# CHAPTER III
# METHODOLOGY

## 3.1 Materials and Equipment

3.1.1 Equipment

1. Laptop (Lenovo, Y580 ,Intel(R) Core(TM) i7-3630QM CPU @ 2.40GHz RAM 4.00 GB, Microsoft Office 2007)

3.1.2 Software

1) Aspen Plus (version 7.1)
2) Online Cost Estimator

## 3.2 Process Simulation Procedures

3.2.1 Literature Survey

1) Study and review the background, technical operation, feasibility and problems of the MEA-based post combustion $CO_2$ capture process.

2) Study the promising ILs used in $CO_2$ capture process (replacing conventional MEA-based process) by determining their $CO_2$ solubility, $CO_2$ selectivity, ease of regeneration, viscosity and cost of ILs.

3.2.2 Process Simulation

*3.2.2.1 Developing the MEA-based $CO_2$ Capture Process*

Build up MEA flow diagram by using electrolyte template in Aspen Plus. The ENRTL is used for a global thermodynamics model. The flowsheet consisting of absorber and stripper is modeled by using RADFRAC column. The design specifications in the simulation are as follows:

Vent $CO_2$: the absorber is designed to meet the specification of the vent gas with 90 % $CO_2$ recovery ($CO_2$ concentration is less than 1.0 vol. %). This specification can be achieved by varying the loading and mass flow rate of MEA.

Stripper Reflux Ratio: closed-loop simulation can be achieved when the composition between two streams (outlet from second heat exchanger next to desorber and inlet stream to the absorber) are equivalent. This is done by matching the loading (mol $CO_2$/mol MEA) of these two streams. Loading is defined as the ratio of $CO_2$ carrying species over MEA carrying species. After the specification of stripper column is set to strip off 90 % of $CO_2$, mass reflux ratio of stripper column is varied until the loading of stripper outlet and amine inlet stream are equivalent.

Cross-heat exchanger duty: at the starting of the simulation, the cross-heat exchanger is simulated as two separated heat exchangers. It is necessary to match the heat duties between two heat exchangers, so they can effectively function as a cross-heat exchanger. The approach temperature is also set to 5 °C.

Water and MEA balance: water and MEA balance is necessary in order to have the closed-loop convergence. For this purpose, the flow rate of the makeup water and MEA stream are varied to achieve an overall mass balance.

*3.2.2.2 Developing the IL-based $CO_2$ Capture Process*

When doing the simulation using Aspen Plus, the property parameters of selected components will be automatically retrieved. Since the databases of Aspen Plus do not provide any pure component data for [emim][Ac], the direct input information of its properties and data regression mode in Aspen Plus are essentially employed.

For the critical properties of ILs, the so-called group contribution method, "modified Lyndersen-Joback-Reid" method is used to estimate the critical properties of IL, since the ILs start to decompose at the temperature near their normal boiling point. For the temperature dependent properties, the parameters of five property models that are shown in Figure 3.1 are regressed based on the reported properties of [emim][Ac] available in the literature. The IL-based system involves the mixture system, which is composed of the solubility of gases in IL ($N_2$ and $CO_2$ in [emim][Ac]) and solubility of liquid in liquid ([emim][Ac] in water).

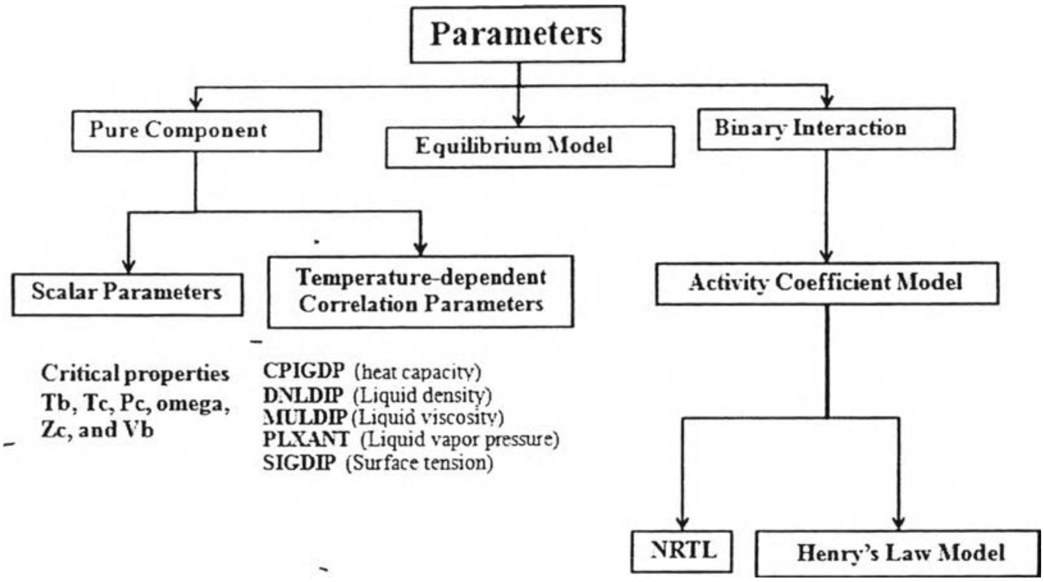


**Figure 3.1** Flowchart defining information about ionic liquid into Aspen Plus.

The binary interaction parameters of Non-Random Two Liquid (NRTL) are used to calculate the activity coefficient of the binary system ([emim][Ac] + water) and Henry's constant model is used to calculate the Henry's constant of $N_2$ and $CO_2$ soluble in [emim][Ac]. Both binary interaction parameters and parameters of Henry's constant model are taken from the regression of the experimental data (P-x diagram) available in the literature. The reaction data of [emim][Ac] with $CO_2$ are taken from the literature for equilibrium calculation. The accuracy of all parameters obtained from the data regression must be checked by using these parameters to calculate back for each property and then compare it with the experimental data. Based on all of these parameters, a process simulation of IL [emim][Ac] can be carried out to meet the same target of MEA-based process. IL flow diagram is similar to MEA flow diagram, but there is the difference in the regeneration section, by replacing the stripper column in the MEA to the flash tank in IL flow diagram (Aspen-RCSTR). Therefore, equilibrium model in the Aspen Plus is employed to calculate the reactions of [emim][Ac] in the reactor. IL flow diagram in this study is similar to the one used by (Shiflett *et al.*, 2010). The optimization of IL flow diagram is done by varying the absorber pressure and IL flow rate.

3.2.3 <u>The Capital Investment Cost Evaluation</u>

The steps of evaluation are as follows:

*3.2.3.1 Equipment Cost Estimation*

To estimate the equipment cost, a major equipment list was prepared and followed by quantity of equipment, type of equipment, material of construction and size of equipment into the program. Material of equipments is selected by the typical specification from the literature. Size parameters such as diameter, height and area are given from the simulation. After getting all the information, an online cost estimator (http://highered.mcgraw-hill.com) is used to calculate the cost of equipment.

*3.2.3.2 Capital Investment Cost Evaluation*

Capital investment cost is classified into two groups, fixed capital investment and working capital costs. Fixed capital investment cost is divided into manufacturing fixed-capital investment cost, or direct cost, and nonmanufacturing fixed-capital investment cost, or indirect cost. There are many methods to calculate the investment cost. In this study the percentage of delivered-equipment cost method is used. The cost of delivering the equipment is represents as a percentage of the delivered-equipment cost. The percentage of each element is shown in Table 3.1.

**Table 3.1** Total Capital Investment (TCI)

| Manufacturing Fixed-Capital Investment (Direct Cost) | Percentage |
|---|---|
| Purchased Equipment Delivered | 1.1 |
| Purchased Equipment Installation | 0.47 |
| Instrumentation and Controls (installed) | 0.36 |
| Piping (installed) | 0.68 |
| Electrical Systems (installed) | 0.11 |
| Buildings (Including Services) | 0.18 |
| Yard Improvement | 0.1 |

| Manufacturing Fixed-Capital Investment (Direct Cost) | Percentage |
|---|---|
| Service Facilities (installed) | 0.7 |
| Manufacturing Fixed-Capital Investment (Direct Cost) | 2.8 |
| **Nonmanufacturing Fixed-Capital Investment (Indirect Cost)** | |
| Engineering and Supervision | 0.33 |
| Construction Expenses | 0.41 |
| Legal Expenses | 0.04 |
| Contractor's Fees | 0.22 |
| Contingency | 0.44 |
| **Fixed-Capital Investment** | |
| Fixed-Capital Investment (FCI) | |
| **Working Capital Investment** | |
| Working Capital Investment (WC) | 0.89 |
| **Total Capital Investment (TCI)** | |

Another cost that needs to be accounted in the investment cost is cost of absorbent. In this study, MEA and IL price is on the basis of \$2.25/kg and \$20/kg, respectively. After finishing the investment cost evaluation, the costs of MEA and IL-based processes are compared to look at the potential of IL cost benefit.