



## CHAPTER III EXPERIMENTAL

### 3.1 Materials

Chemicals/materials used in this research are as follows:

Cyclohexene purum ( $C_6H_{10}$ : purum  $\gg$  99%, Fluka) was used as the precursor for cyclohexene epoxidation.

Ruthenium (III) chloride hydrate ( $RuCl_3 \cdot xH_2O$ , Aldrich) was used to prepare metal oxide additive.

Aqueous solution of 30 wt.% hydrogen peroxide ( $H_2O_2$ , Carlo Erba) was used as the oxidant.

*tert*-Butanol ( $C_4H_{10}O$ , Ajax finechem) was used as the solvent.

Dodecane ( $C_{12}H_{26}$ , Fluka) was used as internal standard.

Cyclohexene oxide ( $C_6H_{10}O$ , Fluka), 2-cyclohexen-1-ol ( $C_6H_9OH$ , Fluka), 2-cyclohexen-1-one ( $C_6H_8O$ , Fluka), and (1*S*,2*S*)-*trans*-1,2-cyclohexanediol ( $C_6H_{12}O_2$ , Fluka) was used as standard.

Silica ( $SiO_2$ , HiSil<sup>®</sup>255 Modified Silica), alumina ( $\gamma-Al_2O_3$ ), and non-mesoporous-assembled titania ( $TiO_2$ , Degussa P-25, J.J. Degussa Huls Co.,Ltd.) were commercial grade, obtained from Tokuyama, Saint-Gobain Norpro, and Aeroxide; respectively.

Iron (II) chloride tetrahydrate ( $FeCl_2 \cdot 4H_2O$ , Fluka), iron (III) chloride hexahydrate ( $FeCl_3 \cdot 6H_2O$ , Riedel-deHaen), and ammonium hydroxide 30% ( $NH_4OH$ , Malinckrodt) were used to synthesize  $Fe_3O_4$  (magnetite).

Tetraisopropyl orthotitanate (TIPT,  $Ti(OCH(CH_3)_2)_4$ , synthesis grade, Merck), laurylamine hydrochloride (LAHC,  $CH_3(CH_2)_{11}NH_2 \cdot HCl$ , synthesis grade, Merck), acetylacetone (ACA,  $CH_3COCH_2COCH_3$ , synthesis grade, Rasayan), distilled water, and hydrochloric acid (HCl) were used for the synthesis of mesoporous-assembled  $TiO_2$  ( $TiO_2$  (SG)).

**Table 3.1** Physical properties of substances used in cyclohexene epoxidation

Material	Molecular weight	Boiling point (°C)	Density (g/cm <sup>3</sup> )
Cyclohexene	82.14	82.8	0.81
Cyclohexene oxide	98.14	131.0	0.97
2-Cyclohexen-1-ol	98.14	164.0	0.99
2-Cyclohexen-1-one	96.13	168.0	0.99
(1S,2S)- <i>trans</i> -1,2-Cyclohexanediol	116.16	117.0	-
Dodecane	170.34	213.0	0.75
Hydrogen peroxide	34.01	150.2	1.40
<i>tert</i> -Butanol	74.12	82.4	0.78

### 3.2 Equipments

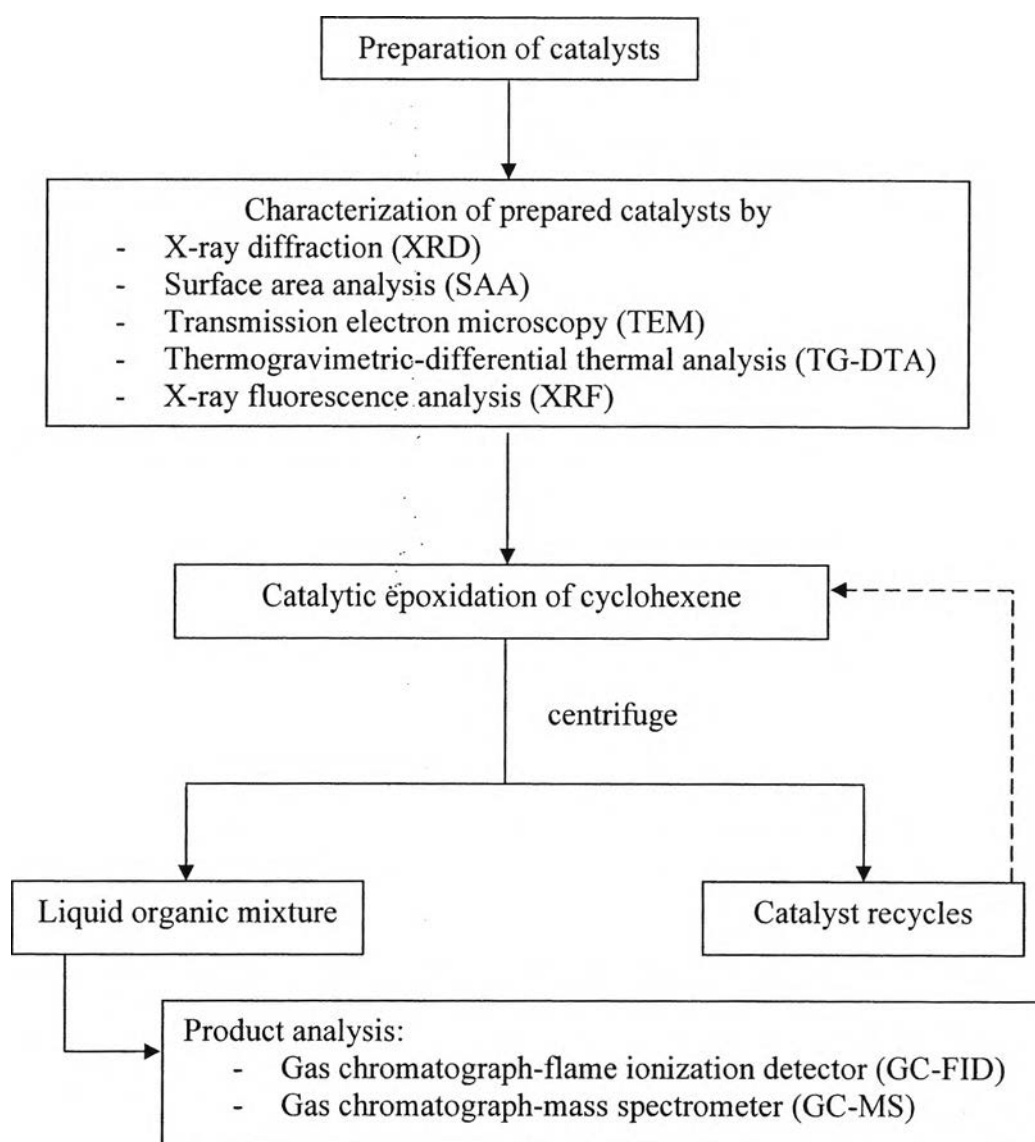
Equipments used in this research are as follows:

1. Gas chromatograph (Agilent GC 6890) with FID detector and ZB-5 HT column (30 m × 0.32 mm ID × 0.10 μm film thickness)
2. Gas chromatograph with mass spectrometer
3. Surface area analyzer (SAA, Quantachrome/ Autosorb-1 model)
4. X-ray diffractometer (Rigaku, Rint 2200 HV model)
5. Transmission electron microscope (JEOL JEM-200CX)
6. Thermogravimetric-differential thermal analyzer (TG-DTA, Perkin Elmer/ Pyris Diamond)
7. X-ray fluorescence (Philips, PW2400)
8. Oven (CARBOLITE/CWE 1100)
9. Hot plate and stirrer (Cole-Parmer, Stable Temp model)
10. Circulating bath (Huber model)
11. Centrifuge machine (Labnet, spectrafugal)
12. Glasswares (Duran, Germany)
13. Magnetic stirrer

### 3.3 Methodology

#### 3.3.1 Experimental Procedure

Overview of the experimental procedure covering the scope of the research is shown in Figure 3.1.

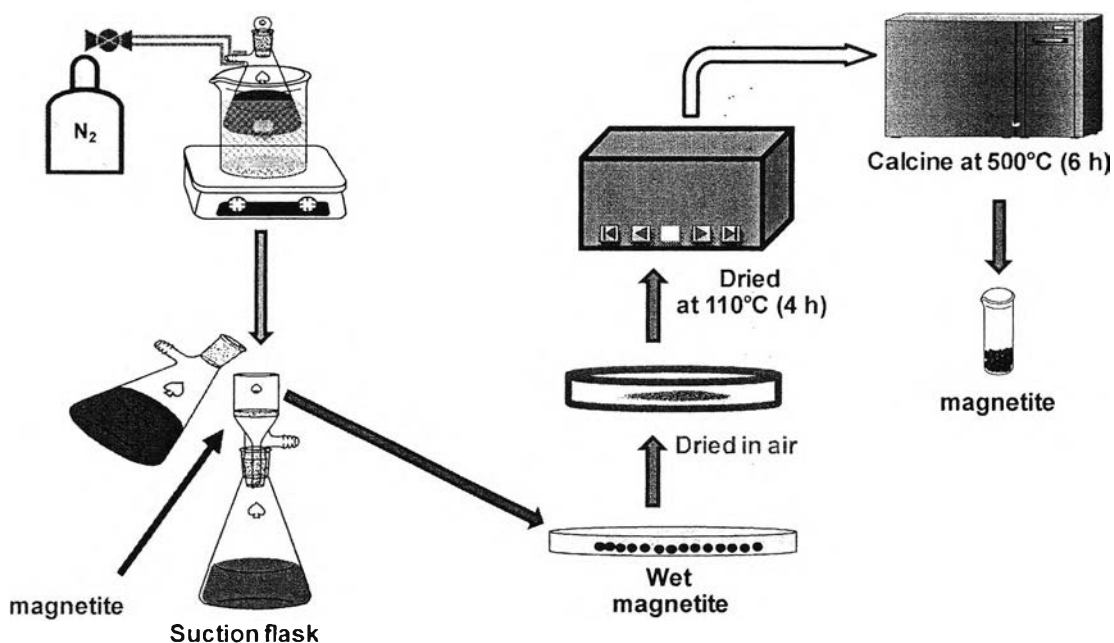


**Figure 3.1** Overview of experimental procedure.

### 3.3.2 Preparation of Magnetite ( $\text{Fe}_3\text{O}_4$ )

In this research, the magnetite ( $\text{Fe}_3\text{O}_4$ ) is prepared by precipitation method, as shown in Figure 3.2.

For the magnetite preparation, a 100 ml of distilled water is placed in a temperature-controlled bath at  $70^\circ\text{C}$  and purged with nitrogen gas in order to remove dissolved molecular oxygen. In each preparation, 1.075 g of  $\text{FeCl}_2\cdot 4\text{H}_2\text{O}$  and 2.900 g of  $\text{FeCl}_3\cdot 6\text{H}_2\text{O}$  are dissolved in prepared distilled water under continuous stirring and heating at  $70^\circ\text{C}$ . The pH of solution is between 9 and 10, which can be adjusted by adding 3.75 ml of  $\text{NH}_4\text{OH}$  when  $\text{FeCl}_2\cdot 4\text{H}_2\text{O}$  and  $\text{FeCl}_3\cdot 6\text{H}_2\text{O}$  are dissolved completely. After 1 h of further stirring, the magnetite is obtained and then filtered by suction instrument. The magnetite is washed by distilled water and acetone, dried at room temperature overnight, and placed in an oven kept at  $110^\circ\text{C}$  for 4 h. The dried magnetite was calcined at  $500^\circ\text{C}$  for 6 h and kept in desiccator.



**Figure 3.2** Schematic of the synthetic procedure of magnetite (Gupta, A.K., and Gupta, M., 2005).

### 3.3.3 Preparation of TiO<sub>2</sub> (SG) and RuO<sub>2</sub>/TiO<sub>2</sub> (SSSG)

The mesoporous-assembled TiO<sub>2</sub> nanocrystal support (TiO<sub>2</sub> (SG)), and RuO<sub>2</sub>-loaded mesoporous-assembled TiO<sub>2</sub> nanocrystal catalyst (RuO<sub>2</sub>/TiO<sub>2</sub> (SSSG)) were synthesized according to the following procedure:

a. A specified amount of analytical grade ACA was introduced into TIPT with the molar ratio of unity.

b. The mixed solution was then gently shaken until homogeneous mixing. Afterwards, a 0.1 M LAHC aqueous solution with pH of 4.2 was added into the ACA-modified TIPT solution, in which the molar ratio of TIPT to LAHC was adjusted to a value of 4.

c. The mixture was kept continuously stirring at 40°C overnight to obtain transparent yellow sol.

(d. and e. are the additional steps for the preparation of RuO<sub>2</sub>-loaded mesoporous-assembled TiO<sub>2</sub> by single-step sol-gel method (RuO<sub>2</sub>/TiO<sub>2</sub> (SSSG)))

d. To the aged TiO<sub>2</sub> sol solution, ruthenium (III) chloride hydrate (RuCl<sub>3</sub>·xH<sub>2</sub>O) was added with various RuO<sub>2</sub> loadings.

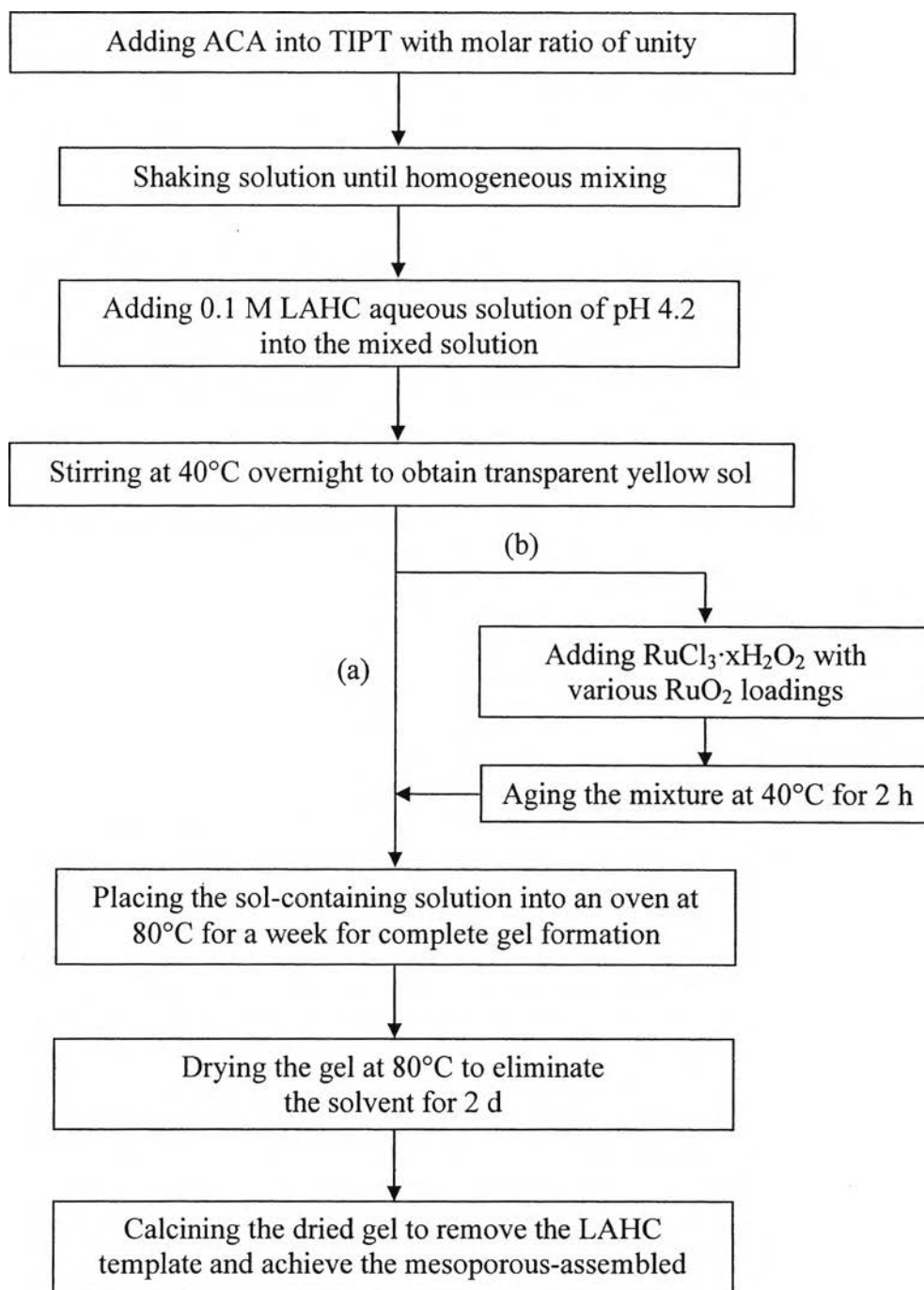
e. The final mixture was further aged at 40°C for 2 h to acquire homogeneous solution.

f. Then, the sol-containing solution was placed into an oven at 80°C for a week in order to obtain complete gel formation.

g. Subsequently, the gel was dried at 80°C to eliminate the solvent for 2 d, which is mainly the distilled water used in the preparation of surfactant aqueous solution.

h. The dried sample was finally calcined to remove LAHC template and consequently produce the TiO<sub>2</sub> (SG) and RuO<sub>2</sub>/TiO<sub>2</sub> (SSSG).

The steps for the synthesis of  $\text{TiO}_2$  (SG) and  $\text{RuO}_2/\text{TiO}_2$  (SSSG) are shown in Figure 3.3.

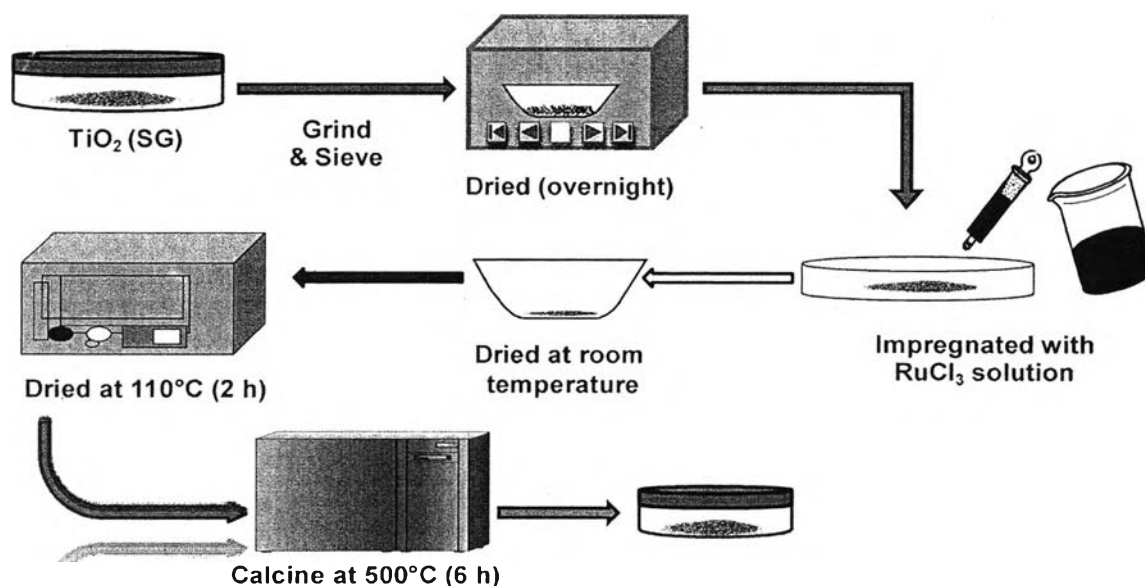


**Figure 3.3** Synthesis procedure for mesoporous-assembled  $\text{TiO}_2$  nanocrystal: (a) for  $\text{TiO}_2$  (SG) (Sreethawong *et al.*, 2005) and (b) for  $\text{RuO}_2/\text{TiO}_2$  (SSSG).

### 3.3.4 Preparation of RuO<sub>2</sub>/TiO<sub>2</sub> (IWI)

In this study, the RuO<sub>2</sub> activator is loaded onto TiO<sub>2</sub> (SG) by incipient wetness impregnation (IWI) method, as shown in Figure 3.4.

In the first step, the TiO<sub>2</sub> (SG) is ground, sieved, and dried in an oven at 110°C overnight. RuCl<sub>3</sub>·xH<sub>2</sub>O is weighed for an appropriate amount and dissolved in distilled water in suitable amount of catalyst. After that, the catalyst is impregnated by slowly dropping the ruthenium chloride solution. Subsequently, the RuO<sub>2</sub>, which is loaded onto the prepared catalyst, is dried at room temperature for 1 h before being dried in an oven at 110°C for 2 h and finally calcined at 500°C for 6 h. The resulting supported catalyst is labeled and stored in a desiccator.



**Figure 3.4** Schematic of the catalyst preparation of the RuO<sub>2</sub>/TiO<sub>2</sub> (IWI) catalyst.

### 3.3.5 Catalyst Characterization

The different properties may affect the conversion and selectivity; therefore, it is necessary to verify them by several techniques. In this work, several characterization techniques are employed.

#### *X-Ray Diffraction (XRD)*

X-ray diffraction (XRD) is used to identify phases present in the samples. The crystalline structure of oxide support and the mean particle diameter of ruthenium (IV) oxide (or RuO<sub>2</sub>) are analyzed by means of a Rigaku X-ray Diffractometer system (RINT-2200) with copper tube for generating CuK $\alpha$  radiation (1.54056 Å) and nickel filter. It is also possible to achieve a relative analysis by the intensity of the peak. For the same crystalline substance, the higher intensity of the peak indicates the higher content of that phase.

RINT-2200 system is used to obtain XRD pattern at a generator voltage of 40 kV and generator current of 30 mA. The goniometer parameters are divergent slit = 1° (2 $\theta$ ); scattering slit = 1° (2 $\theta$ ); and receiving slit = 0.3 mm. The scan speed of 1° (2 $\theta$ )/min with scan step of 0.02 (2 $\theta$ ) is used for the continuous run in 20 to 60° (2 $\theta$ ) range. Sample should be ground to the fine homogeneous powder and held in a beam direction in a thin-walled glass container. The signal is sent to the online computer to record and analyze. Scherrer equation as expressed in Equation 3.1 shows the relationship between the crystalline thickness ( $D_b$ ) and the broadening ( $B_d$ ) of the diffraction line corresponding to the Bragg angle ( $\theta$ ) using wavelength ( $\lambda$ ).

$$D_b = \frac{K \cdot \lambda}{B_d \cdot \cos \theta} \quad (3.1)$$

where:

$D_b$  = mean crystalline diameter (nm)

K = Scherrer constant, 0.89

$\lambda$  = X-ray wavelength (0.15418 nm for CuK $\alpha$ )

$B_d$  = full width half maximum (FWHM) of diffraction peak measured at 2 $\theta$

$\theta$  = Bragg angle of the reflection (degree)



It is significant to note here that the results from the Scherrer equation are a crystalline thickness that is perpendicular to the diffraction planes rather than an actual particle size. It is necessary to apply a correction factor that depends on the actual shape of the crystallinities and on the Millers indices of the diffraction planes in order to obtain the actual crystallite size from the thickness.

*Surface Area Analysis (SAA)*

Autosorb-1 Gas Sorption System (Quantachrome Corporation) is used to measure the surface area, total pore volume, and average pore diameter of the catalysts. The equipment measurement is based on Brunauer-Emmet-Teller (BET) equation. This technique is done by calculating the physical multi-layer adsorption of nitrogen. Volatile adsorbents on the surface are eliminated by heating under vacuum at 250°C for at least 4 h prior to the analysis. Nitrogen gas with the cross-sectional area of  $1.62 \times 10^{-19} \text{ m}^2/\text{molecule}$  is adsorbed on the catalyst surface at liquid nitrogen temperature (-196°C). The surface area is calculated from the 22-points nitrogen adsorption. The average pore diameter and pore volume are obtained at  $P/P_0$  ratios close to unity. The result is analyzed by Autosorb Anygas Software version 2.1 using the BET equation, as shown in Equation 3.2.

$$\frac{1}{W \cdot \left( \frac{P_0}{P} - 1 \right)} = \frac{1}{W_m \cdot C} + \frac{(C-1)}{(W_m \cdot C)} \cdot \left( \frac{P_0}{P} \right) \quad (3.2)$$

where:

P = pressure of gas

$P_0$  = saturated vapor pressure of the liquid at the operating temperature

W = weight of gas adsorbed at a relative pressure,  $P/P_0$

$W_m$  = weight of adsorbate constituting a monolayer of surface coverage

C = constant that is related to the energy of adsorption in the first adsorbed layer and magnitude of the adsorbent/adsorbate interaction

The surface area is calculated by Equation 3.3.

$$S = \frac{W_m \cdot A_{N_2} \cdot (6.02 \times 10^{23})}{M_{W, N_2}} \quad (3.3)$$

where:

$S$  = specific surface area ( $\text{m}^2/\text{g}$ )

$A_{N_2}$  = cross-sectional area of one molecule of  $N_2$  ( $0.162 \text{ nm}^2$  at  $-196^\circ\text{C}$ )

$M_{w,N_2}$  = molecule weight of nitrogen ( $28 \text{ g/g-mol}$ )

#### *Transmission Electron Microscopy (TEM)*

The transmission electron micrographs are applied for investigating the average particle size and identifying morphological structure of the synthesized catalysts. The catalyst samples are ground into fine powder and ultrasonically dispersed in ethanol. A small droplet of the suspension is deposited on a copper grid, and the solvent is evaporated prior to loading the sample into the microscope. TEM is carried out using in a JEOL JEM-200CX operated at and accelerating voltage of 200 kV in bright field modes. A beam is passed through a series of lenses to form a magnified image of a sample that is inserted in the area of the objective lens. The image from selected area is viewed through projection onto a view of screen. However, electron beams can be easily scattered by air molecules, and TEM columns must be kept under high vacuum. Additionally, the electromagnetic lenses is used for focusing the electron beam. The elemental analysis of photocatalyst is also investigated by an energy-dispersive X-ray (EDX) analyzer attached to TEM.

#### *Thermogravimetric-Differential Thermal Analysis (TG-DTA)*

Simultaneous thermogravimetry and differential thermal analysis (TG-DTA) of uncalcined  $\text{TiO}_2$  gel was used to obtain suitable calcination temperature for removing the LAHC surfactant. Moreover, TG-DTA is investigated for determination of the surface OH density ( $\text{OH}/\text{nm}^2$ ) and surface OH-to-catalyst weight ratio ( $\text{OH}/\text{g}$ ) of  $\text{TiO}_2$  (SG),  $\text{RuO}_2/\text{TiO}_2$  (IWI), and  $\text{RuO}_2/\text{TiO}_2$  (SSSG). The uncalcined gel of 5-20 mg was heated from 30 to  $700^\circ\text{C}$  with a heating rate of  $20^\circ\text{C}/\text{min}$  in nitrogen gas with  $\alpha\text{-Al}_2\text{O}_3$  as the reference. The OH surface density of the catalysts is calculated by using the TGA weight loss and the SAA, as shown in Equation 3.4 (Zou and Lin, 2004).

$$n\text{OH}/\text{nm}^2 = \alpha \left( \frac{(n\text{OH}/\text{nm}^2)_{T_2} \times \text{SSA} \times \text{wt}_{T_2} + \left( \frac{2(\text{wt}_{T_1} - \text{wt}_{T_2}) N_A}{\text{MW}_{\text{H}_2\text{O}}} \right)}{\text{SSA} \times \text{wt}_{T_1}} \right) \quad (3.4)$$

where:

$\text{wt}_{T_i}$  = the sample weight at the corresponding temperature  $T_i$

$\text{MW}_{\text{H}_2\text{O}}$  = the molecular weight of water (18 g/g-mol)

$N_A$  = Avogadro's constant ( $6.02 \times 10^{23} \text{ mol}^{-1}$ )

$\text{SSA}$  = Specific surface area ( $\text{m}^2/\text{g}$ )

$\alpha$  = a calibration factor given as 0.625

$(n\text{OH}/\text{nm}^2)_{T_2}$  = free of OH surface groups as  $1 \text{ nm}^{-2}$

$n\text{OH}/\text{nm}^2$  = the OH surface density ( $\text{nm}^{-2}$ )

A temperature range from 100 to 120°C was found for removal of physically adsorbed water; therefore, this range is not crucial for powder characterization as it depends even on humidity during sample preparation. But for a temperature range from 120 to 500°C, it represents the weight loss by the removal of hydroxyl groups from the powder surface and possibly desorption of volatile organic compounds associated with powder synthesis or processing (Mueller *et al.*, 2003).

#### *X-Ray Fluorescence Analysis (XRF)*

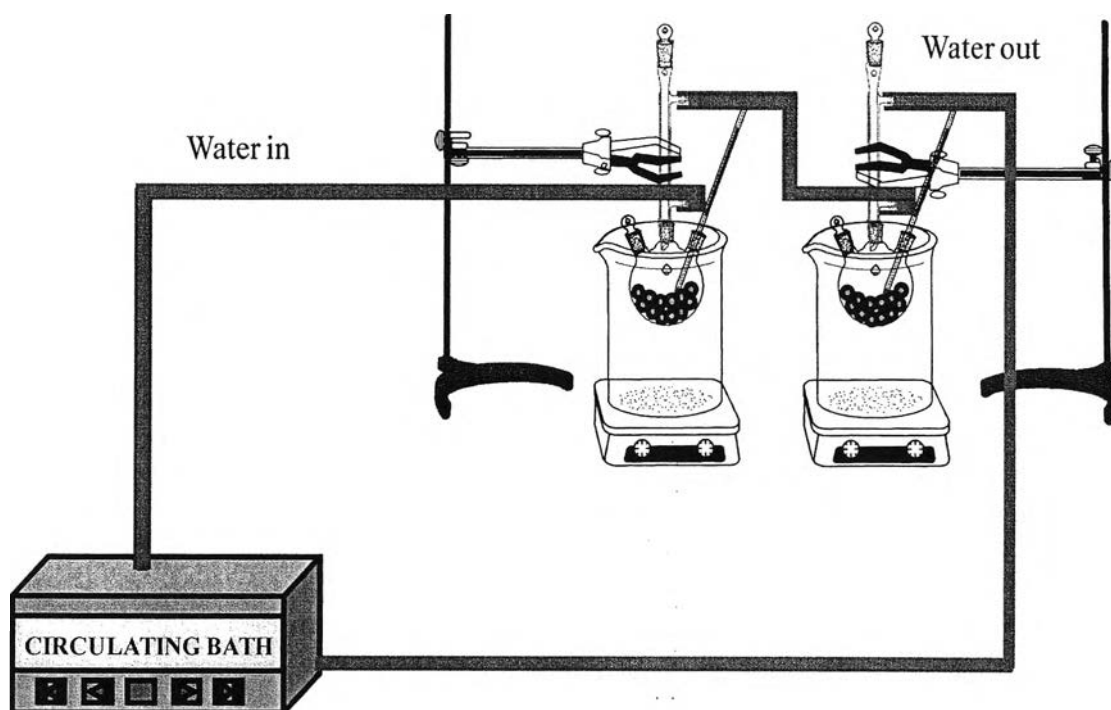
The XRF method is widely used to measure the elemental composition of materials. Since this method is fast and non-destructive to the sample, it is the method of choice for field applications and industrial production for control of materials. The analysis of major and trace elements in geological materials by x-ray fluorescence is made possible by the behavior of atoms when they interact with radiation. When materials are excited with high-energy, short wavelength radiation (e.g., X-rays), they can become ionized. If the energy of the radiation is sufficient to dislodge a tightly-held inner electron, the atom becomes unstable and an outer electron replaces the missing inner electron. When this happens, energy is released due to the decreased binding energy of the inner electron orbital compared with an

outer one. The emitted radiation is of lower energy than the primary incident X-rays and is termed fluorescent radiation. Because the energy of the emitted photon is characteristic of a transition between specific electron orbitals in a particular element, the resulting fluorescent X-rays can be used to detect the abundances of elements that are present in the sample.

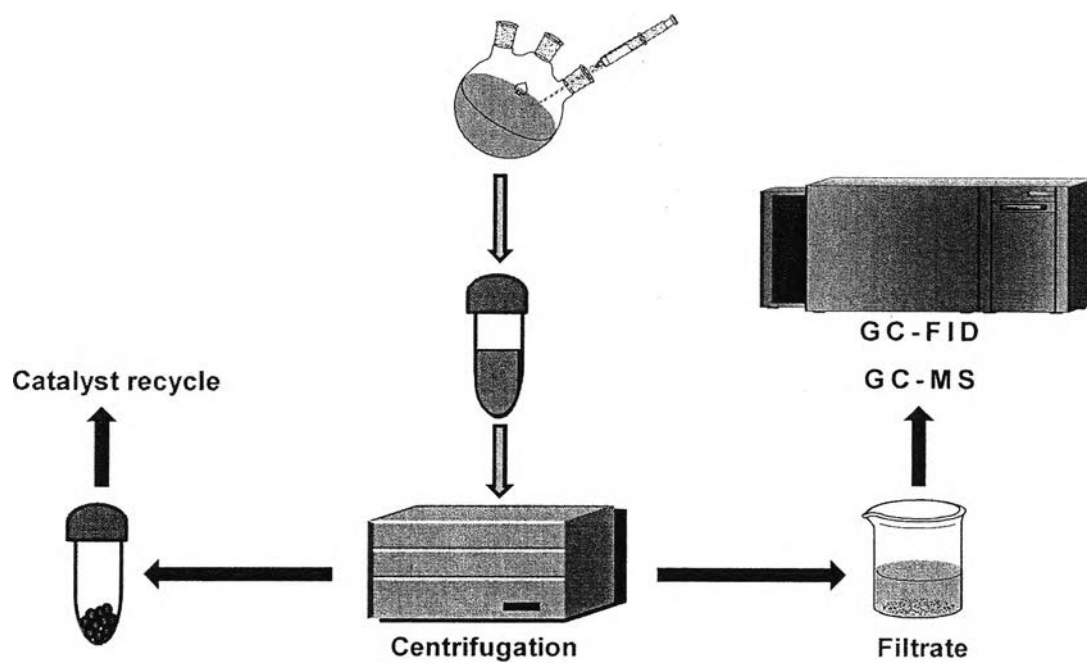
### 3.3.6 Catalytic Activity Testing

The catalytic experiments are carried out using cyclohexene as the precursor and *tert*-butanol as the solvent. In typical reaction, 100 ml three-neck round-bottomed flask is fitted with a reflux condenser and placed in temperature-controlled water bath, and to this is added with 30 mmol cyclohexene, catalyst, and 30 ml *tert*-butanol. The reaction mixture is magnetically stirred and heated until the reaction temperature is finally maintained at a desired value. The reaction is then started by adding the oxidant into the mixture. For every 1 h of further stirring, the chemical mixture in the reactor is sampled. After that, the catalyst is separated by centrifugation, and then the filtrate (or liquid organic mixture) is analyzed by a gas chromatograph (Agilent 6890) equipped with a flame ionization detector (GC-FID) for determination of product composition. The identification of the products is also examined by a gas chromatograph equipped with a mass spectrometer (GC-MS). The schematic of catalyst testing is shown 3.5-3.6.

Many parameters affecting the conversion and selectivity of the prepared catalysts are studied in this research, such as the effects of various supports, calcination temperature, calcination time, RuO<sub>2</sub> content, reaction temperature, catalyst content, H<sub>2</sub>O<sub>2</sub>-to-cyclohexene ratio, and also recyclability of selected spent catalysts.



**Figure 3.5** Schematic of epoxidation reaction experiment.



**Figure 3.6** Flow diagram of catalyst recycle.

#### *Effect of Calcination Temperature*

The effect of calcination temperature for the RuO<sub>2</sub>/TiO<sub>2</sub> (IWI) is studied on the conversion of cyclohexene and selectivity of epoxide. The calcination temperature is varied from 500 to 700°C.

#### *Effect of Calcination Time*

The effect of calcination time for the RuO<sub>2</sub>/TiO<sub>2</sub> (IWI) is studied on the conversion of cyclohexene and selectivity of epoxide. The calcination time is varied from 3 to 6 h with 1 h increment at calcination temperature of 550°C.

#### *Effect of RuO<sub>2</sub> Content*

The effect of RuO<sub>2</sub> content for the RuO<sub>2</sub>/TiO<sub>2</sub> (IWI) and RuO<sub>2</sub>/TiO<sub>2</sub> (SSSG) with calcination temperature of 550°C and calcination time of 4 h is studied on the conversion of cyclohexene and selectivity of epoxide. The RuO<sub>2</sub> contents of 0.5, 1, 1.5, and 2 mol% are studied. The suitable RuO<sub>2</sub> content is chosen for the next study.

#### *Effect of Reaction Temperature*

The effect of reaction temperature is studied on the conversion of cyclohexene and selectivity of epoxide. The reaction temperature is varied from 50 to 80°C, whereas the other factors are kept constant at 0.5 g catalyst, 30 mmol cyclohexene, 30 ml solvent, and 30 mmol H<sub>2</sub>O<sub>2</sub>. The suitable reaction temperature is chosen for the next study.

#### *Effect of Catalyst Amount*

The effect of catalyst amount with the reaction temperature of 70°C is studied on the conversion of cyclohexene and selectivity of epoxide. The catalyst amount is varied from 0.20 to 0.80 g with 0.15 g increment, whereas the other factors are kept constant at 30 mmol cyclohexene, 30 ml solvent, and 30 mmol H<sub>2</sub>O<sub>2</sub>. The suitable catalyst content is chosen for the next study.

#### *Effect of H<sub>2</sub>O<sub>2</sub>-to-cyclohexene Ratio*

The effect of H<sub>2</sub>O<sub>2</sub>-to-cyclohexene ratio with the reaction temperature of 70°C and catalyst amount of 0.5 g is studied on the conversion of cyclohexene and selectivity of epoxide. The H<sub>2</sub>O<sub>2</sub>-to-cyclohexene ratio is varied from 0.1 to 6.67. The suitable H<sub>2</sub>O<sub>2</sub>-to-cyclohexene ratio is chosen for the next study.

### *Effect of Recycling of Selected Spent Catalysts*

The appropriate catalysts with the optimum reaction temperature, catalyst amount, and H<sub>2</sub>O<sub>2</sub>-to-cyclohexene ratio are used for recyclability studies in regard to cyclohexene epoxidation. Each catalyst is recovered from the reaction mixture by centrifugation, and the recovered catalyst is washed with *tert*-butanol and then with distilled water to remove all of the organic phases adsorbed on the catalyst surface, and dried in oven overnight. The recovered catalyst was reused to study its recyclability for the epoxidation reaction for three cycles.

#### 3.3.7 Product Analysis by GC-FID

The filtrate (or liquid organic mixture), which is separated from the catalyst by centrifugation, is analyzed by a gas chromatograph (Agilent GC 6890) - flame ionization detector (FID) for determination of product composition. The liquid products from the cyclohexene epoxidation contain non-polar hydrocarbon. The non-polar hydrocarbon can be determined by using ZB-5 column (non-polar column), of which the composition is 5% diphenyl polysiloxane and 95% dimethyl polysiloxane. Firstly, the mixture between the standard substances and internal standard, which is dodecane, is injected into column to determine the response factor from peak area of GC. Secondly, before sample injection to GC, the liquid organic mixture has to be mixed with the internal standard. Finally, the conversion percentage and the selectivity percentage are calculated from peak area and response factor.

In this research, a gas chromatograph-flame ionization detector (GC-FID, Agilent 6890) is used as liquid product analyzer. The GC operating condition is summarized in Table 3.2.

**Table 3.2** GC conditions for the product analysis

Setting	Condition
Oven temperature	50°C for 5 min, 10°C/min to 160°C, 160°C for 5 min
Injector temperature	250°C
Detector temperature	250°C
Carrier gas	Helium 99.99% purity
Sample volume	1 µl
Column type	ZB-5 HT column (30 m × 0.32 mm ID × 0.10 µm Film Thickness)

To determine the quantity of the products, dodecane (C<sub>12</sub>H<sub>26</sub>) was used as the internal standard. The response factors of each product are calculated based on Equation 3.5:

$$R_x = \left( \frac{m_{is}}{A_{is}} \right) \left( \frac{A_x}{m_x} \right) \quad (3.5)$$

Where

$R_x$  is response factor of reference substance x

$m_{is}$  is mass in g of internal standard

$m_x$  is mass in g of reference substance x

$A_x$  is peak area of reference substance x

$A_{is}$  is peak area of internal standard

The composition (yield) percentage of each product is calculated by Equation 3.6:



$$\text{wt.}\% = \left( \frac{1}{R_x} \right) \left( \frac{m_{is}}{A_{is}} \right) \left( \frac{A_x}{m_x} \right) \times 100 \quad (3.6)$$

where

wt.% is percentage of mass of component x in sample

$R_x$  is response factor of component x in sample

$m_{is}$  is mass in g of internal standard in sample

$m_x$  is mass in g of sample

$A_x$  is peak area of component x in sample

$A_{is}$  is peak area of internal standard in sample

The conversion percentage of the substrate and the selectivity percentage of the product in epoxidation reaction are calculated by Equations 3.7 and 3.8, respectively. Conversion of feed is defined as the weight ratio of cyclohexene converted to the initial cyclohexene, as shown in Equation 3.7. Selectivity is defined as the ratio of the number of weight of the products formation to cyclohexene converted, as shown in Equation 3.8.

$$\text{Cyclohexene conversion (\%)} = \frac{\text{cyclohexene converted (wt.\%)}}{\text{initial cyclohexene (wt.\%)}} \times 100 \quad (3.7)$$

$$\text{Selectivity of product i (\%)} = \frac{\text{product i produced (wt.\%)}}{\text{cyclohexene converted (wt.\%)}} \times 100 \quad (3.8)$$