure at 0°C

P_t = Pressure at t°C

T_b = Temperature at 0°C = 273.15 K

T_t = Temperature at t°C = 273.15 + t K

V = Constant volume

Then, $P_b = (273.15/T_t) \times P_t = 1$ atm

Partial pressure

$$P = \frac{[\text{Flow of } (He + N_2) - \text{Flow of } He]}{\text{Flow of } (He + N_2)} \qquad (C5)$$

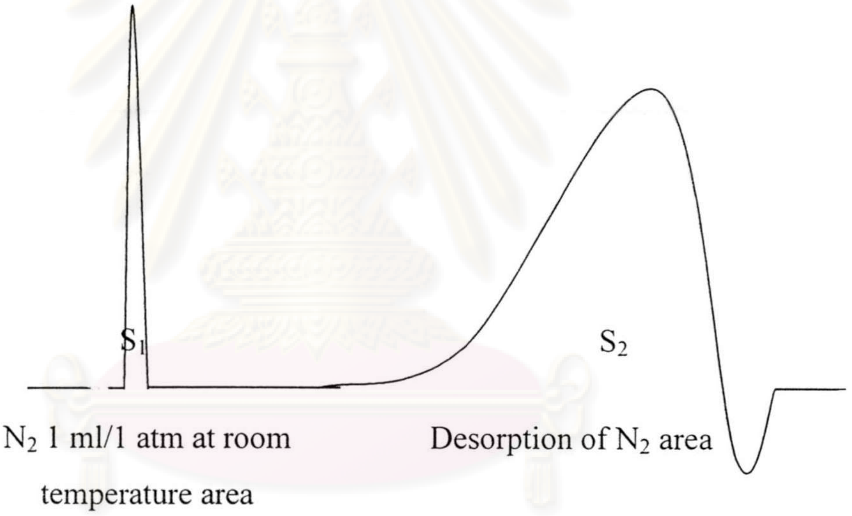
$$= 0.3 \text{ atm}$$

For nitrogen gas, the saturated vapor pressure equals to

P_0 = 1.1 atm

then, $p = P/P_0 = 0.3/1.1 = 0.2727$

To measure the volume of nitrogen adsorbed, n



$$n = \frac{S_2}{S_1} \times \frac{1}{W} \times \frac{273.15}{T} \text{ ml. /g of catalyst} \qquad (C6)$$

Where, S_1 = N_2 1 ml/1 atm at room temperature area

S_2 = Desorption of N_2 area

W = Sample weight, g

T = Room temperature, K

Therefore,

$$n_m = \frac{S_2}{S_1} \times \frac{1}{W} \times \frac{273.15}{T} \times (1 - p)$$

$$n_m = \frac{S_2}{S_1} \times \frac{1}{W} \times \frac{273.15}{T} \times 0.7272 \qquad \text{(C2.1)}$$

Whereas, the surface area of nitrogen gas from literature equal to

S_b = 4.373 m^2/ml of nitrogen gas

Then,

$$S = \frac{S_2}{S_1} \times \frac{1}{W} \times \frac{273.15}{T} \times 0.7272 \times 4.343$$

$$S = \frac{S_2}{S_1} \times \frac{1}{W} \times \frac{273.15}{T} \times 3.1582 \text{ m}^2/\text{g} \qquad \text{(C7)}$$

APPENDIX D

CALIBRATION CURVE

Flame ionization detector gas chromatographs Shimadzu model 9A equipped with a Chromosorb WAW column is used to analyze the concentrations of phthalic anhydride, maleic anhydride, acetic acid, ethylbenzene, toluene, and benzene.

The Porapak-Q and Molecular Sieve 5-A column are used with a gas chromatograph equipped with a thermal conductivity detector, Shimadzu model 8A, to analyze the concentration of CO_2 and CO.

The calibration curves of phthalic anhydride, maleic anhydride, acetic acid, ethylbenzene, toluene, and benzene are illustrated in the following figures.

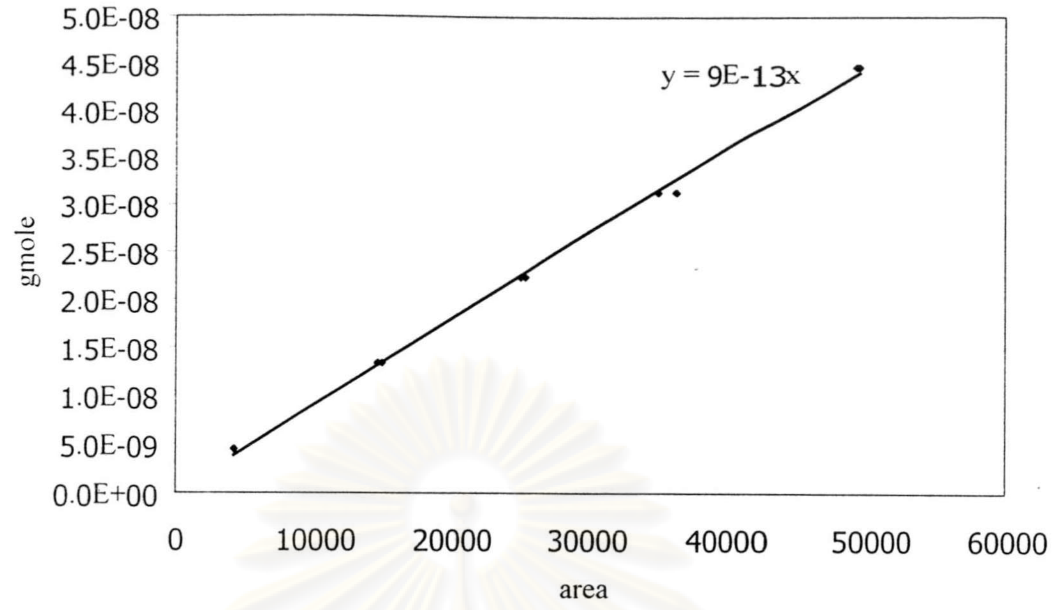


Figure D1 The calibration curve of phthalic anhydride

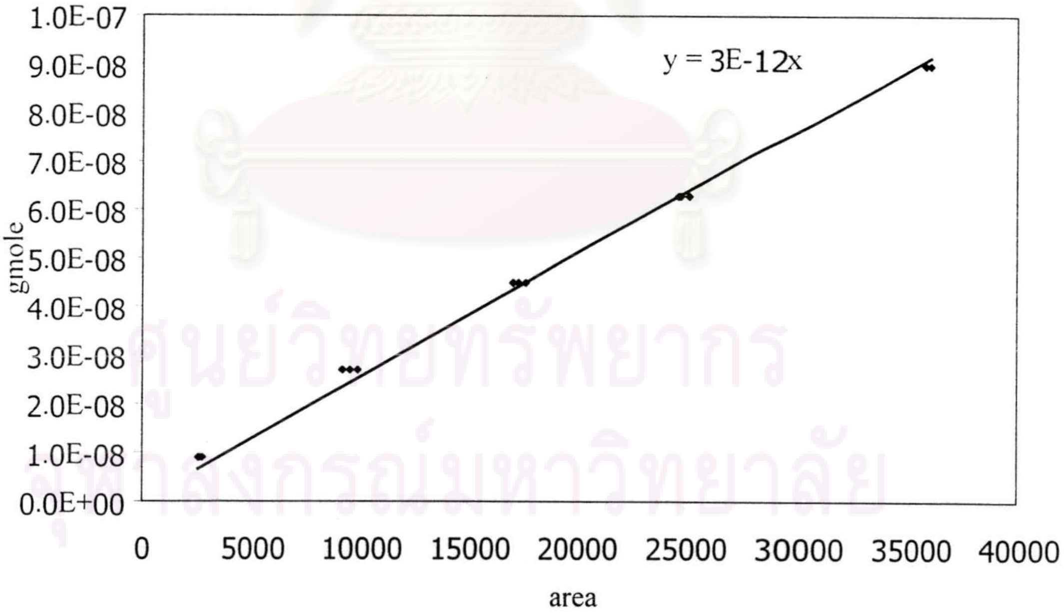


Figure D2 The calibration curve of maleic anhydride

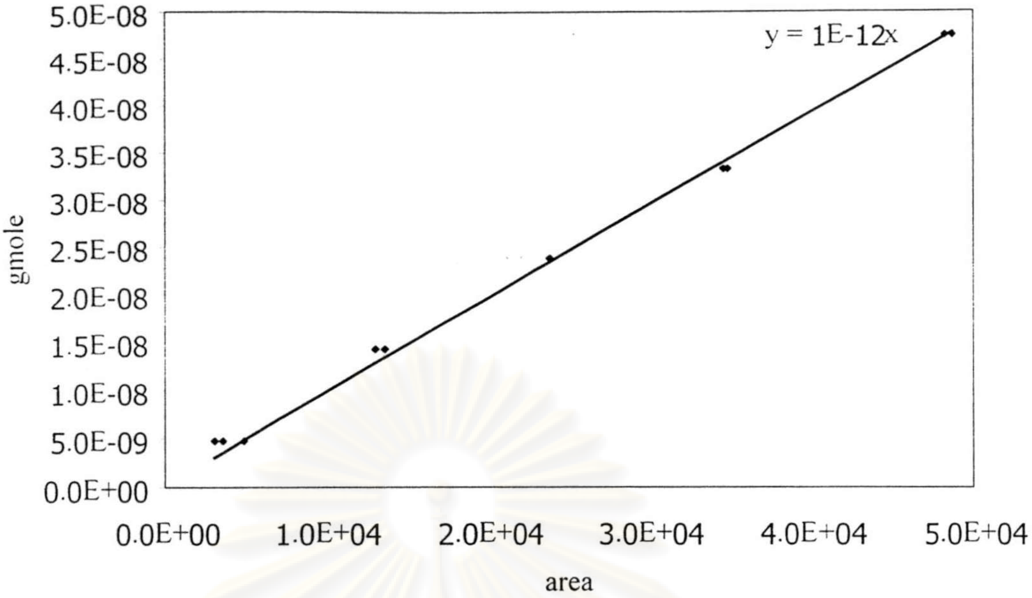


Figure D3 The calibration curve of acetic acid

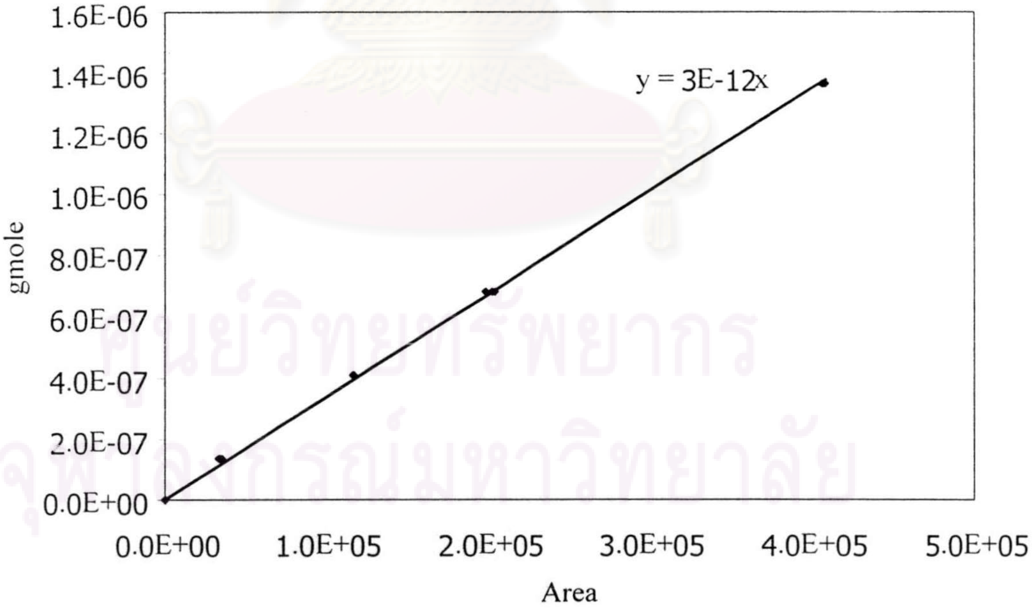


Figure D4 The calibration curve of ethylbenzene

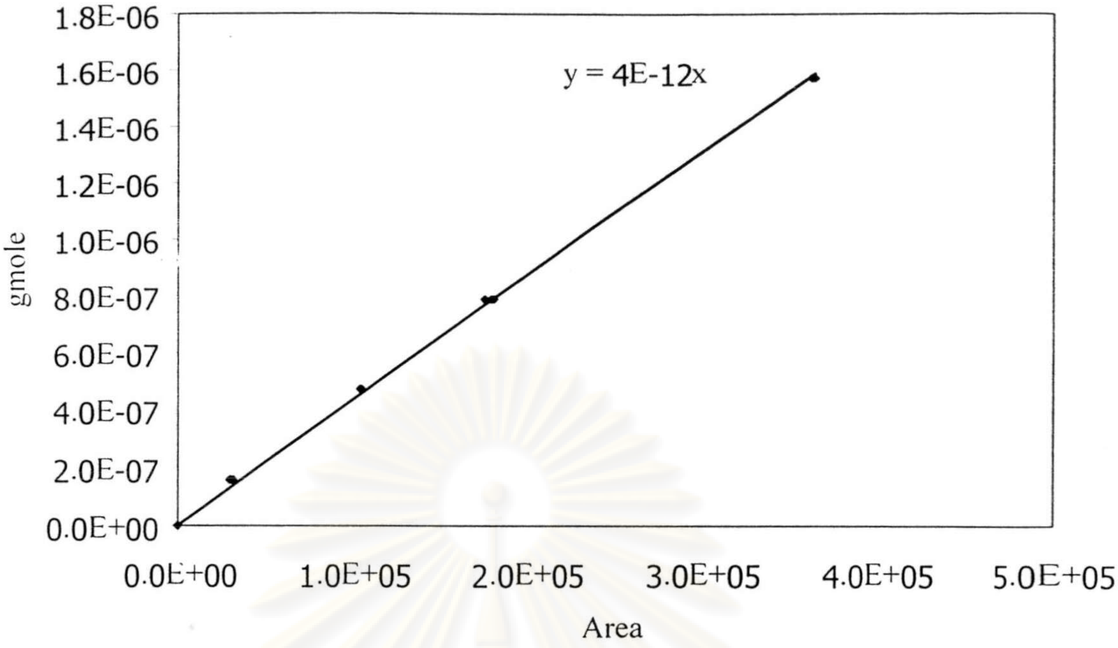


Figure D5 The calibration curve of toluene

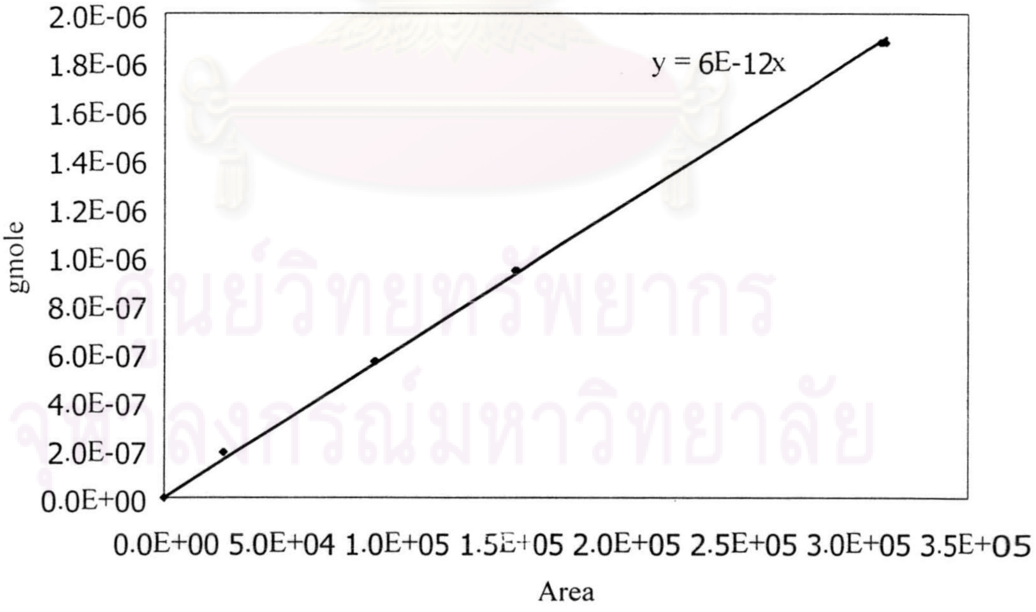


Figure D6 The calibration curve of benzene

APPENDIX E

DATA OF EXPERIMENTS

Table E1 Data of figure 5.5

Temp (^oC)	Phthalic anhydride conversion (%)				
	Blank	$CoMgO/Al_2O_3$	Co_3O_4/Al_2O_3	MgO/Al_2O_3	Al_2O_3
200	2.18	29.08	25.03	4.01	5.27
250	2.65	51.53	27.74	11.48	17.66
300	5.93	84.46	40.48	14.10	37.06
350	15.37	84.74	50.61	29.10	41.66
400	22.36	87.34	55.42	39.86	49.51
450	27.83	88.73	63.55	51.28	55.23
500	34.41	90.73	69.11	63.92	65.48
550	43.49	91.21	94.65	81.25	79.62

Table E2 Data of figure 5.6

Temp (^oC)	Maleic anhydride conversion (%)				
	Blank	$CoMgO/Al_2O_3$	Co_3O_4/Al_2O_3	MgO/Al_2O_3	Al_2O_3
200	1.65	12.01	5.03	2.91	2.36
250	1.87	30.25	17.63	7.95	8.59
300	3.42	43.95	30.16	9.06	20.69
350	20.00	68.23	38.70	23.07	24.87
400	38.26	94.64	62.42	43.93	50.09
450	61.50	94.76	90.51	79.38	85.74
500	67.05	95.29	91.05	84.78	86.61
550	68.69	97.63	93.36	85.43	89.89

Table E3 Data of figures 5.7-5.9

Temp.(°C)	Benzene conversion (%)		Toluene conversion (%)		Ethylbenzene conversion (%)	
	Blank	Co-Mg-O/Al_2O_3	Blank	Co-Mg-O/Al_2O_3	Blank	Co-Mg-O/Al_2O_3
200	0.00	3.39	0.00	1.08	0.00	4.79
250	0.00	16.22	0.00	20.59	0.00	7.79
300	0.00	32.28	0.00	47.79	0.00	12.21
350	0.00	44.15	0.00	75.49	0.00	86.49
400	0.00	69.24	5.00	93.77	10.00	100.00
450	32.70	76.64	30.00	100.00	38.00	100.00
500	43.15	89.06	42.85	100.00	48.00	100.00
550	55.00	96.64	56.10	100.00	62.00	100.00

Table E4 Data of figure 5.10

Temp(°C)	Acetic acid conversion (%)				
	Blank	Co-Mg-O/Al_2O_3	Co_3O_4/Al_2O_3	MgO/Al_2O_3	Al_2O_3
100		2.08	1.21	0.02	0.89
150		14.17	5.01	1.54	5.09
200	5.76	22.38	10.43	11.26	6.43
250	12.73	29.16	37.41	19.48	27.86
300	15.39	94.28	94.81	93.08	95.37
350	89.15	94.80	95.31	94.72	96.43
400	94.71	95.17	95.22	94.88	96.95
450	95.79	95.46	95.31	95.48	96.92
500	96.46	96.83	97.24	97.79	97.36
550	96.82	96.93	97.33	98.05	97.47

Table E5 Data of figure 5.11

Temp (°C)	Phthalic anhydride conversion (%)			
	8Co3MgO/Al_2O_3	8Co2MgO/Al_2O_3	8Co1MgO/Al_2O_3	8Co0.5MgO/Al_2O_3
200	14.4	14.59	29.08	14.47
250	22.65	24.44	51.53	22.85
300	52.94	38.72	84.46	40.35
350	87.52	78.81	84.74	56.69
400	89.61	85.79	87.34	63.42
450	91.05	86.11	88.73	82.30
500	92.09	87.97	90.73	85.39
550	92.35	90.09	91.21	86.01

Table E6 Data of figure 5.12

Temp (°C)	Maleic anhydride conversion (%)			
	8Co3MgO/Al_2O_3	8Co2MgO/Al_2O_3	8Co1MgO/Al_2O_3	8Co0.5MgO/Al_2O_3
200	2.28	7.59	12.01	0.27
250	18.31	20.01	30.25	2.27
300	26.29	33.75	43.95	3.88
350	39.52	50.68	68.23	39.23
400	74.95	91.66	94.64	90.62
450	90.89	92.58	94.76	92.53
500	90.9	92.81	95.29	95.50
550	92.72	95.16	97.63	95.52

Table E7 Data of figure 5.13

Temp (°C)	Phthalic anhydride conversion (%)				
	10Co1MgO/Al_2O_3	9Co1MgO/Al_2O_3	8Co1MgO/Al_2O_3	7Co1MgO/Al_2O_3	6Co1MgO/Al_2O_3
200	19.36	17.02	29.08	15.29	18.18
250	30.52	23.44	51.53	17.86	25.61
300	70.96	60.35	84.46	52.97	63.61
350	85.41	74.11	84.74	66.71	76.87
400	90.06	82.07	87.34	78.06	90.87
450	91.21	82.53	88.73	78.95	90.95
500	91.54	83.03	90.73	79.12	91.05
550	91.63	84.17	91.21	80.02	91.21

Table E8 Data of figure 5.14

Temp (°C)	Maleic anhydride conversion (%)				
	10Co1MgO/Al_2O_3	9Co1MgO/Al_2O_3	8Co1MgO/Al_2O_3	7Co1MgO/Al_2O_3	6Co1MgO/Al_2O_3
200	1.93	10.97	12.01	5.59	0.35
250	25.26	11.67	30.25	7.78	18.59
300	38.46	20.68	43.95	10.43	31.43
350	64.63	53.15	68.23	31.61	55.27
400	92.71	77.39	94.64	87.27	87.11
450	94.21	78.41	94.76	88.7	87.89
500	94.67	80.81	95.29	90.00	90.58
550	97.60	81.61	97.63	90.32	90.84

APPENDIX F

MATERIAL SAFETY DATA SHEETS OF PHTHALIC ANHYDRIDE AND MALEIC ANHYDRIDE

Safety data for phthalic anhydride

General

Synonyms: 1,2-benzenedicarboxylic acid anhydride, phthalic acid anhydride

Molecular formula: $C_8H_4O_3$

Physical data

Appearance: white crystalline solid with choking odour

Melting point: 131°C

Boiling point: 295°C

Vapour density: 5.1 (air=1)

Vapour pressure:

Density (g cm^{-1}): 1.53

Flash point: 152°C (closed cup)

Explosion limit: 1.7-10.5%

Autoignition temperature:

Water solubility: slight

Stability

Stable. Combustible. Incompatible with strong oxidizing agents, strong bases, moisture, nitric acid, alkalies. Dust may form an explosive mixture with air.

Toxicology

Corrosive - causes burns. Harmful if swallowed or inhaled. Skin or eye contact may cause severe irritation. Typical TLV/TWA 1 ppm. Typical STEL 4 ppm. Typical PEL 2 ppm.

Personal protection

Safety glasses, gloves, adequate ventilation.

Safety data for maleic anhydride

General

Synonyms: cis-butenedioc anhydride, 2,5-furanedione, toxilic anhydride, dihydro-2,5-dioxofuran, lytron 810, lytron 820, NCI-C54660

Molecular formula: $C_4H_2O_3$

Physical data

Appearance: colourless or white solid with an acrid odour

Melting point: 53°C

Boiling point: 201°C

Vapour density: 3.4 (air=1)

Vapour pressure: 0.16 mm Hg at 20°C

Density (g cm^{-3}): 1.43

Flash point: 102°C (closed cup)

Explosion limits:

Autoignition temperature:

Water solubility: soluble; decomposes in hot solution

Stability

Stable. Combustible. Incompatible with water, strong oxidizing agents, alkali metals, strong bases, amines, most common metals, polymerisation catalysts and accelerators.

Toxicology

Harmful if swallowed, inhaled or absorbed through the skin. Corrosive - causes burns. Irritant. Typical TLV/TWA 0.25 ppm. Typical PEL 0.25 ppm.

Personal protection

Safety glasses, gloves, adequate ventilation.

VITA

Miss. Surangkana Umpo was born on October 4th, 1978 in Chonburi, Thailand. She received the Bachelor Degree of Chemical Engineering from Faculty of Engineering, King's Mongkut Institute of Technology Ladkrabang in 2000. She continued her Master's Study at Chulalongkorn University in June, 2000.