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APPENDICES

APPENDIX A
CALCULATION OF CATALYST PREPARATION

Preparation of 8Co-Mg-O/TiO_2 and 8Co-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 - Titanium dioxide [TiO_2]
- Alumina [Al_2O_3]

Calculation for the preparation of the 8Co-Mg-O/TiO_2 catalyst.

The 8Co-Mg-O/TiO_2 aqueous solution used in catalyst preparation consists of Co 8wt% and TiO_2 92wt%. The amount of cobalt in 8Co-Mg-O/TiO_2 catalyst is calculated as follows:

Basis: TiO_2 1 g.
If the weight of catalyst was 100 gram, 8Co-Mg-O/TiO_2 would compose of cobalt 8 g. and TiO_2 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 1% was loaded on $8Co/TiO_2$ 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-Mg-O/ Al_2O_3 catalyst.

The calculation for the preparation of $8Co\text{-}Mg\text{-}O/Al_2O_3$ catalyst is the same as the preparation of $8Co\text{-}Mg\text{-}O/TiO_2$ catalyst.

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 1-propanal oxidation 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, 8% 1-propanol, 5% O_2 balance with nitrogen was used as the unique reactant in the system. Molecular weight of 1-propanol and air (O_2 5%) are 60 and 28.2, respectively. Thus, the average molecular weight of the gas mixture was calculated as follows:

$$M_{AB} = 0.08\times60 + 0.92\times28.2$$
$$= 30.744 \text{ g/mol}$$

Calculation of reactant gas density

Consider the 1-propanol oxidation 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.

$$\rho = \frac{PM}{RT} = \frac{1.0\times10^{5}\times30.744\times10^{-3}}{8.314T}$$

We obtained : $\rho = 0.782$ kg/m^3 at T = 200°C

$\rho = 0.706$ kg/m^3 at T = 250°C

$\rho = 0.645$ kg/m^3 at T = 300°C

$\rho = 0.594$ kg/m^3 at T = 350°C

Calculation of the gas mixture viscosity

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 1-propanol and 2 to air (O_2 5%)

$M_1 = 60$ and $M_2 = 28.2$

From Perry the viscosity of pure 1-propanol at 200°C, 250°C, 300°C, 350°C, 400°C, 450°C and 500°C are 0.0124, 0.0135, 0.015 and 0.0162 cP, respectively. The viscosity of pure air at 200°C, 250°C, 300°C and 350°C are 0.0248, 0.0265, 0.0285 and 0.030 cP, respectively.

At 200°C :

$$\phi_{12} = \frac{\left[1+\left(\frac{0.0124}{0.0248}\right)^{1/2}\left(\frac{28.2}{60}\right)^{1/4}\right]^2}{\left[8\left(1+\frac{60}{28.2}\right)\right]^{1/2}} = 0.502$$

$$\phi_{21} = 0.502\left(\frac{0.0248}{0.0124}\right)\left(\frac{60}{28.2}\right) = 2.14$$

$$\mu_m = \frac{0.08\times 0.0124}{0.08+0.92\times 0.502} + \frac{0.92\times 0.0248}{0.92+0.08\times 2.14} = 0.0227cP = 2.27\times 10^{-5}\, kg/m-\sec$$

At 250°C :

$$\phi_{12} = \frac{\left[1+\left(\frac{0.0135}{0.0265}\right)^{1/2}\left(\frac{28.2}{60}\right)^{1/4}\right]^2}{\left[8\left(1+\frac{60}{28.2}\right)\right]^{1/2}} = 0.506$$

$$\phi_{21} = 0.506\left(\frac{0.0265}{0.0135}\right)\left(\frac{60}{28.2}\right) = 2.113$$

$$\mu_m = \frac{0.08\times 0.0135}{0.08+0.92\times 0.506} + \frac{0.92\times 0.0265}{0.92+0.08\times 2.113} = 0.0244cP = 2.44\times 10^{-5}\, kg/m-\sec$$

At 300°C :

$$\phi_{12} = \frac{\left[1+\left(\frac{0.015}{0.0285}\right)^{1/2}\left(\frac{28.2}{60}\right)^{1/4}\right]^2}{\left[8\left(1+\frac{60}{28.2}\right)\right]^{1/2}} = 0.512$$

$$\phi_{21} = 0.512\left(\frac{0.0285}{0.015}\right)\left(\frac{60}{28.2}\right) = 2.07$$

$$\mu_m = \frac{0.08\times 0.015}{0.08+0.92\times 0.512} + \frac{0.92\times 0.0285}{0.92+0.08\times 2.07} = 0.0263cP = 2.63\times 10^{-5}\, kg/m-\sec$$

At 350°C :

$$\phi_{12} = \frac{\left[1+\left(\frac{0.0162}{0.030}\right)^{1/2}\left(\frac{28.2}{60}\right)^{1/4}\right]^2}{\left[8\left(1+\frac{60}{28.2}\right)\right]^{1/2}} = 0.517$$

$$\phi_{21} = 0.517\left(\frac{0.030}{0.0162}\right)\left(\frac{60}{28.2}\right) = 2.037$$

$$\mu_m = \frac{0.08\times 0.0162}{0.08+0.92\times 0.517} + \frac{0.92\times 0.030}{0.92+0.08\times 2.037} = 0.0278cP = 2.78\times 10^{-5}\, kg/m-\text{sec}$$

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

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

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 air and propanol are as follows: (Reid,1988)

For C_3H_7OH : $\sigma(C_3H_7OH) = 4.549\ ^0A$, $\varepsilon/k = 576.7$

For air : σ (air) $= 3.711\ ^0A$, $\varepsilon/k = 78.6$

The sample rules are usually employed.

$$\sigma_{AB} = \frac{\sigma_A + \sigma_B}{2} = \frac{4.549 + 3.711}{2} = 4.13$$

$$\varepsilon_{AB}/k = \left(\frac{\varepsilon_A \varepsilon_B}{k^2}\right)^{1/2} = (576.7 \times 78.6)^{1/2} = 212.9$$

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 $T^* = \frac{473}{212.9} = 2.222$ at 200°C

$T^* = \frac{523}{212.9} = 2.456$ at 250°C

$T^* = \frac{573}{212.9} = 2.691$ at 300°C

$T^* = \frac{623}{212.9} = 2.926$ 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 = 1.038 ; 200°C

Ω_D = 1.006 ; 250°C

Ω_D = 0.979 ; 300°C

Ω_D = 0.956 ; 350°C

With Equation of D_{AB},

$$\underline{\text{At } 200^\circ\text{C}} : D(C_3H_7OH\text{-air}) = \frac{\left(3.03 - \frac{0.98}{30.24^{0.5}}\right)(10^{-3})473^{3/2}}{1 \times 30.24^{0.5} \times 4.13^2 \times 1.038}$$

$$= 3.01 \times 10^{-5} \quad m^2/s$$

$$\underline{\text{At } 250^\circ\text{C}} : D(C_3H_7OH\text{-air}) = \frac{\left(3.03 - \frac{0.98}{30.24^{0.5}}\right)(10^{-3})523^{3/2}}{1 \times 30.24^{0.5} \times 4.13^2 \times 1.006}$$

$$= 3.62 \times 10^{-5} \quad m^2/s$$

$$\underline{\text{At } 300^\circ\text{C}} : D(C_3H_7OH\text{-air}) = \frac{\left(3.03 - \frac{0.98}{30.24^{0.5}}\right)(10^{-3})573^{3/2}}{1 \times 30.24^{0.5} \times 4.13^2 \times 0.979}$$

$$= 4.26 \times 10^{-5} \quad m^2/s$$

$$\underline{\text{At } 350^\circ\text{C}} : D(C_3H_7OH\text{-air}) = \frac{\left(3.03 - \frac{0.98}{30.24^{0.5}}\right)(10^{-3})623^{3/2}}{1 \times 30.24^{0.5} \times 4.13^2 \times 0.956}$$

$$= 5.04 \times 10^{-5} \quad m^2/s$$

Reactant gas mixture was supplied at 100 ml/min. in tubular microreactor used in the 1-propanol oxidation system at 30°C

1-propanol flow rate through reactor = 100 ml/min. at 30°C

The density of 1-propanol , $\rho = \frac{1.0\times10^{5}\times30.744\times10^{-3}}{8.314(273+30)} = 1.236$ kg/s

Mass flow rate = $1.236\left(\frac{100\times10^{-6}}{60}\right) = 2.06\times10^{-6}$ kg/s

Diameter of quartz tube reactor = 8 mm

Cross-sectional area of tube reactor = $\frac{\pi(8\times10^{-3})^{2}}{4} = 5.03\times10^{-5}$ m^2

Mass Velocity , $G = \frac{2.06\times10^{-6}}{5.03\times10^{-5}} = 0.04$ 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:

$$Re_p = \frac{d_p G}{\mu}$$

We obtained

At 200°C : $Re_p = \frac{(0.152\times10^{-3}\times0.04)}{2.27\times10^{-5}} = 0.268$

At 250°C : $Re_p = \frac{(0.152\times10^{-3}\times0.04)}{2.44\times10^{-5}} = 0.249$

At 300°C : $Re_p = \frac{(0.152\times10^{-3}\times0.04)}{2.63\times10^{-5}} = 0.231$

At 350°C : $Re_p = \frac{(0.152\times10^{-3}\times0.04)}{2.78\times10^{-5}} = 0.219$

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> ; $j_D = \frac{0.458}{0.5}(0.268)^{-0.407} = 1.565$

<u>At 250°C</u> ; $j_D = \frac{0.458}{0.5}(0.249)^{-0.407} = 1.613$

At 300°C : $j_D = \frac{0.458}{0.5}(0.231)^{-0.407} = 1.663$

At 350°C : $j_D = \frac{0.458}{0.5}(0.219)^{-0.407} = 1.699$

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

$$j_D = \frac{\varepsilon k_m \rho}{G}(\mu / \rho D)^{2/3}$$

Where ε is the porosity of the single screen.

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

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

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

At 200°C : $Sc = \frac{2.27 * 10^{-5}}{0.782 * 3.01 * 10^{-5}} = 0.964$

At 250°C : $Sc = \frac{2.44 * 10^{-5}}{0.706 * 3.62 * 10^{-5}} = 0.955$

At 300°C : $Sc = \frac{2.63 * 10^{-5}}{0.645 * 4.26 * 10^{-5}} = 0.957$

At 350°C : $Sc = \frac{2.78 * 10^{-5}}{0.594 * 5.04 * 10^{-5}} = 0.928$

Find k_m : At 200°C, $k_m = \left(\frac{1.565 \times 0.04}{0.782}\right)(0.964)^{-2/3} = 0.082$ m/s

At 250°C, $k_m = \left(\frac{1.613 \times 0.04}{0.706}\right)(0.955)^{-2/3} = 0.094$ m/s

At 300°C, $k_m = \left(\frac{1.663 \times 0.04}{0.645}\right)(0.957)^{-2/3} = 0.106$ m/s

At 350°C, $k_m = \left(\frac{1.699 \times 0.04}{0.594}\right)(0.928)^{-2/3} = 0.12$ 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 = $\frac{\pi(0.152 \times 0^{-1})^3 \times 0.375}{6} = 6.895 * 10^{-7}$ g/particle

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

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

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

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

1-propanol molar feed rate = $0.08 \times 6.62 \times 10^{-5} = 5.29 \times 10^{-6}$ mol/s

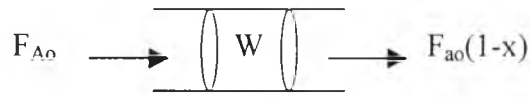
1-propanol conversion (experimental data): 1.78 % at 200°C

5.73 % at 250°C

28.07 % at 300°C

59.93 % at 350°C

The estimated rate of 1-propanol 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 }

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

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

$$r_W = \frac{F_{Ao}x}{W} = \frac{5.29\times10^{-6}\times0.0178}{0.1} = 4.717\times10^{-7} \text{ mol/s-gram catalyst at } 200^{\circ}C$$

$$r_W = \frac{F_{Ao}x}{W} = \frac{5.29\times10^{-6}\times0.0573}{0.1} = 1.518\times10^{-6} \text{ mol/s-gram catalyst at } 250^{\circ}C$$

$$r_W = \frac{F_{Ao}x}{W} = \frac{5.29\times10^{-6}\times0.28}{0.1} = 7.42\times10^{-6} \text{ mol/s-gram catalyst at } 300^{\circ}C$$

$$r_W = \frac{F_{Ao}x}{W} = \frac{5.29\times10^{-6}\times0.599}{0.1} = 1.587\times10^{-5} \text{ mol/s-gram catalyst at } 350^{\circ}C$$

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:

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

$$= \frac{1\text{-propanol converted (mole)}}{(\text{time})(\text{gram of catalyst})}$$

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

$$\underline{\text{At } 200^{\circ}\text{C}},\ (C_b\text{-}C_s) = \frac{r_{obs}}{k_m a_m} = \frac{4.717\times10^{-7}}{0.082\times1.052\times10^{-1}} = 5.47\times10^{-4}\ \text{mol/m}^3$$

$$\underline{\text{At } 250^{\circ}\text{C}},\ (C_b\text{-}C_s) = \frac{r_{obs}}{k_m a_m} = \frac{1.518\times10^{-6}}{0.094\times1.052\times10^{-1}} = 1.53\times10^{-4}\ \text{mol/m}^3$$

$$\underline{\text{At } 300^{\circ}\text{C}},\ (C_b\text{-}C_s) = \frac{r_{obs}}{k_m a_m} = \frac{7.42\times10^{-6}}{0.106\times1.052\times10^{-1}} = 6.65\times10^{-3}\ \text{mol/m}^3$$

$$\underline{\text{At } 350^{\circ}\text{C}},\ (C_b\text{-}C_s) = \frac{r_{obs}}{k_m a_m} = \frac{1.587\times10^{-5}}{0.12\times1.052\times10^{-1}} = 1.26\times10^{-3}\ \text{mol/m}^3$$

From C_b (1-propanol) = 1.59 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 1-propanol oxidation reaction rate.

2. Internal diffusion limitation

Next, consider the internal diffusion limitation of the 1-propanol 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 1-propanol oxidation is an irreversible reaction A→B and first order reaction, so that for isothermal conditions $r = f(C_A) = k_1 C_A$. 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,

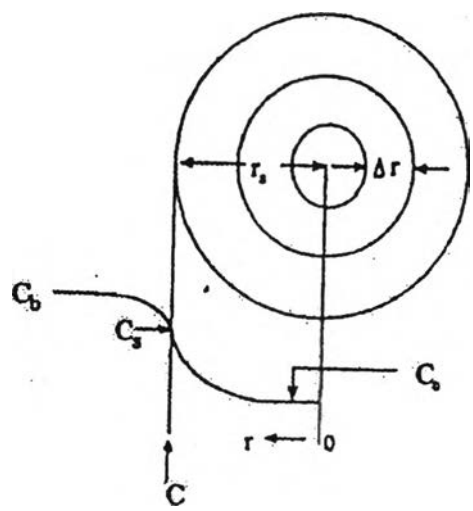


Figure B1. Reactant (A) concentration vs. position for first-order reaction on a spherical catalyst pellet.

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

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

$C = C_s$ 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.

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

At 200°C. $D_e = (0.5)^2 (3.01\times10^{-5}) = 7.53\times10^{-6}$

At 250°C. $D_e = (0.5)^2 (3.62\times10^{-5}) = 9.04\times10^{-6}$

At 300°C. $D_e = (0.5)^2 (4.26\times10^{-5}) = 1.06\times10^{-5}$

Substitute radius of catalyst pellet, $r_s = 0.107\times10^{-3}$ m with ϕ_s equation

$$\phi_s = \frac{0.076\times10^{-3}\text{ m}}{3}\sqrt{\frac{k(\text{m}^3/\text{s - kg cat.})\times 1000(\text{kg/m}^3)}{7.53\times10^{-6}(\text{m}^2/\text{s})}}, \text{ at 200°C}$$

$$\phi_s = 0.292\sqrt{k} \text{ (dimensionless) at 200°C}$$

$\phi_s = 0.266\sqrt{k}$ (dimensionless) at 250°C

$\phi_s = 0.246\sqrt{k}$ (dimensionless) at 300°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. $$kC_A = \frac{F_{Ao}\, dx}{dW}$$

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

$$W = \frac{F_{Ao}}{kC_{Ao}} \int_0^{0.1} \frac{1}{1-x}\, dx$$

$$W = \frac{F_{Ao}}{kC_{Ao}} \left[-\ln(1-x)\right]_0^{0.1} = \frac{F_{Ao}}{kC_{Ao}}(-\ln(0.9))$$

$$k = \frac{F_{Ao}}{WC_{Ao}}(-\ln(0.9822))$$

$$k = \frac{5.29\times10^{-6}\ (\text{mol/s})}{0.1\times10^{-3}\ (\text{kg})\times 1.03(\text{mol/m}^3)}(-\ln(0.9822))$$

$$= 0.92 \times 10^{-4}\ \text{m}^3\text{/s-kg catalyst}$$

Calculate $\phi_s : \phi_s = 0.292\sqrt{0.92\times10^{-4}} = 0.0028$ at 200°C

$$\phi_s = 0.266\sqrt{3.03\times10^{-3}} = 0.015 \text{ at } 250°C$$

$$\phi_s = 0.246\sqrt{1.68\times10^{-2}} = 0.032 \text{ at } 300°C$$

For such small values of ϕ_s it was concluded that the internal mass transport has no effect on the rate of 1-propanol oxidation reaction.

APPENDIX C

CALCULATION OF SPECIFIC SURFACE AREA

From Brunauer-Emmett-Teller (BET) equation

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

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 = Quantity of gas adsorbed at pressure P, ml. at the NTP/g of sample

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

C = 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

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

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

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

$$S = S_b \times n_m \qquad (C3)$$

From the gas law

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

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

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

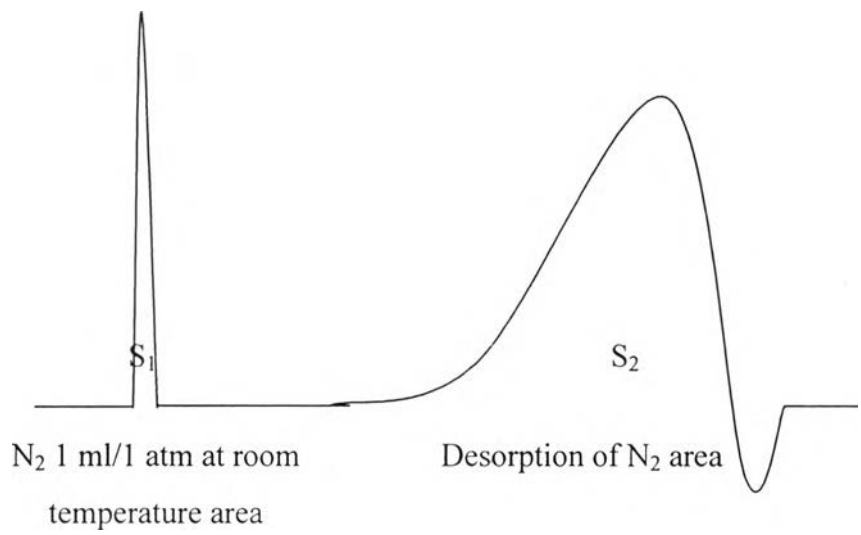
$$= 0.3 \text{ atm}$$

For nitrogen gas, the saturated vapor pressure equals to

$$P_0 = 1.1 \text{ atm}$$

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

To measure the volume of nitrogen adsorbed, n



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

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,

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

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

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

S_b = 4.373 m^2/ml of nitrogen gas

Then,

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

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

APPENDIX D
CALIBRATION CURVE

Flame ionization detector gas chromatographs, model 14A and 14B, were used to analyze the concentrations of oxygenated compounds and light hydrocarbons, respectively. 1-propanol, 2-propanol, formaldehyde, acetaldehyde, and propionaldehyde were analyzed by GC model 14A while methane, ethylene, propane, and propylene were analyzed by GC model 14B.

Gas chromatograph with the thermal conductivity detector, model 8A, was used to analyze the concentration of CO_2 by using Porapak-Q column.

The calibration curves of methane, ethylene, propane, propylene, 1-propanol, 2-propanol, CO_2, formaldehyde, acetaldehyde, and propionaldehyde are illustrated in the following figures.

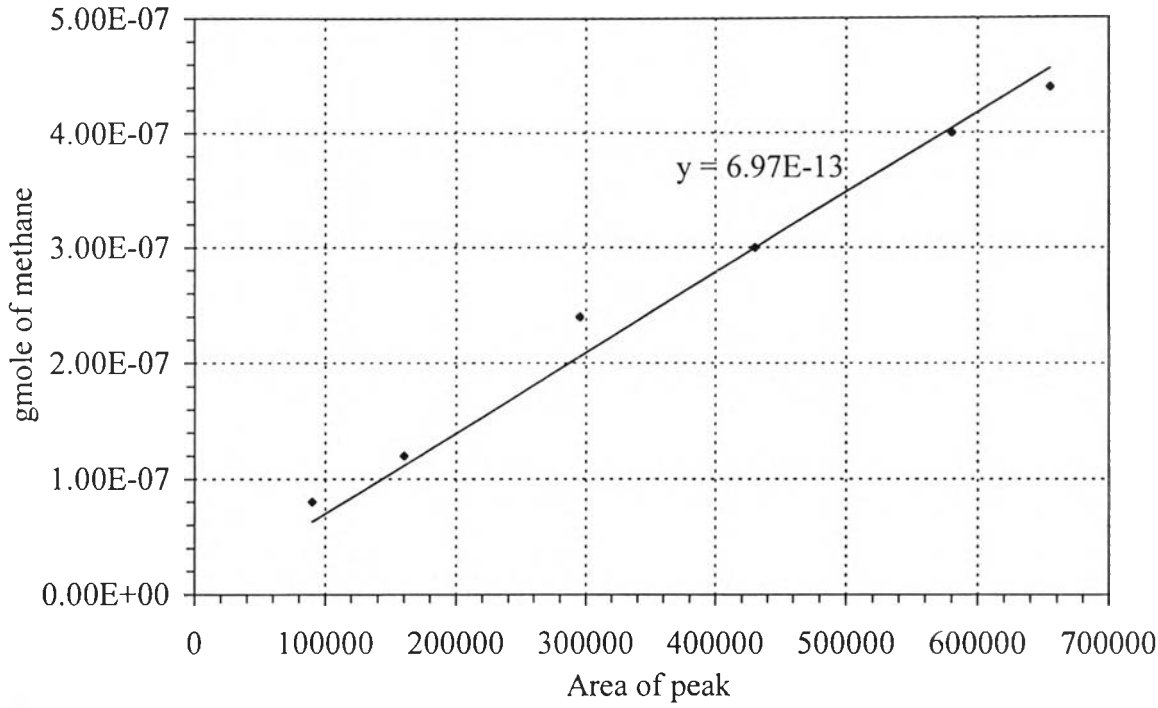


Figure D1 The calibration curve of methane

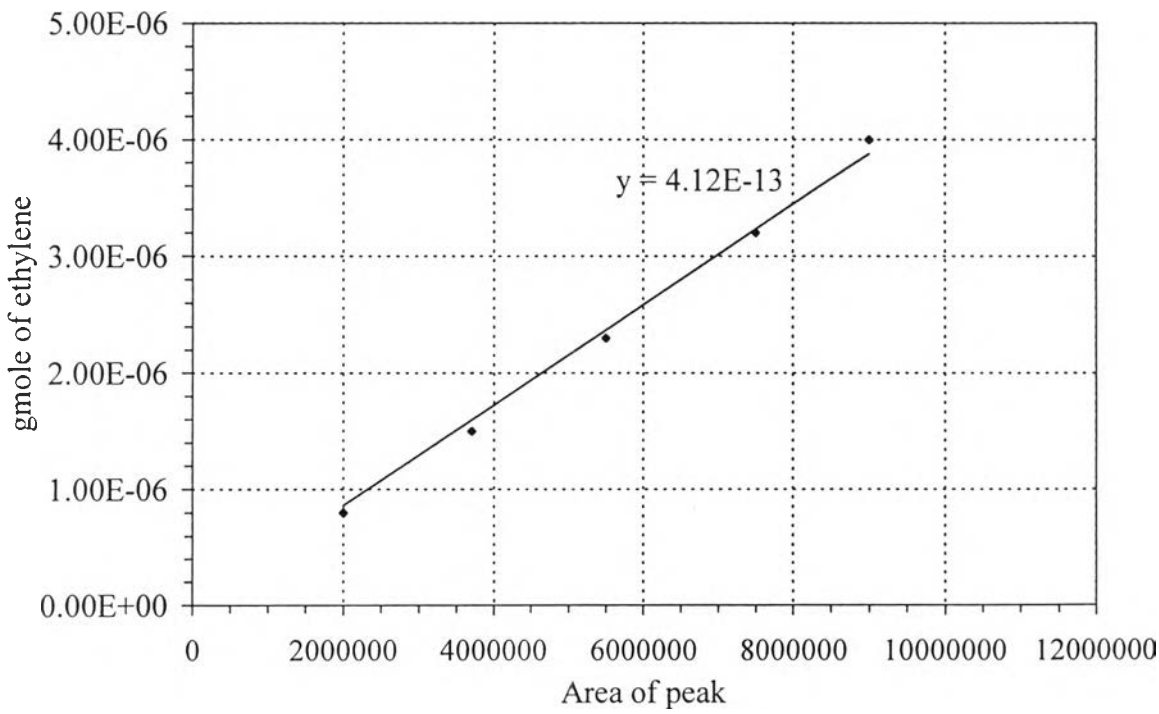


Figure D2 The calibration curve of ethylene

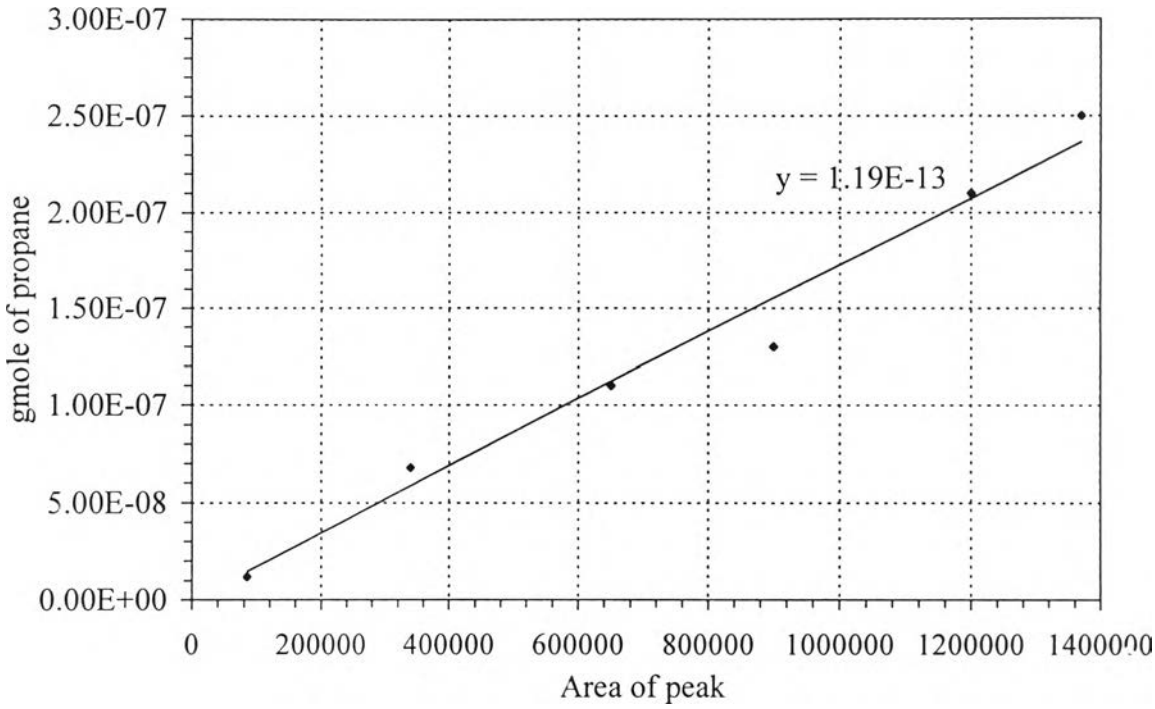


Figure D3 The calibration curve of propane

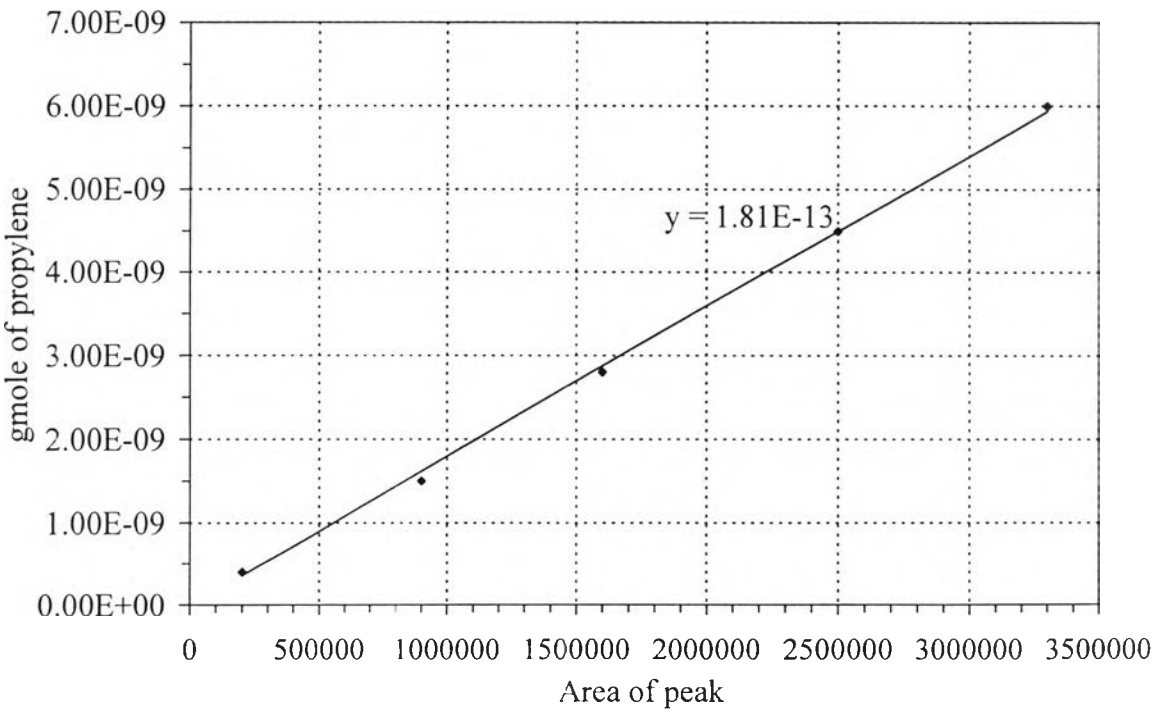


Figure D4 The calibration curve of propylene

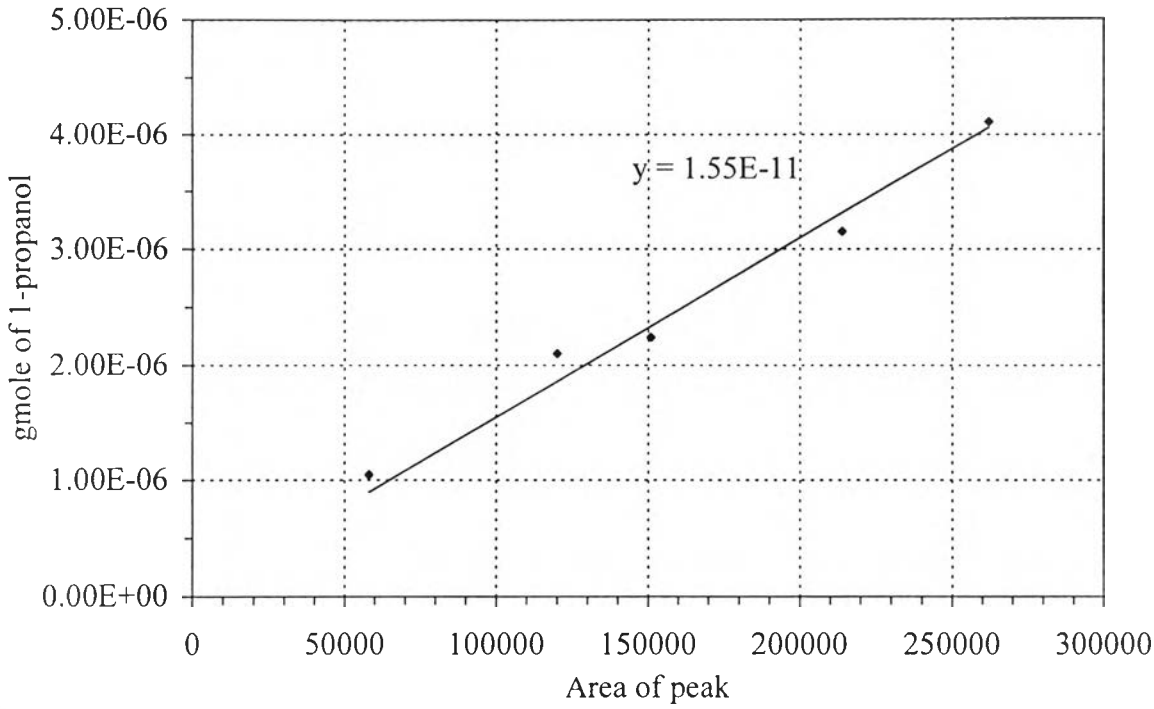


Figure D5 The calibration curve of 1-propanol

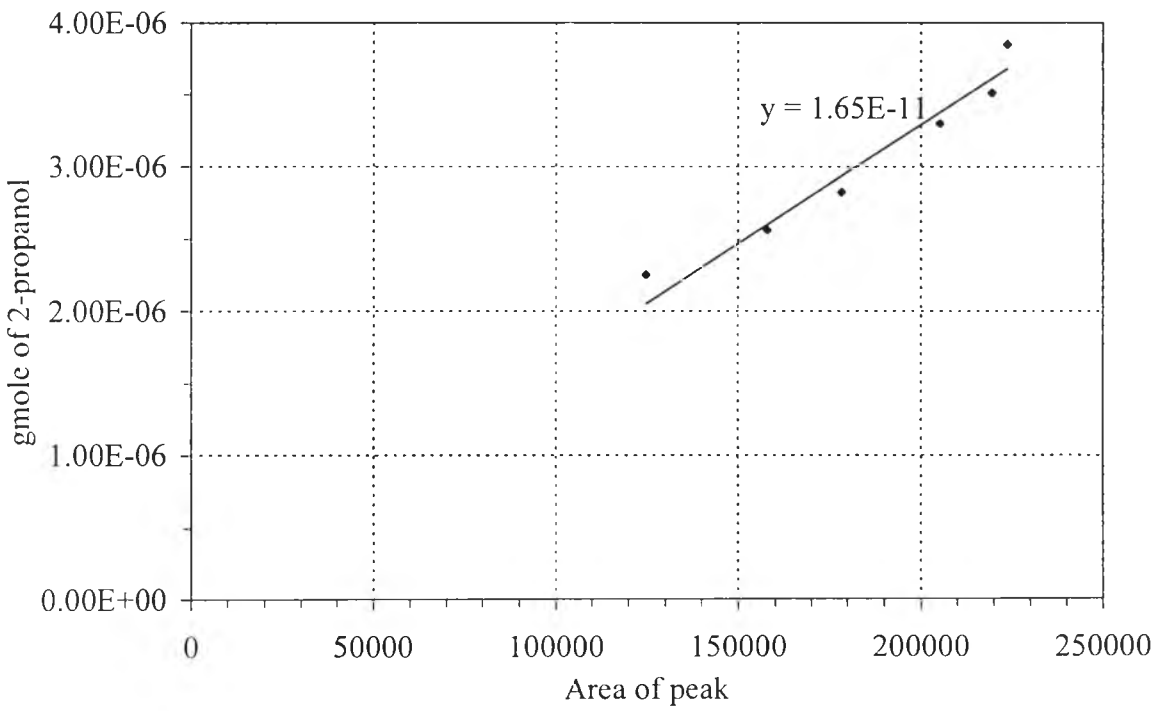


Figure D6 The calibration curve of 2-propanol

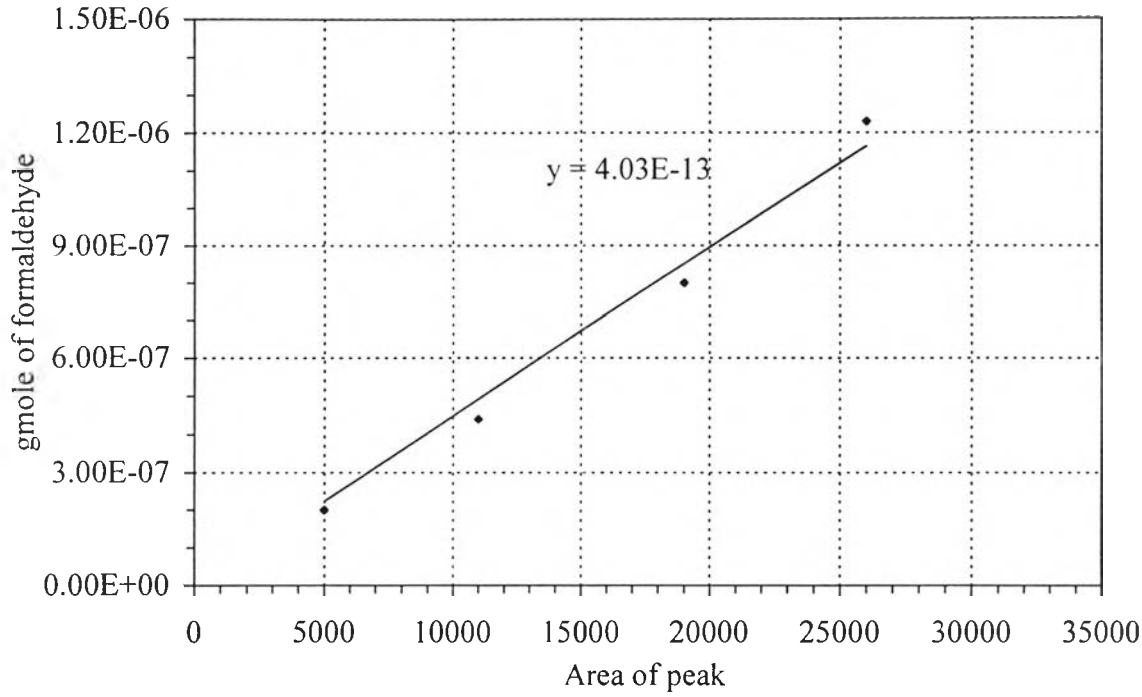


Figure D7 The calibration curve of formaldehyde

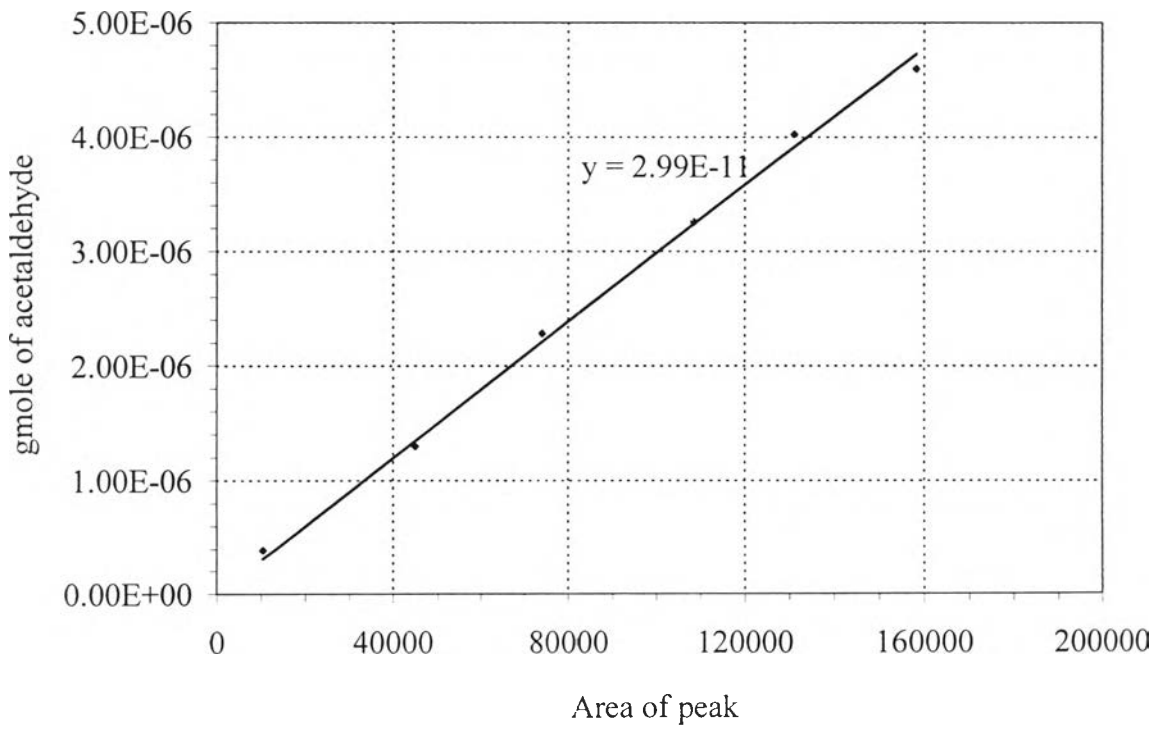


Figure D8 The calibration curve of acetaldehyde

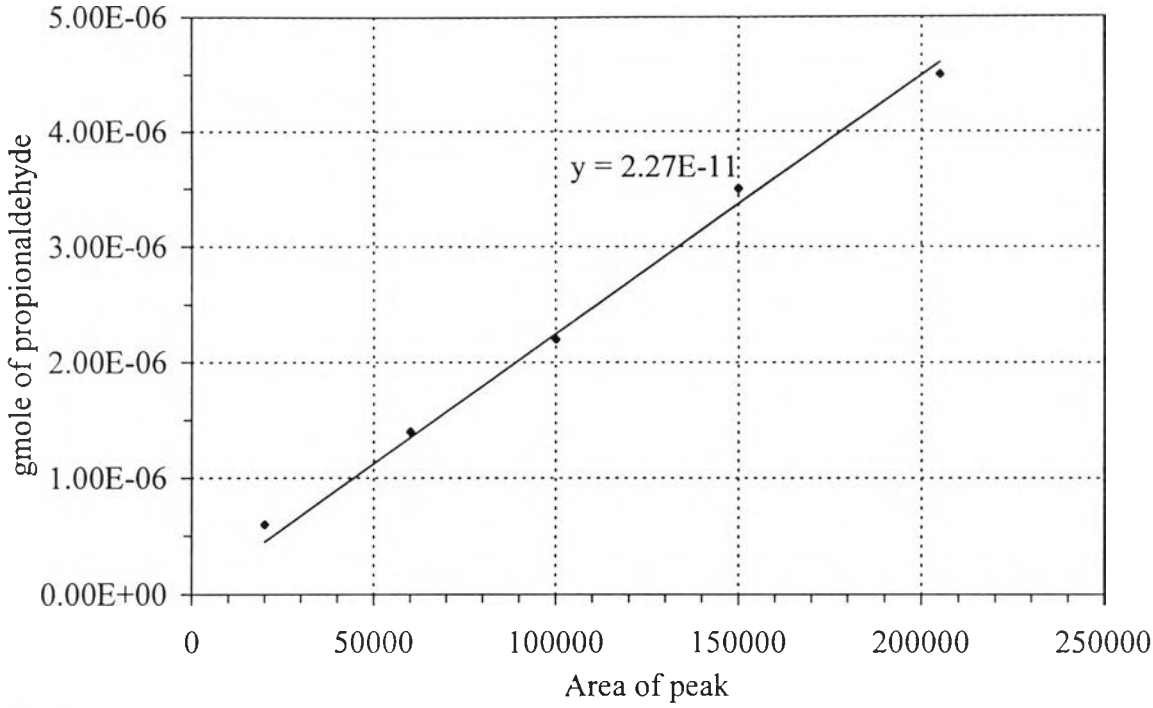


Figure D9 The calibration curve of propionaldehyde

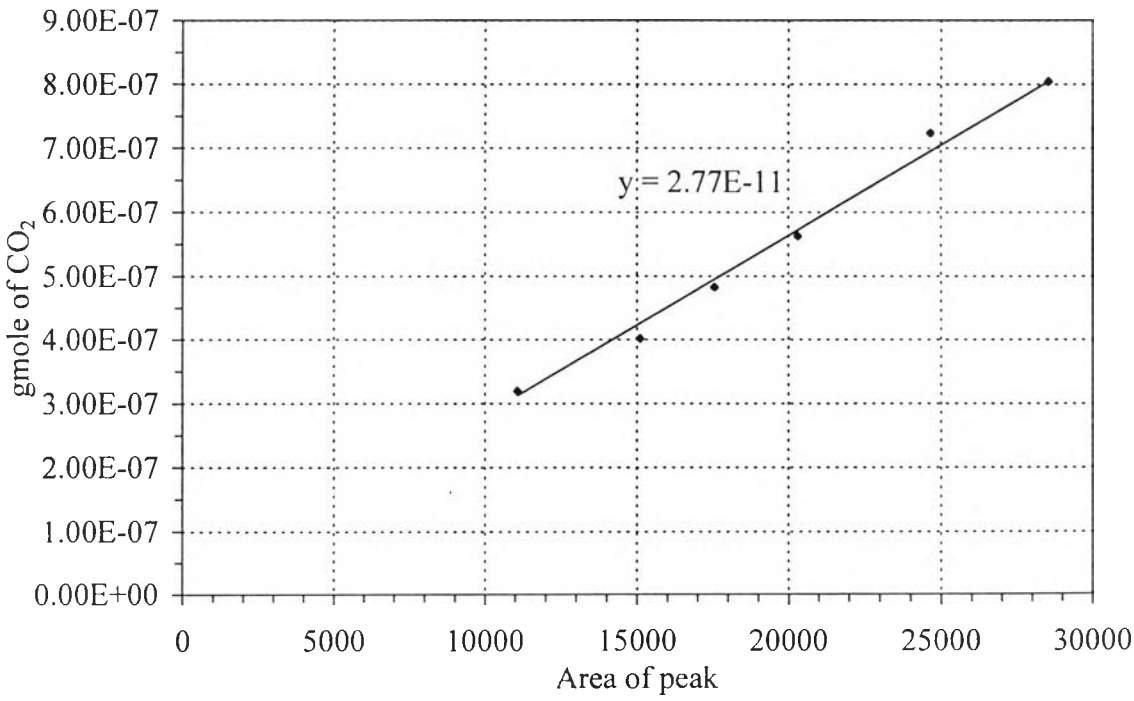


Figure D10 The calibration curve of carbondioxide

APPENDIX E

DATA OF EXPERIMENTS

Table E1 data of figure 5.1a

Time	%1-Propanol Conversion	% Formaldehyde Selectivity	% Acetaldehyde Selectivity	%Propanal Selectivity	%Methane Selectivity	% Ethylene Selectivity	% propylene Selectivity	%Carbondioxide Selectivity
3	45.39	0.03	1.41	74.57	0.02	0.65	9.59	12.91
4	43.86	0.02	1.26	74.54	0.02	0.70	9.66	12.88
5	44.68	0.03	1.39	73.93	0.02	0.64	9.66	12.30
7	43.00	0.02	1.52	74.43	0.03	0.68	10.10	12.97
9	43.56	0.03	1.56	72.67	0.03	0.72	9.90	13.29
11	43.72	0.03	1.47	74.89	0.02	0.68	9.70	12.80
13	43.53	0.03	1.43	74.48	0.03	0.67	10.01	12.50
15	41.87	0.03	1.45	75.06	0.02	0.65	10.07	12.40
17	43.15	0.03	1.44	73.06	0.02	0.75	9.76	12.81
19	40.23	0.03	1.76	73.32	0.03	0.72	10.55	13.06
22	41.36	0.03	1.98	73.23	0.03	0.74	10.25	13.03
25	40.21	0.03	1.43	73.91	0.03	0.75	10.47	13.10
28	38.60	0.03	1.51	73.38	0.02	0.61	10.89	13.17
31	39.62	0.02	0.93	72.11	0.04	0.80	10.76	13.88
35	37.72	0.02	0.83	72.90	0.03	0.83	11.24	13.89
39	38.31	0.02	1.74	72.34	0.03	0.78	10.97	13.20
43	37.83	0.02	1.82	72.33	0.03	0.81	11.17	12.94
46	36.90	0.02	1.64	73.36	0.03	0.82	11.51	12.27
48	36.17	0.02	1.81	71.98	0.03	0.83	11.64	12.90

Table E2 data of figure 5.1b

Time	%1-Propanol Conversion	% Formaldehyde Selectivity	% Acetaldehyde Selectivity	%Propanal Selectivity	%Methane Selectivity	% Ethylene Selectivity	% propylene Selectivity	%Carbondioxide Selectivity
2.25	26.57	0.02	0.75	83.98	0.03	0.40	5.18	8.31
3.25	24.91	0.02	0.83	85.17	0.04	0.42	5.20	8.07
4.25	24.77	0.02	0.76	85.41	0.03	0.38	4.59	7.70
5.5	23.93	0.02	0.81	87.81	0.03	0.32	3.81	7.12
7	24.71	0.02	1.04	86.81	0.03	0.31	3.66	7.10
9	22.70	0.02	0.75	85.94	0.03	0.32	3.99	7.79
11	21.72	0.02	0.73	85.54	0.03	0.38	5.01	7.35
14	21.56	0.02	0.78	86.90	0.02	0.23	4.22	6.03
17	22.13	0.02	0.72	85.82	0.02	0.32	5.02	7.31
20	21.18	0.02	0.68	85.67	0.02	0.36	4.57	7.79
23	21.43	0.02	0.81	87.23	0.05	0.28	3.63	7.47
26	20.71	0.02	0.66	85.63	0.02	0.32	3.81	8.35
29	20.42	0.02	0.78	87.05	0.02	0.26	3.63	5.85
32	15.43	0.02	0.84	85.04	0.03	0.36	4.71	8.16
35	17.18	0.02	0.81	85.87	0.03	0.37	5.54	7.19
38	16.18	0.02	0.96	86.37	0.02	0.33	4.64	7.37
41	15.64	0.02	0.76	85.27	0.04	0.41	6.36	7.11
44	15.73	0.02	0.74	85.33	0.03	0.39	6.09	7.14
46	15.30	0.02	0.71	85.02	0.03	0.40	6.27	7.48
48	15.35	0.02	0.79	85.25	0.04	0.42	6.42	6.54

Table E3 data of figure 5.1c

Time	%1-Propanol Conversion	% Formaldehyde Selectivity	% Acetaldehyde Selectivity	%Propanal Selectivity	%Methane Selectivity	% Ethylene Selectivity	% propylene Selectivity	%Carbondioxide Selectivity
2.25	47.17	0.00	1.32	96.49	0.06	0.03	0.06	0.00
3.5	46.43	0.00	1.03	94.40	0.06	0.03	0.09	0.31
5	45.95	0.00	0.82	96.36	0.03	0.03	0.06	0.29
7.25	44.96	0.00	0.63	97.33	0.02	0.03	0.04	0.33
10.25	45.75	0.00	0.58	96.12	0.02	0.03	0.01	0.37
13	45.00	0.00	0.53	96.99	0.02	0.06	0.00	1.00
15.5	46.50	0.00	0.65	96.33	0.00	0.09	0.00	1.79
18	46.21	0.00	0.74	95.37	0.00	0.10	0.00	2.22
20	44.29	0.00	0.90	95.67	0.00	0.07	0.00	1.55
22	46.72	0.00	0.92	94.87	0.00	0.10	0.00	2.22
24	46.66	0.00	0.93	95.20	0.00	0.09	0.00	2.11
26	46.96	0.00	1.05	94.60	0.00	0.08	0.00	1.92
28	45.65	0.00	1.09	94.94	0.00	0.04	0.04	1.85
30	47.48	0.00	0.81	95.85	0.00	0.04	0.02	1.83
33	46.12	0.00	0.58	94.33	0.00	0.04	0.00	1.97
36	44.16	0.00	0.66	95.56	0.00	0.08	0.00	1.79
40	44.63	0.00	0.76	94.41	0.00	0.12	0.00	1.75
42	46.29	0.00	0.78	93.73	0.00	0.09	0.00	1.80
45	42.69	0.00	0.80	93.12	0.01	0.09	0.00	2.13
48	42.54	0.00	0.83	92.53	0.02	0.12	0.00	2.19

Table E4 data of figure 5.2a

Time	%1-Propanol Conversion	% Formaldehyde Selectivity	% Acetaldehyde Selectivity	%Propanal Selectivity	%Methane Selectivity	% Ethylene Selectivity	% propylene Selectivity	%Carbondioxide Selectivity
3	33.74	0.04	0.00	78.12	0.05	0.46	11.36	8.07
4	33.63	0.06	0.00	76.39	0.07	0.61	14.23	8.28
5	32.46	0.06	0.00	74.13	0.06	0.61	15.49	8.47
6	30.89	0.06	0.00	75.74	0.06	0.56	16.33	6.72
7	30.02	0.05	0.00	71.81	0.06	0.60	17.98	9.31
9	29.56	0.06	0.00	70.52	0.06	0.60	18.61	9.31
11	30.23	0.06	0.00	71.75	0.05	0.60	17.96	9.09
13	28.90	0.06	0.00	70.97	0.05	0.55	18.41	9.29
15	29.55	0.06	0.00	70.37	0.05	0.58	18.64	9.13
17	30.18	0.07	0.00	71.30	0.05	0.60	18.71	8.82
20	30.43	0.07	0.00	71.57	0.05	0.60	18.24	8.44
24	28.29	0.07	0.00	71.48	0.06	0.67	18.06	9.41
28	28.36	0.07	0.00	70.42	0.05	0.68	18.18	9.96
31	29.30	0.06	0.00	71.34	0.05	0.53	17.87	8.51
34	29.03	0.06	0.00	71.94	0.05	0.50	17.14	8.71
37	28.79	0.07	0.00	72.15	0.05	0.53	17.43	8.70
40	28.88	0.06	0.00	72.53	0.05	0.55	16.38	8.56
44	29.05	0.07	0.00	72.26	0.05	0.58	17.44	8.01
48	28.91	0.07	0.00	72.45	0.05	0.55	17.55	8.72

Table E5 data of figure 5.2b

Time	%1-Propanol Conversion	% Formaldehyde Selectivity	% Acetaldehyde Selectivity	%Propanal Selectivity	%Methane Selectivity	% Ethylene Selectivity	% propylene Selectivity	%Carbondioxide Selectivity
2	35.61	0.07	0.00	70.99	0.03	0.19	19.30	8.27
3	35.35	0.07	0.00	70.20	0.05	0.15	18.39	9.84
4	35.09	0.06	0.00	69.23	0.02	0.15	19.07	10.84
6	35.53	0.06	0.00	70.38	0.03	0.14	18.24	8.92
8	35.20	0.06	0.00	71.06	0.03	0.13	19.12	8.90
10	36.01	0.05	0.00	69.95	0.04	0.13	18.86	9.42
13	35.24	0.05	0.00	70.66	0.03	0.13	19.34	9.71
14	34.65	0.05	0.00	69.06	0.02	0.15	19.87	10.23
16	35.45	0.05	0.00	70.01	0.02	0.15	20.10	9.55
18	34.71	0.05	0.00	69.91	0.03	0.18	19.56	9.71
20	35.05	0.04	0.00	70.89	0.03	0.18	18.82	9.02
22	34.00	0.05	0.00	71.11	0.05	0.19	19.04	9.35
24	32.20	0.04	0.00	70.87	0.03	0.19	18.19	9.59
27	31.87	0.04	0.00	70.61	0.05	0.36	18.01	10.83
30	32.23	0.05	0.00	70.25	0.04	0.30	17.80	10.73
33	32.72	0.04	0.00	69.41	0.04	0.36	20.27	9.77
36	31.32	0.04	0.00	70.27	0.04	0.34	18.36	10.75
40	32.74	0.05	0.00	69.65	0.04	0.36	18.77	10.66
44	32.15	0.04	0.00	69.15	0.05	0.38	20.32	9.63
48	32.06	0.05	0.00	69.67	0.05	0.37	19.40	10.07

Table E6 data of figure 5.2c

Time	%1-Propanol Conversion	% Formaldehyde Selectivity	% Acetaldehyde Selectivity	%Propanal Selectivity	%Methane Selectivity	% Ethylene Selectivity	% propylene Selectivity	%Carbondioxide Selectivity
2.25	46.99	0.00	9.42	60.02	0.11	0.03	30.11	0.16
3.5	50.04	0.00	10.43	63.66	0.12	0.03	25.45	0.21
5	49.39	0.00	10.96	63.72	0.13	0.00	24.15	0.24
7	45.03	0.00	9.51	67.65	0.08	0.04	21.95	0.09
8.5	41.79	0.00	7.45	64.34	0.11	0.05	23.87	0.29
10	39.78	0.00	7.58	75.21	0.07	0.05	16.78	0.25
12	30.35	0.00	5.47	77.31	0.06	0.04	14.64	0.06
14	28.30	0.00	4.88	80.93	0.11	0.04	11.71	0.25
17.5	32.56	0.00	6.04	77.22	0.08	0.09	15.10	0.57
19	36.39	0.00	6.50	72.91	0.07	0.09	15.61	0.59
21	29.97	0.00	5.54	77.47	0.10	0.07	14.42	0.44
24	28.13	0.00	4.32	78.51	0.10	0.24	14.22	1.56
26	31.62	0.00	6.04	80.64	0.06	0.13	10.15	1.42
28	30.27	0.00	5.18	72.82	0.09	0.24	18.29	3.05
30	33.81	0.00	6.19	77.01	0.10	0.18	13.71	2.51
34	30.27	0.00	5.75	74.23	0.09	0.21	15.44	3.51
40	34.05	0.00	6.54	72.92	0.13	0.22	13.98	3.87
43	34.74	0.00	6.52	75.17	0.13	0.29	13.25	3.72
46	37.71	0.00	7.08	74.67	0.11	0.28	11.90	4.33
48	35.65	0.00	6.96	73.53	0.07	0.27	13.03	4.44

Table E7 data of figure 5.3a

Time	%1-Propanol Conversion	% Formaldehyde Selectivity	% Acetaldehyde Selectivity	%Propanal Selectivity	%Methane Selectivity	% Ethylene Selectivity	% propylene Selectivity	%Carbondioxide Selectivity
3.75	52.00	0.17	0.00	36.64	0.01	0.01	59.47	2.54
4.75	49.34	0.28	0.00	35.56	0.02	0.02	60.18	3.34
6	47.45	0.29	0.00	34.99	0.02	0.02	61.19	3.41
8	47.63	0.18	0.00	33.10	0.01	0.02	64.37	2.03
10	47.56	0.19	0.00	33.48	0.01	0.01	62.36	2.26
12	48.05	0.19	0.00	34.83	0.01	0.01	61.32	2.39
14	48.19	0.23	0.00	34.40	0.01	0.01	60.93	2.98
16	47.99	0.18	0.00	34.37	0.01	0.02	61.65	2.46
19	45.95	0.26	0.00	34.61	0.01	0.01	62.40	2.55
22	44.21	0.18	0.00	35.70	0.02	0.02	60.67	2.47
25	42.83	0.19	0.00	35.58	0.02	0.02	61.09	2.31
27	42.38	0.19	0.00	35.63	0.02	0.02	60.34	2.66
29	42.49	0.22	0.00	36.35	0.02	0.02	60.18	2.35
31	42.82	0.16	0.00	35.11	0.01	0.01	61.97	2.41
34	43.16	0.18	0.00	36.59	0.01	0.01	59.87	2.81
37	42.46	0.16	0.00	35.28	0.01	0.01	61.37	3.00
40	43.27	0.16	0.00	37.03	0.01	0.01	59.30	2.65
43	42.40	0.20	0.00	36.11	0.01	0.01	60.80	2.79
46	42.72	0.19	0.00	36.22	0.02	0.02	59.88	2.92
48	42.62	0.17	0.00	36.94	0.02	0.02	60.40	2.25

Table E8 data of figure 5.3b

Time	%1-Propanol Conversion	% Formaldehyde Selectivity	% Acetaldehyde Selectivity	%Propanal Selectivity	%Methane Selectivity	% Ethylene Selectivity	% propylene Selectivity	%Carbondioxide Selectivity
3	51.11	0.14	0.00	59.62	0.01	0.01	33.22	2.79
4.5	48.74	0.15	0.00	63.07	0.01	0.01	33.19	3.01
6	47.65	0.18	0.00	60.63	0.01	0.01	35.23	2.99
8	49.03	0.17	0.00	63.76	0.01	0.01	31.75	2.98
10	47.25	0.18	0.00	65.48	0.01	0.01	30.90	3.03
12	45.90	0.19	0.00	61.57	0.01	0.01	33.83	3.04
14	46.73	0.18	0.00	58.33	0.01	0.01	38.32	2.94
15.5	45.13	0.21	0.00	58.29	0.01	0.01	38.17	3.12
19	45.09	0.22	0.00	58.61	0.01	0.01	36.83	2.96
22.5	44.38	0.25	0.00	59.75	0.01	0.01	36.62	2.93
24.5	41.40	0.20	0.00	54.97	0.01	0.01	41.29	2.75
26.5	38.45	0.20	0.00	53.58	0.01	0.01	40.88	2.60
29	38.86	0.20	0.00	52.16	0.01	0.01	44.50	2.69
31.5	41.89	0.18	0.00	50.10	0.01	0.01	43.60	2.55
34.5	41.25	0.20	0.00	49.90	0.01	0.01	43.80	2.39
38	38.43	0.21	0.00	52.87	0.01	0.01	43.28	2.64
42	42.11	0.20	0.00	49.27	0.01	0.01	43.13	2.62
45.5	40.66	0.21	0.00	53.51	0.01	0.01	43.21	2.45
48	39.91	0.23	0.00	52.47	0.01	0.01	42.94	2.65

Table E9 data of figure 5.3c

Time	%1-Propanol Conversion	% Formaldehyde Selectivity	% Acetaldehyde Selectivity	%Propanal Selectivity	%Methane Selectivity	% Ethylene Selectivity	% propylene Selectivity	%Carbondioxide Selectivity
2	72.27	0.16	0.00	95.38	0.00	0.00	2.80	1.10
3	73.94	0.21	0.00	93.95	0.00	0.00	2.58	1.48
4	67.57	0.27	0.00	94.35	0.00	0.00	2.27	1.10
7	68.91	0.33	0.00	91.20	0.00	0.00	4.15	1.81
8.5	73.51	0.34	0.00	92.31	0.00	0.00	4.77	2.20
10	69.31	0.38	0.00	91.48	0.00	0.00	4.81	2.25
11.7	69.97	0.35	0.00	90.43	0.00	0.00	4.20	1.99
13	64.26	0.38	0.00	87.85	0.00	0.00	4.87	2.32
16	75.81	0.37	0.00	87.93	0.00	0.00	5.54	3.10
18	69.04	0.42	0.00	89.60	0.00	0.00	5.18	2.42
20	73.40	0.41	0.00	90.26	0.00	0.00	5.70	2.78
22	68.52	0.47	0.00	88.15	0.00	0.00	5.83	2.68
24	77.99	0.20	0.00	93.39	0.00	0.00	3.11	1.89
26	69.06	0.25	0.00	91.47	0.00	0.00	2.79	1.52
28	69.43	0.29	0.00	90.03	0.00	0.00	3.55	1.75
30	72.55	0.25	0.00	88.52	0.00	0.00	3.69	1.82
34	75.47	0.31	0.00	89.65	0.00	0.00	5.28	2.44
38	76.44	0.37	0.00	88.80	0.02	0.00	5.47	2.72
42	72.94	0.38	0.00	89.43	0.00	0.00	3.79	2.43
46	76.44	0.26	0.00	92.08	0.00	0.00	2.98	1.52
48	72.33	0.30	0.00	90.99	0.00	0.00	4.48	2.10

Table E10 data of figure 5.4a

Time	%1-Propanol Conversion	% Formaldehyde Selectivity	% Acetaldehyde Selectivity	%Propanal Selectivity	%Methane Selectivity	% Ethylene Selectivity	% propylene Selectivity	%Carbondioxide Selectivity
1.75	96.10	0.26	0.00	3.75	0.00	0.00	95.21	0.00
4	96.00	0.31	0.00	5.34	0.00	0.00	92.80	0.03
6	96.27	0.29	0.00	4.94	0.00	0.00	92.78	0.03
8	96.15	0.32	0.00	5.78	0.00	0.00	92.46	0.03
10	96.07	0.31	0.00	5.87	0.00	0.00	91.77	0.04
13	95.98	0.29	0.00	6.00	0.00	0.00	92.61	0.03
15	95.86	0.34	0.00	5.56	0.00	0.00	92.36	0.03
17	96.01	0.37	0.00	8.46	0.00	0.00	89.87	0.04
19	96.27	0.37	0.00	9.16	0.00	0.00	90.04	0.04
22	96.14	0.35	0.00	9.53	0.00	0.00	89.88	0.09
25	96.03	0.34	0.00	8.78	0.00	0.00	90.12	0.06
28	96.24	0.34	0.00	8.70	0.00	0.00	90.60	0.05
31	95.93	0.38	0.00	9.11	0.00	0.00	89.88	0.08
34	96.09	0.34	0.00	9.12	0.00	0.00	89.53	0.06
37	95.96	0.34	0.00	8.89	0.00	0.00	88.62	0.07
39.5	96.13	0.32	0.00	8.36	0.00	0.00	90.80	0.06
43	96.03	0.31	0.00	8.02	0.00	0.00	91.14	0.07
46	96.24	0.32	0.00	9.00	0.00	0.00	90.47	0.06
48	95.88	0.37	0.00	9.45	0.00	0.00	89.46	0.06

Table E11 data of figure 5.4b

Time	%1-Propanol Conversion	% Formaldehyde Selectivity	% Acetaldehyde Selectivity	%Propanal Selectivity	%Methane Selectivity	% Ethylene Selectivity	% propylene Selectivity	%Carbondioxide Selectivity
2.5	93.83	0.00	0.00	35.78	0.00	0.00	61.96	0.00
4	94.69	0.00	0.00	35.75	0.00	0.00	63.19	0.00
5	94.00	0.00	0.00	34.72	0.00	0.00	64.84	0.02
7	93.68	0.00	0.00	36.39	0.00	0.00	62.95	0.01
8.5	94.18	0.00	0.00	37.12	0.00	0.00	61.04	0.02
10	93.93	0.00	0.00	36.16	0.00	0.00	61.83	0.01
12	94.91	0.00	0.00	34.42	0.00	0.00	64.43	0.02
14	95.60	0.00	0.00	33.53	0.00	0.00	64.15	0.01
16	95.12	0.00	0.00	34.77	0.00	0.00	61.34	0.03
18	94.56	0.00	0.00	35.56	0.00	0.00	62.57	0.03
21	95.24	0.00	0.00	35.32	0.00	0.00	64.31	0.02
23	95.36	0.00	0.00	35.74	0.00	0.00	63.74	0.03
26	94.88	0.00	0.00	33.71	0.00	0.00	65.05	0.03
29	95.26	0.00	0.00	35.97	0.00	0.00	63.49	0.03
32	95.59	0.00	0.00	35.38	0.00	0.00	63.36	0.02
35	95.57	0.00	0.00	35.93	0.00	0.00	62.06	0.03
38	95.13	0.00	0.00	34.80	0.00	0.00	62.33	0.02
41	95.34	0.00	0.00	35.33	0.00	0.00	63.51	0.02
45	95.41	0.00	0.00	35.23	0.00	0.00	64.12	0.03
48	95.55	0.00	0.00	35.84	0.00	0.00	63.36	0.03

Table E12 data of figure 5.4c

Time	%1-Propanol Conversion	% Formaldehyde Selectivity	% Acetaldehyde Selectivity	%Propanal Selectivity	%Methane Selectivity	% Ethylene Selectivity	% propylene Selectivity	%Carbondioxide Selectivity
3	100.00	1.32	0.00	87.34	0.00	0.00	10.03	0.00
4.25	100.00	1.30	0.00	84.61	0.00	0.00	12.69	0.00
5.5	100.00	1.15	0.00	87.10	0.00	0.00	9.95	0.00
6.5	100.00	1.15	0.00	89.49	0.00	0.00	7.37	0.00
7.5	100.00	0.89	0.00	91.49	0.00	0.00	6.98	0.00
9	100.00	0.86	0.00	93.55	0.00	0.00	5.24	0.00
11.42	100.00	0.73	0.00	90.87	0.00	0.00	5.63	0.07
15	100.00	0.60	0.00	90.25	0.00	0.00	5.58	0.00
17.5	100.00	0.57	0.00	93.57	0.00	0.00	5.67	0.08
18.5	100.00	0.48	0.00	92.70	0.00	0.00	3.76	0.08
20.25	100.00	0.51	0.00	89.93	0.00	0.00	6.28	0.15
22	93.99	0.72	0.00	86.70	0.00	0.00	10.11	0.00
24	93.85	0.66	0.00	89.78	0.00	0.00	7.94	0.00
26	89.83	0.62	0.00	92.98	0.00	0.00	5.36	0.08
28	85.31	0.69	0.00	89.55	0.00	0.00	6.74	0.16
30	87.97	0.60	0.00	87.08	0.00	0.00	7.52	0.32
33	88.76	0.55	0.00	85.18	0.00	0.00	8.71	1.06
36	83.78	0.61	0.00	87.00	0.00	0.00	8.21	1.69
39	77.90	0.57	0.00	91.13	0.00	0.00	4.91	1.25
42	88.54	0.61	0.00	82.90	0.00	0.00	11.21	1.19
45	87.99	0.71	0.00	85.90	0.00	0.00	11.60	1.23
48	91.77	0.60	0.00	83.27	0.00	0.00	13.57	0.89
49	89.16	0.71	0.00	82.36	0.00	0.00	14.64	1.18
51	88.79	0.79	0.00	78.12	0.00	0.00	16.28	1.26

Table E13 data of figure 5.5a

Time	%1-Propanol Conversion	% Formaldehyde Selectivity	% Acetaldehyde Selectivity	%Propanal Selectivity	%Methane Selectivity	% Ethylene Selectivity	% propylene Selectivity	%Carbondioxide Selectivity
3.17	69.09	0.05	7.71	65.61	0.48	4.48	7.26	14.33
4.42	71.67	0.13	2.35	72.59	0.46	4.19	5.43	13.87
5.58	76.35	0.06	6.42	68.97	0.52	4.69	5.51	13.79
6.58	74.63	0.06	6.63	68.40	0.52	4.64	4.85	14.58
7.50	75.76	0.61	6.24	68.57	0.57	4.91	4.71	14.10
8.50	71.59	0.06	4.90	69.47	0.56	4.88	4.84	15.16
9.50	76.59	0.07	5.56	69.11	0.46	3.95	3.62	15.97
10.67	72.82	0.06	5.46	68.86	0.57	4.58	3.85	16.52
11.75	76.27	0.07	5.84	69.41	0.39	3.36	3.00	16.35
12.83	77.53	0.07	5.08	64.59	0.62	5.21	4.59	15.38
14.25	76.21	0.08	5.31	69.19	0.47	4.01	3.39	16.98
15.25	77.24	0.07	5.68	68.74	0.52	4.47	3.65	16.71
16.37	72.77	0.08	4.49	69.81	0.38	3.28	2.66	18.13
17.30	75.40	0.05	7.38	68.90	0.36	3.42	4.76	14.67
18.25	73.01	0.11	2.33	75.42	0.35	3.40	3.26	14.85
20.25	74.85	0.08	4.60	70.21	0.51	4.59	3.70	14.65
22.25	73.29	0.08	4.56	69.29	0.62	5.35	4.16	14.72
24.25	71.90	0.08	4.21	70.40	0.62	5.18	3.95	15.46
26.25	73.09	0.08	3.62	68.96	0.45	3.84	2.78	15.28
29.25	74.22	0.08	3.86	69.38	0.57	4.81	3.32	15.16
32.25	76.14	0.12	0.00	70.37	0.60	4.97	3.65	16.77
38.75	77.35	0.08	5.53	67.81	0.60	5.01	3.34	17.55
44.75	73.31	0.08	3.55	70.07	0.57	4.89	3.31	15.87
48.40	72.59	0.08	3.83	73.82	0.38	3.16	2.06	15.57

Table E14 data of figure 5.5b

Time	%1-Propanol Conversion	% Formaldehyde Selectivity	% Acetaldehyde Selectivity	%Propanal Selectivity	%Methane Selectivity	% Ethylene Selectivity	% propylene Selectivity	%Carbondioxide Selectivity
0.83	78.83	0.10	10.80	56.09	1.16	10.29	6.77	14.39
5.25	78.97	0.10	6.72	58.09	1.71	11.19	5.56	16.00
6.50	77.22	0.10	6.70	59.01	1.66	9.75	4.84	17.85
8.50	76.79	0.11	6.83	56.13	3.18	10.85	4.50	18.25
9.83	77.09	0.11	3.62	58.37	1.54	10.80	4.12	20.52
11.00	75.48	0.12	2.55	59.39	2.05	10.42	4.96	20.25
13.50	81.22	0.10	3.24	57.99	1.70	10.90	4.21	21.59
15.50	77.43	0.10	7.04	54.71	1.61	9.99	3.85	22.55
18.25	78.81	0.11	7.01	54.85	1.59	9.82	3.58	22.08
20.00	80.92	0.11	7.85	54.15	1.35	10.08	2.79	23.10
22.00	80.87	0.10	6.43	56.20	1.58	9.82	3.22	21.84
23.50	81.18	0.11	7.98	54.61	1.99	9.66	3.30	21.63
25.50	81.37	0.07	4.59	55.97	1.76	10.83	3.51	22.33
28.00	80.27	0.11	6.40	56.52	1.86	9.54	3.62	21.15
31.00	81.97	0.12	6.15	56.62	1.83	9.46	4.72	20.86
34.00	81.29	0.11	7.22	56.37	1.35	8.86	4.19	21.24
39.50	78.10	0.05	3.35	61.35	1.31	10.15	3.15	20.25
43.25	78.56	0.07	4.87	56.86	1.46	10.51	3.21	21.66
46.00	75.15	0.07	4.70	57.31	1.48	10.80	2.96	22.43
48.00	77.91	0.09	5.81	56.76	1.62	10.48	3.74	20.75

Table E15 data of figure 5.5c

Time	%1-Propanol Conversion	% Formaldehyde Selectivity	% Acetaldehyde Selectivity	%Propanal Selectivity	%Methane Selectivity	% Ethylene Selectivity	% propylene Selectivity	%Carbondioxide Selectivity
3.20	65.32	0.10	4.34	67.20	0.82	9.92	5.90	11.07
4.00	65.12	0.10	4.60	72.32	1.16	12.73	7.86	0.39
5.00	64.28	0.09	4.18	66.51	0.95	9.91	5.63	12.52
6.67	63.32	0.09	3.44	66.76	1.04	9.86	5.50	12.61
8.00	64.03	0.09	2.85	66.87	1.08	9.38	5.29	14.03
9.00	63.60	0.08	3.25	68.22	0.97	8.08	4.33	14.02
10.00	65.59	0.08	2.80	65.06	0.97	7.56	4.30	19.07
12.00	64.62	0.07	4.34	66.50	1.06	7.42	4.31	15.81
14.00	66.06	0.07	2.75	66.05	0.75	5.28	3.09	21.94
16.00	66.54	0.07	2.69	67.12	1.18	7.68	4.16	16.84
18.00	64.70	0.11	4.00	68.96	0.92	10.91	4.61	8.89
22.00	60.14	0.08	2.05	63.34	1.20	12.22	5.66	13.54
26.00	53.63	0.09	2.21	80.32	1.23	9.53	4.91	0.61
30.00	56.98	0.07	2.23	72.43	1.07	6.80	3.69	12.91
36.00	61.78	0.07	2.24	70.71	1.04	6.66	3.18	15.65
42.00	63.72	0.10	2.32	72.03	0.90	10.48	3.79	9.59
48.00	64.05	0.08	1.10	77.21	0.85	6.49	2.79	10.78

Table E16 data of figure 5.6a

Time	%1-Propanol Conversion	% Formaldehyde Selectivity	% Acetaldehyde Selectivity	%Propanal Selectivity	%Methane Selectivity	% Ethylene Selectivity	% propylene Selectivity	%Carbondioxide Selectivity
2.67	100.00	0.11	47.52	7.23	3.09	13.64	20.29	5.61
4.00	99.26	0.16	57.31	27.97	0.61	2.49	7.13	3.21
5.08	99.55	0.00	45.70	29.09	1.81	7.93	13.09	1.08
6.50	99.53	0.00	40.55	32.22	1.76	7.58	15.82	0.72
7.75	98.64	0.10	31.15	41.56	1.83	8.06	14.86	0.87
9.08	97.19	0.09	32.48	44.49	1.60	7.25	12.17	0.89
10.50	93.42	0.00	46.35	48.09	0.17	0.81	2.12	0.95
11.75	92.81	0.00	38.61	42.68	1.27	5.41	10.40	0.93
13.83	89.75	0.13	22.16	47.86	2.27	10.23	14.10	1.00
17.25	90.59	0.14	20.33	47.88	2.86	12.94	13.04	1.35
19.42	93.62	0.00	34.01	41.45	2.45	10.74	9.06	1.04
21.42	79.87	0.10	25.11	45.01	1.95	10.29	15.65	1.05
23.00	68.71	0.09	25.96	47.34	1.54	7.89	15.34	0.00
26.00	57.73	0.10	21.54	51.30	1.73	7.73	15.73	1.32
29.00	61.74	0.10	20.35	55.97	2.06	8.57	12.10	0.00
32.00	68.00	0.12	18.38	57.93	2.41	10.28	9.92	0.00
36.25	79.49	0.11	21.17	52.29	2.48	10.37	9.06	0.00
41.00	85.38	0.00	31.80	45.29	2.65	10.94	7.36	0.00
43.25	95.23	0.00	37.64	39.58	2.57	10.54	5.80	0.00
48.00	69.16	0.15	12.18	62.71	1.82	10.40	11.34	0.00

Table E17 data of figure 5.6b

Time	%1-Propanol Conversion	% Formaldehyde Selectivity	% Acetaldehyde Selectivity	%Propanal Selectivity	%Methane Selectivity	% Ethylene Selectivity	% propylene Selectivity	%Carbondioxide Selectivity
4.67	98.04	0.03	51.70	31.67	0.32	1.32	13.46	0.00
6.58	98.12	0.03	44.68	39.24	0.26	1.31	11.94	0.58
9.83	95.97	0.00	36.25	41.92	0.52	2.95	17.86	0.00
11.00	93.45	0.00	33.51	41.70	0.54	3.08	19.59	0.00
13.08	87.89	0.00	28.89	50.74	0.60	3.68	14.67	0.00
15.33	81.85	0.00	21.68	55.30	0.55	3.51	8.89	9.39
16.83	74.80	0.00	19.85	64.43	0.70	4.55	8.35	0.82
18.33	68.06	0.05	12.42	72.79	0.74	4.85	7.02	1.04
19.83	68.19	0.06	11.10	76.02	0.70	4.81	5.44	0.94
31.08	69.96	0.00	18.23	67.16	0.62	4.00	7.67	0.91
32.42	63.22	0.04	11.98	75.46	0.65	4.20	5.80	0.85
38.83	66.00	0.13	2.29	89.20	0.46	3.27	2.33	1.11
40.75	62.67	0.13	2.06	87.59	0.62	4.43	3.06	1.19
48.00	44.74	0.00	6.07	89.66	0.06	0.16	3.24	0.00

Table E18 data of figure 5.6c

Time	%1-Propanol Conversion	% Formaldehyde Selectivity	% Acetaldehyde Selectivity	%Propanal Selectivity	%Methane Selectivity	% Ethylene Selectivity	% propylene Selectivity	%Carbondioxide Selectivity
3.78	97.13	0.13	1.00	25.27	1.19	6.82	43.26	21.03
4.83	86.08	0.32	3.14	65.73	0.48	3.00	14.17	11.15
6.00	83.32	0.27	2.26	62.96	0.61	3.92	17.77	12.01
7.50	78.72	0.23	2.50	67.29	0.57	3.96	12.64	12.01
8.50	74.65	0.25	2.95	81.49	0.02	0.10	0.23	14.42
9.50	79.73	0.11	2.48	62.67	0.84	6.06	14.69	12.58
10.50	73.01	0.10	2.33	69.58	0.53	4.10	8.98	13.00
12.00	75.15	0.08	2.34	66.81	0.69	5.27	9.66	13.77
13.00	76.74	0.07	2.44	68.31	0.55	4.26	6.74	16.53
14.00	72.67	0.07	2.26	70.11	0.56	4.51	7.13	14.94
16.00	73.19	0.06	2.24	68.35	0.58	4.75	6.69	15.84
18.00	71.22	0.06	2.17	70.00	0.54	4.46	5.98	16.25
20.00	88.20	0.33	0.41	61.19	0.53	2.88	20.99	12.22
22.00	83.65	0.23	2.34	68.24	0.50	3.28	13.27	11.58
24.00	78.59	0.13	2.35	71.68	0.40	2.88	9.05	11.56
28.00	77.07	0.06	2.27	67.90	0.67	5.26	7.17	15.95
32.00	74.37	0.04	2.19	66.78	0.56	4.57	4.65	18.30
36.00	74.90	0.04	2.30	66.76	0.57	4.66	4.43	19.43
42.00	73.35	0.04	1.93	67.07	0.71	5.75	5.30	19.01
48.00	73.10	0.04	2.07	68.52	0.75	5.96	5.40	16.15

Table E19 data of figure 5.7a

Time	%1-Propanol Conversion	% Formaldehyde Selectivity	% Acetaldehyde Selectivity	%Propanal Selectivity	%Methane Selectivity	% Ethylene Selectivity	% propylene Selectivity	%Carbondioxide Selectivity
2.83	74.50	0.24	0.00	83.46	0.13	0.08	15.10	0.44
4.00	72.66	0.21	0.00	82.40	0.16	0.10	15.44	1.24
5.00	73.30	0.17	0.00	78.32	0.19	0.11	17.29	3.76
6.00	72.55	0.16	0.00	78.41	0.21	0.11	15.47	4.29
7.00	75.59	0.17	0.36	80.34	0.20	0.10	14.58	4.20
8.00	73.69	0.16	0.37	79.54	0.21	0.11	15.31	3.97
9.00	72.93	0.14	0.33	79.49	0.21	0.11	14.48	4.10
11.25	76.13	0.16	0.52	84.82	0.16	0.08	8.92	4.34
13.00	77.60	0.15	0.48	81.52	0.16	0.09	9.26	4.64
14.00	76.53	0.16	0.57	82.70	0.19	0.10	10.73	4.90
15.00	75.51	0.14	0.43	80.99	0.21	0.11	11.31	5.38
16.00	76.43	0.14	0.52	84.16	0.20	0.10	10.04	4.78
18.33	77.82	0.16	0.58	83.62	0.18	0.10	9.76	5.29
20.50	79.06	0.14	0.59	80.62	0.24	0.13	11.81	5.67
22.00	76.55	0.15	0.46	81.79	0.21	0.11	10.67	5.88
25.00	76.15	0.14	0.61	85.90	0.14	0.07	7.36	5.38
29.00	79.29	0.22	0.00	82.60	0.13	0.12	7.45	9.18
31.00	93.81	0.48	0.00	72.34	0.13	0.08	23.69	1.84
35.00	93.74	0.34	0.00	70.60	0.54	0.23	18.01	2.19
37.60	91.80	0.46	0.00	74.37	0.59	0.23	17.06	2.09
40.47	88.60	0.73	0.00	62.12	1.76	0.37	24.94	1.57
42.00	90.45	0.24	8.19	56.86	1.89	0.21	20.87	4.42
43.00	87.47	0.39	4.55	56.71	3.69	0.29	23.80	5.64
48.00	88.84	0.04	4.51	55.08	5.29	0.37	22.97	6.11

Table E20 data of figure 5.7b

Time	%1-Propanol Conversion	% Formaldehyde Selectivity	% Acetaldehyde Selectivity	%Propanal Selectivity	%Methane Selectivity	% Ethylene Selectivity	% propylene Selectivity	%Carbondioxide Selectivity
3.00	100.00	0.00	43.36	16.94	0.09	0.06	36.43	0.04
4.25	100.00	0.00	39.58	18.18	0.10	0.07	39.18	0.47
5.50	100.00	0.00	35.50	19.42	0.12	0.08	43.84	0.42
6.50	92.39	0.00	36.63	18.90	0.13	0.08	42.56	0.45
8.50	88.91	0.00	33.35	17.23	0.15	0.09	46.59	0.53
10.50	86.54	0.00	33.89	19.81	0.16	0.09	44.62	0.61
14.50	79.76	0.00	30.38	20.69	0.19	0.10	44.74	0.57
16.00	76.70	0.00	30.06	22.06	0.20	0.10	45.47	0.62
17.50	71.88	0.00	29.76	25.50	0.20	0.10	41.50	0.63
19.50	72.33	0.00	29.44	27.27	0.20	0.10	40.95	0.58
25.25	75.03	0.00	30.13	24.78	0.21	0.11	41.81	0.45
29.00	71.75	0.00	26.90	25.75	0.26	0.15	44.64	0.49
30.33	69.54	0.00	27.03	27.67	0.26	0.15	40.67	0.52
38.00	71.36	0.00	26.94	28.69	0.32	0.17	40.22	0.65
42.00	75.84	0.00	27.58	30.39	0.34	0.19	36.38	0.75
46.00	74.61	0.00	29.84	31.44	0.27	0.14	32.86	0.70
48.00	76.44	0.00	29.08	25.43	0.34	0.18	38.53	0.71

Table E21 data of figure 5.7c

Time	%1-Propanol Conversion	% Formaldehyde Selectivity	% Acetaldehyde Selectivity	%Propanal Selectivity	%Methane Selectivity	% Ethylene Selectivity	% propylene Selectivity	%Carbondioxide Selectivity
1.63	80.74	0.20	0.25	80.58	0.16	0.12	13.27	4.48
2.27	81.16	0.21	0.00	80.47	0.17	0.11	13.29	4.24
3.40	79.05	0.22	0.64	83.45	0.15	0.10	10.84	5.14
4.50	80.35	0.21	0.00	80.91	0.10	0.07	12.96	5.81
7.00	80.30	0.20	0.00	84.71	0.13	0.09	9.89	5.00
8.00	80.57	0.21	0.12	82.37	0.12	0.05	11.04	5.24
9.00	79.71	0.22	0.66	83.11	0.09	0.06	11.41	5.10
10.40	80.67	0.21	0.00	82.64	0.08	0.06	10.75	6.16
12.00	80.75	0.21	0.68	83.80	0.04	0.03	5.54	7.38
14.00	83.89	0.17	0.73	74.06	0.13	0.10	15.06	6.94
16.00	84.29	0.18	0.83	83.35	0.13	0.06	10.44	5.83
22.00	84.67	0.14	0.00	83.64	0.13	0.05	8.91	6.40
23.25	85.04	0.15	0.20	86.16	0.13	0.10	9.02	4.37
24.50	85.08	0.14	0.00	84.26	0.13	0.10	9.42	5.83
31.83	86.12	0.15	0.00	87.67	0.11	0.10	5.51	5.87
33.25	85.93	0.13	0.00	88.06	0.14	0.10	6.28	5.91
34.67	84.64	0.15	0.00	73.83	0.13	0.08	14.84	9.64
36.00	83.57	0.14	0.16	81.67	0.11	0.12	12.73	6.03
38.22	83.71	0.19	0.00	80.00	0.09	0.18	12.78	6.04
40.33	83.23	0.20	0.00	80.31	0.09	0.16	7.66	9.77
42.00	80.63	0.21	0.00	82.65	0.08	0.10	10.98	5.60
45.50	77.40	0.18	0.00	84.24	0.08	0.04	5.55	6.06
48.00	76.08	0.19	0.00	87.59	0.07	0.04	5.85	6.12

Table E22 data of figure 5.8a

Time	%1-Propanol Conversion	% Formaldehyde Selectivity	% Acetaldehyde Selectivity	%Propanal Selectivity	%Methane Selectivity	% Ethylene Selectivity	% propylene Selectivity	%Carbondioxide Selectivity
2.00	100.00	0.00	58.70	25.28	0.12	0.03	15.58	0.17
4.00	100.00	0.00	48.28	30.62	0.09	0.04	18.14	0.38
5.33	100.00	0.00	47.89	33.99	0.08	0.04	16.08	0.41
6.50	100.00	0.00	48.43	34.87	0.07	0.04	14.76	0.43
9.50	100.00	0.00	42.79	41.53	0.08	0.05	14.71	0.54
12.50	87.83	0.00	39.03	48.47	0.07	0.04	10.48	0.80
14.00	81.93	0.00	33.37	50.35	0.11	0.06	14.23	0.87
16.75	74.75	0.00	28.29	59.82	0.09	0.05	9.65	0.89
18.00	79.45	0.00	27.82	61.00	0.10	0.06	9.93	1.04
20.00	74.86	0.00	25.09	64.69	0.09	0.05	8.52	0.99
23.00	69.39	0.00	21.85	67.73	0.08	0.04	6.63	0.98
30.50	77.35	0.00	24.39	72.97	0.07	0.04	0.00	1.20
33.50	76.90	0.00	23.95	74.21	0.07	0.04	0.00	1.55
37.25	74.47	0.00	19.19	77.91	0.06	0.03	0.00	1.98
41.00	75.96	0.00	17.64	80.11	0.06	0.03	0.00	1.93
43.00	71.57	0.00	16.00	77.23	0.05	0.03	2.57	1.96
48.00	78.22	0.00	15.91	81.24	0.06	0.03	0.00	2.28

Table E23 data of figure 5.8b

Time	%1-Propanol Conversion	% Formaldehyde Selectivity	% Acetaldehyde Selectivity	%Propanal Selectivity	%Methane Selectivity	% Ethylene Selectivity	% propylene Selectivity	%Carbondioxide Selectivity
2.58	80.42	0.00	0.00	69.47	0.23	0.07	29.00	0.63
3.75	83.13	0.00	0.00	61.40	0.20	0.08	37.37	0.54
5.08	79.36	0.00	0.00	69.35	0.14	0.06	30.13	0.09
6.50	80.14	0.00	0.00	70.52	0.11	0.06	28.34	0.75
8.50	79.78	0.00	0.00	67.09	0.12	0.07	30.71	1.22
10.50	77.73	0.00	0.00	64.07	0.15	0.09	34.14	0.47
12.17	75.64	0.00	0.00	65.20	0.15	0.09	32.40	1.33
13.50	74.60	0.00	0.00	68.45	0.13	0.08	30.12	0.24
14.75	70.17	0.00	0.00	70.88	0.13	0.08	27.32	0.59
17.33	63.27	0.00	0.00	69.80	0.15	0.09	26.21	2.50
18.67	61.13	0.00	0.00	66.55	0.18	0.10	28.65	3.94
22.50	70.50	0.00	0.00	65.48	0.17	0.09	31.12	2.20
24.25	62.77	0.00	0.00	67.01	0.17	0.10	27.52	4.21
30.00	50.49	0.00	0.00	64.73	0.29	0.18	29.88	3.88
34.50	48.57	0.00	0.00	64.97	0.32	0.21	30.44	3.17
40.75	51.45	0.00	0.00	63.63	0.29	0.20	26.95	8.70
46.50	67.85	0.00	0.00	65.01	0.18	0.10	31.36	2.43
48.00	63.18	0.00	0.00	67.10	0.18	0.10	26.19	5.51

Table E24 data of figure 5.8c

Time	%1-Propanol Conversion	% Formaldehyde Selectivity	% Acetaldehyde Selectivity	%Propanal Selectivity	%Methane Selectivity	% Ethylene Selectivity	% propylene Selectivity	%Carbondioxide Selectivity
3.00	97.98	0.00	0.00	72.22	0.17	0.03	26.56	0.14
4.42	97.87	0.00	0.00	69.31	0.15	0.04	29.73	0.14
5.83	95.84	0.00	0.00	73.09	0.13	0.05	25.95	0.14
6.00	95.17	0.00	0.00	70.66	0.11	0.06	27.84	0.12
7.58	94.29	0.00	0.00	89.57	0.02	0.01	8.96	0.07
10.33	96.32	0.00	0.00	69.07	0.07	0.05	30.45	0.04
11.58	96.14	0.00	0.00	73.64	0.05	0.04	25.91	0.04
12.83	95.91	0.00	0.00	73.15	0.05	0.04	26.56	0.04
15.00	95.36	0.00	0.00	71.58	0.06	0.04	27.19	0.03
16.33	94.01	0.00	0.00	79.07	0.04	0.03	19.70	0.03
17.67	92.79	0.00	0.00	80.28	0.04	0.03	18.41	0.03
19.00	85.09	0.00	0.00	76.26	0.11	0.09	22.05	0.06
21.33	85.66	0.00	0.00	68.43	0.12	0.08	28.90	0.04
24.75	82.55	0.00	0.00	72.37	0.11	0.07	25.17	0.05
27.83	80.20	0.00	0.00	68.04	0.15	0.11	28.19	0.08
30.83	76.72	0.00	0.00	73.69	0.17	0.13	23.05	0.12
33.00	76.34	0.00	0.00	73.08	0.22	0.17	21.19	0.23
36.75	73.22	0.01	0.00	86.86	0.14	0.13	8.59	0.40
40.00	79.46	0.01	0.00	65.72	0.54	0.38	25.59	0.34
46.00	85.03	0.01	0.00	64.91	1.05	0.51	22.95	0.90
48.00	87.20	0.01	0.00	69.12	0.99	0.46	20.46	1.11

Table E25 data of figure 5.9a

Temp	%1-Propanol Conversion	% Formaldehyde Selectivity	% Acetaldehyde Selectivity	%Propanal Selectivity	%Methane Selectivity	% Ethylene Selectivity	% propylene Selectivity	%Carbondioxide Selectivity
200	1.52	0.70	0.00	78.38	0.00	0.00	17.90	0.00
250	16.86	0.34	0.00	33.54	0.00	0.00	63.78	0.00
300	65.61	0.67	0.00	9.63	0.02	0.07	87.83	0.00
350	96.83	0.74	1.80	8.45	0.12	0.35	84.15	0.00
400	100.00	0.83	3.02	2.86	0.14	0.41	87.51	0.30
450	100.00	0.87	3.78	1.05	0.40	1.03	86.94	1.05
500	100.00	0.84	2.74	0.00	1.36	2.69	88.10	2.32

Table E26 data of figure 5.9b

Temp	%1-Propanol Conversion	% Formaldehyde Selectivity	% Acetaldehyde Selectivity	%Propanal Selectivity	%Methane Selectivity	% Ethylene Selectivity	% propylene Selectivity	%Carbondioxide Selectivity
200	7.83	0.06	0.00	9.93	0.00	0.00	86.61	0.00
250	12.86	0.15	0.00	6.13	0.00	0.15	90.17	0.00
300	51.21	0.61	0.00	4.37	0.13	0.07	93.09	0.00
350	85.89	1.14	1.90	5.45	0.11	0.13	90.18	0.00
400	100.00	0.86	2.30	3.32	0.12	0.41	90.28	0.00
450	100.00	0.84	3.02	1.21	0.35	1.01	90.47	0.79
500	100.00	0.70	2.55	0.00	0.66	1.41	90.21	1.33

Table E27 data of figure 5.10a

Temp	%1-Propanol Conversion	% Formaldehyde Selectivity	% Acetaldehyde Selectivity	%Propanal Selectivity	%Methane Selectivity	% Ethylene Selectivity	% propylene Selectivity	%Carbondioxide Selectivity
200	8.93	1.54	0.00	0.00	0.05	0.00	96.11	0.00
250	76.48	0.81	0.00	52.63	0.01	0.01	42.23	0.55
300	88.32	0.48	0.00	50.12	0.01	0.02	43.33	1.50
350	100.00	0.36	0.00	48.96	0.04	0.09	44.65	1.71
400	100.00	0.37	0.41	49.51	0.11	0.13	45.42	1.94
450	100.00	0.36	1.76	51.34	0.04	0.01	43.90	2.17
500	100.00	0.37	1.87	52.20	0.01	0.11	42.51	2.25

Table E28 data of figure 5.10b

Temp	%1-Propanol Conversion	% Formaldehyde Selectivity	% Acetaldehyde Selectivity	%Propanal Selectivity	%Methane Selectivity	% Ethylene Selectivity	% propylene Selectivity	%Carbondioxide Selectivity
200	1.34	0.68	0.00	0.00	0.00	0.00	95.70	0.00
250	48.46	0.75	0.00	3.12	0.01	0.00	92.41	0.00
300	97.20	0.78	0.00	3.96	0.01	0.00	93.32	0.00
350	100.00	0.77	0.00	6.45	0.01	0.01	91.46	0.00
400	100.00	0.77	0.00	6.60	0.01	0.04	90.67	0.00
450	100.00	0.77	0.00	4.09	0.11	0.08	94.59	0.00
500	100.00	0.78	0.00	0.61	0.17	0.08	95.09	0.40

APPENDIX F
BLANK TEST OF OXIDATION REACTION

The oxidation reaction of 1-propanol and 2-propanol at the same reaction condition but have no catalyst (blank test) are shown as follow:

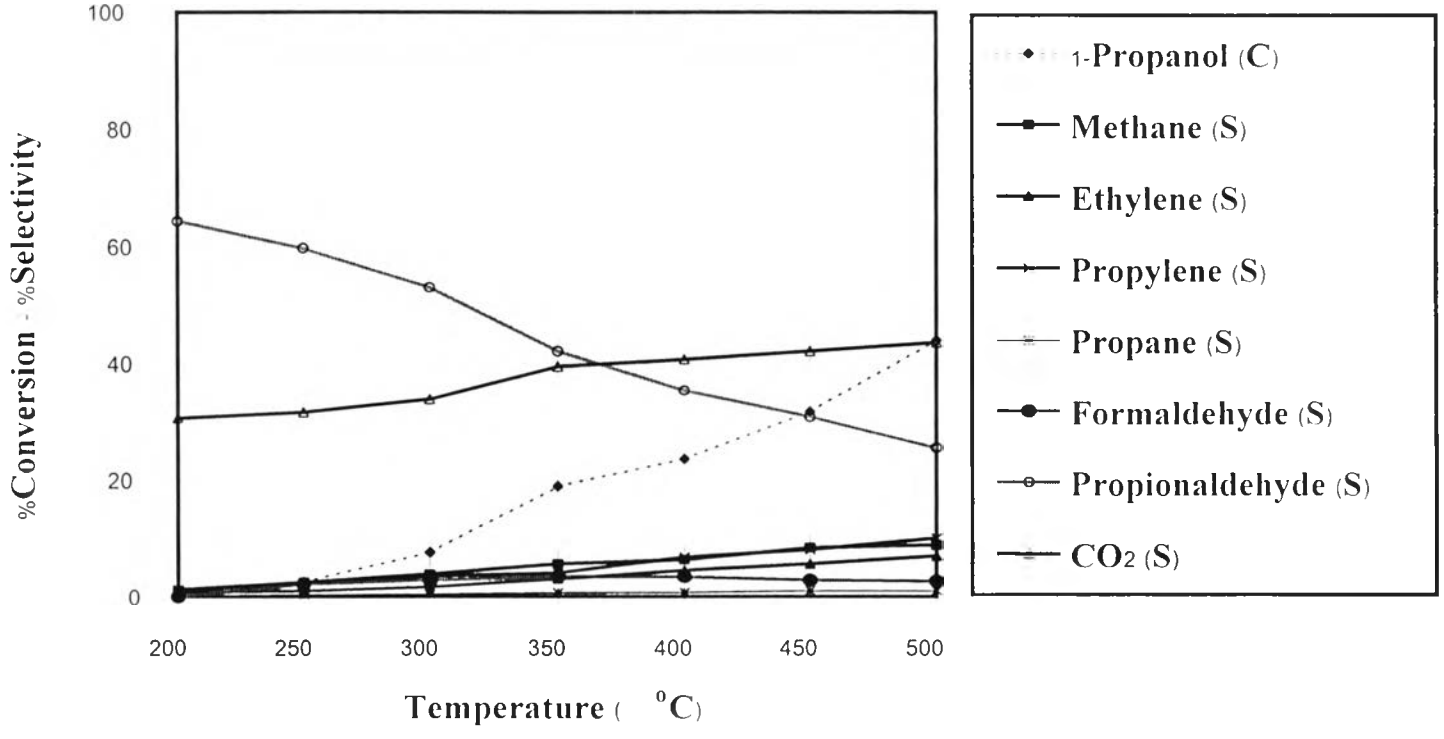


Figure F1 Conversion (C) of 1-propanol and product selectivities (S) in the 1-propanol oxidation.

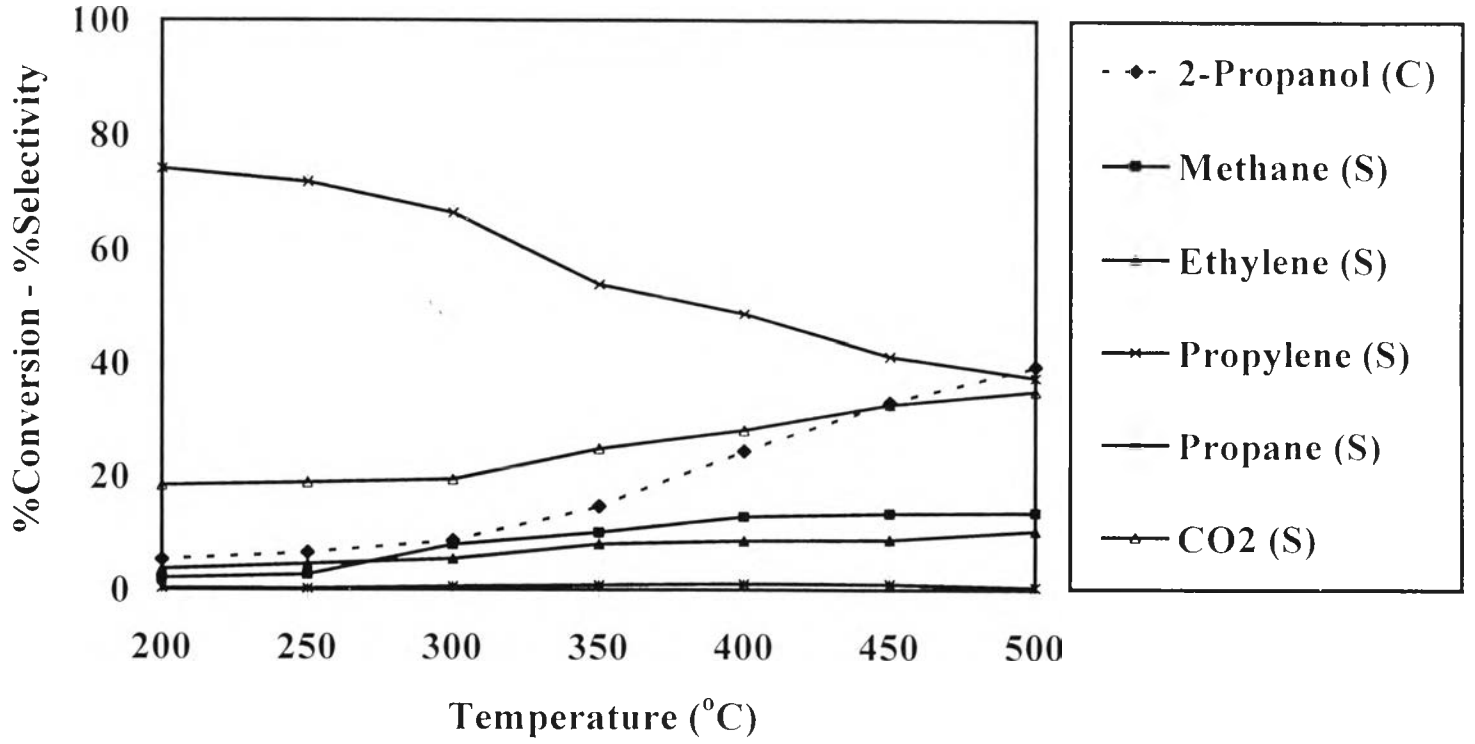


Figure F2 Conversion (C) of 2-propanol and product selectivities (S) in the 2-propanol oxidation.

APPENDIX G

CALIBRATION CURVE OF CARBON DIOXIDE CONTENT

Table G1 Detected area was converted to and estimated weight of carbon by feeding 100%CO_2 0.405 ml./min. mixed with helium in various flow rate through porapak Q column on GC 8AIT at 110°C detector temperature and 90°C column temperature. using (1.5 ml) sampling loop

Carbon content (mg)	Average area (a.u.)
0.001293	2218
0.002138	3738
0.004051	7079
0.005375	9379
0.007239	12587

The assumption of gas content calculation was based on the ideal gas law. Therefore, the data fitted with linear equation can be expressed below;

Amount of carbon (mg), $Y = 5.7410 \times 10^{-7}$

Where least square error, $R^2 = 0.9999$

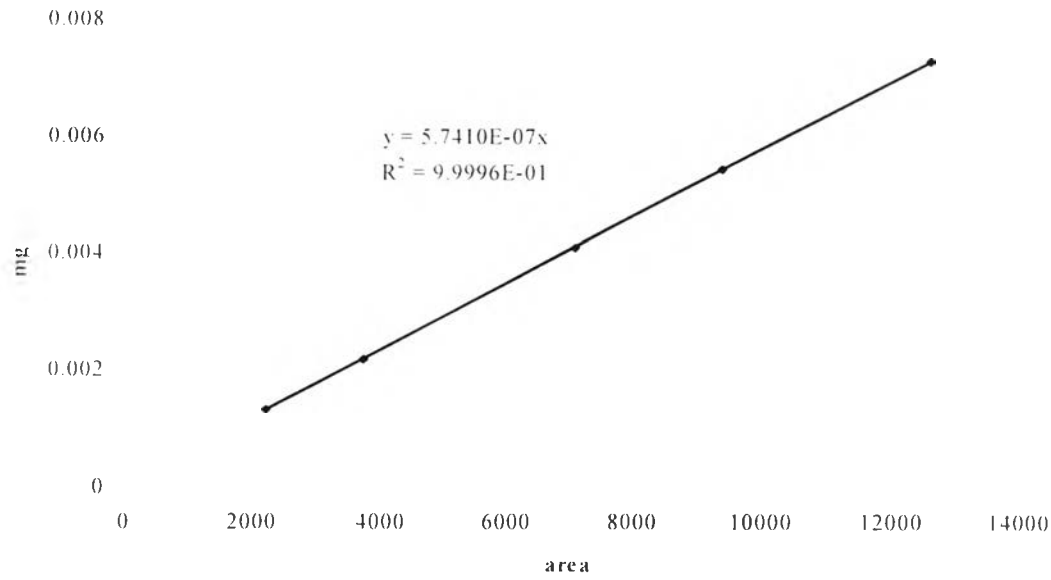


Figure G1 Calibration curve of carbon dioxide on GC 8AIT

VITA

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