CHAPTER III
METHODOLOGY

3.1 Materials and Equipment

3.1.1 Equipment

Laptop (Toshiba, Satellite ,Intel(R) Core(TM) i5-3210M CPU @ 2.50GHz RAM 8.00 GB, Microsoft Office 2012)

3.1.2 Software

Commercial Aspen Plus

3.2 Experimental Procedures

3.2.1 Literature Survey

First, study and review the background, technical operation, feasibility and problems of MEA, ammonia, and ionic liquid post combustion CO_2 capture system. Then, energy requirement in each system was optimized using heat-exchanger network (HEN). Finally, economic evaluation was investigated using commercial software Aspen Plus and cost factor published by Hassan *et al.* (2007)

3.3 Process Simulation

3.3.1 MEA Flow sheet Development

In this study, flue gas from 180 MW_e coal burning power plant with flue gas flow rate of 32 ton/hr, and a gas compositions of 84 % N_2, 12 % CO_2, and 4 % water vapor in standard volume (Khonkaen et al., 2014) was simulated in this flow sheet development. The MEA-based process was designed to capture CO_2 about 90 % by weight with 98 % purity from the flue gas by varying the MEA concentration from 15 to 30 wt. %. A simplified flow sheet development (absorber/stripper configuration) was shown in Figure 3.1.

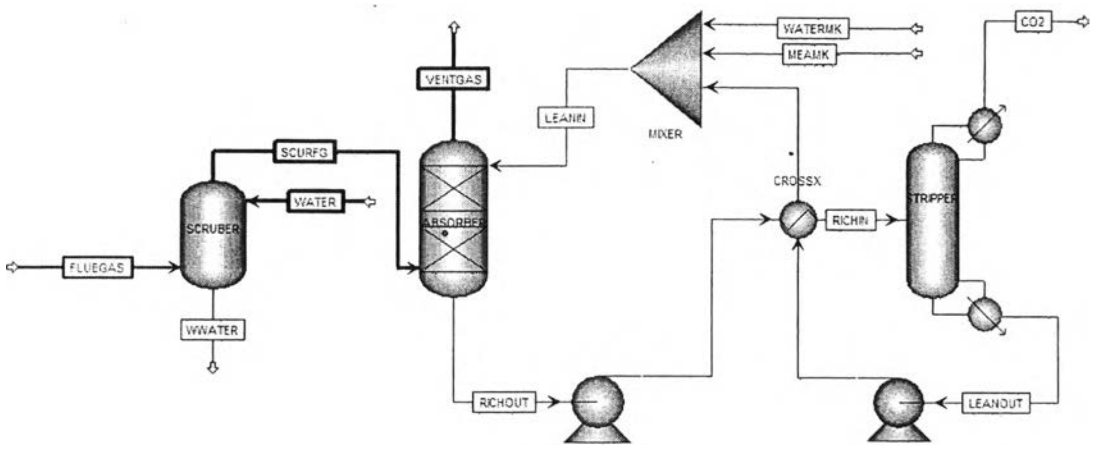

Figure 3.1 Simplified process flow diagram of MEA-based scrubbing system (Aspen plus).

The flue gas at high temperature from coal-fired power plant was cooled down to the pressure near atmospheric pressure in the scrubbing section by cooling water before entering the absorber. Then the scrubbed flue gas with CO_2 contacted the lean as counter-current flow to separate CO_2 out of the flue gas. Vented gas from the top of the absorber contains CO_2 less than 0.02 vol % which meets the environmental emission standards. Rich CO_2 in MEA solution was pumped and heated up before entering the stripper. Then, over 98.2 wt. % of CO_2 purity was stripped out at the top and regenerated MEA went out at the bottom of the stripper. MEA solution was recycled back to the absorber section in order to minimize MEA usage. MEA solution and make-up water were used to maintain the concentration and CO_2 lean loading of MEA solution. MEA flow sheet was simulated by using electrolyte template that already exists in Aspen Plus. The flow sheet was preliminary done in an open-loop simulation in order to converge flow sheet easily. However, the simulation would be capable to converge in the closed loop as well. The design specification in the simulation are shown in Table 3.1.

Table 3.1 Design specification of MEA flow sheet

Parameters	Range of value	Unit
MEA concentration	15-30	wt %
CO_2 lean loading	0.2-0.3	mole CO_2/mole MEA
Temperature of lean MEA stream	308	K
Absorber pressure	1	atm
CO_2 recovery	90	wt%
Stored CO_2 purity	98	wt%

3.3.2 Ammonia Flow sheet Development

Ammonia flow sheet was quite similar to the MEA flow sheet. The Redlich–Kwong equation of state and the Electrolyte-NRTL model were used to compute the properties of the vapour and liquid phases, respectively. Flue gas from a 180 MW_e coal burning power plant with a flow rate of 32 ton/hr, and a gas composition of 84% N_2, 12% CO_2, and 4% water vapor in standard volume (Khonkaen, 2014) was simulated in this study. A simplified flow sheet of aqueous ammonia-based scrubbing system is shown in Figure 3.2.

The flow sheet development was divided into two parts including the CO_2 capture system and the ammonia abatement system. The flow sheet was optimized by varying the concentration of ammonia solution in a range between 2 and 8 wt% and CO_2 lean loading of ammonia solution from 0.20 to 0.35 mole CO_2/mole NH3. Then, 98 % by weight of CO_2 purity entering storage section was specified by varying the reflux ratio (mass), absorption rate and liquid holdup in the stripping section. The ammonia abatement system was used to recycle the volatized ammonia and also minimize ammonia vent to the atmosphere due to restriction of environmental standards. Vented ammonia flow rate was kept below 2 kg per hour based on ammonia emission standards.

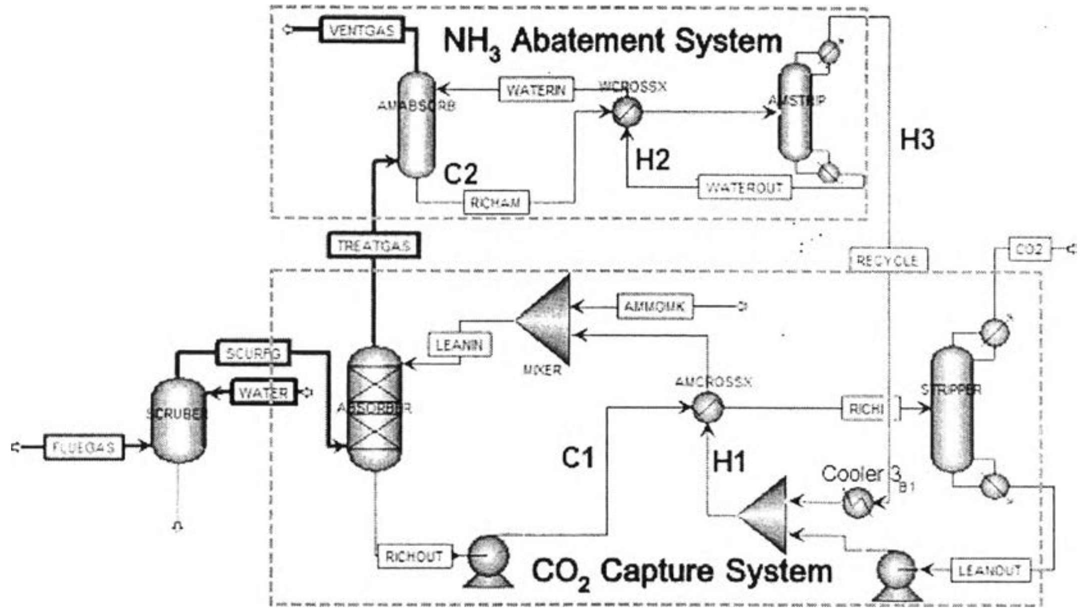

Figure 3.2 Simplified process flow diagram of aqueous ammonia-based scrubbing system (Aspen plus).

This limitation was set as the target of the absorber in the ammonia abatement system and achieved by varying aqueous ammonia concentration at the high loading. Obviously, a sequential optimization was observed (Zhang and Guo, 2013). The design specification in the simulation were shown in Table 3.2

Table 3.2 Design specification of aqueous ammonia flow sheet development

Parameters	Range of value	Unit
Ammonia concentration	4-8	wt %
CO_2 lean loading	0.2-0.3	Mole CO_2/mole NH_3
Temperature of lean NH_3 stream	298	K
Absorber pressure	1	atm
CO_2 recovery	90	wt%
Stored CO_2 purity	98	wt%

3.3.3 IL Flow sheet Development

The IL flow sheet is similar to MEA flow sheet, but it has different types of equipment in the regeneration section. Simplified flow sheet development of IL-based scrubbing system is present in Figure 3. Instead of the stripper column in the MEA process, a flash drum (RCSTR) is used in the IL flow sheet. Since the IL flow sheet does not exist in the Aspen Plus, the data base in Aspen Plus template needs some input such as some thermodynamic properties that accurately represent the solution used. The binary interaction parameters between IL and other components in the flue gas are regressed based on experimental data from relevant research papers.

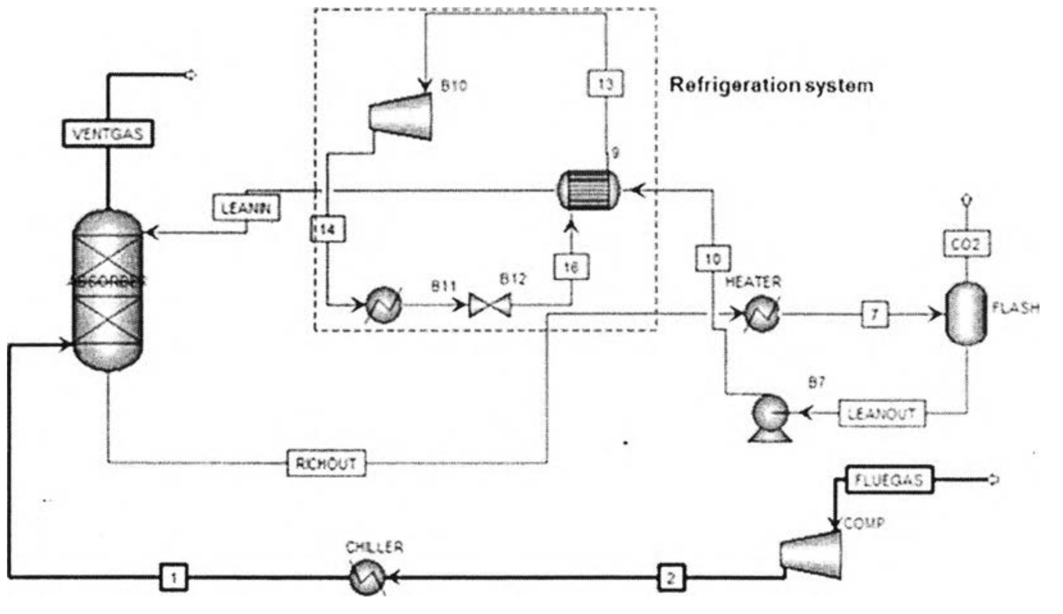

Figure 3.3 Simplified process flow diagram of IL-based scrubbing system (Aspen plus).

The NRTL is used as for a global thermodynamics model. After developing the IL flow sheet, the optimization will be done by determining the absorber pressure and solution circulation rate. The design specification in the simulation are shown in Table 3.3

Table 3.3 Design specification of IL (EmimAc) flow sheet development

Parameters	Range of value	Unit
Temperature of lean IL stream	271	K
Absorber pressure	6.8	atm
CO_2 recovery	90	wt%
Stored CO_2 purity	98	wt%

3.4 Process Heat Integration

Process heat integration is an important tool to reduce energy usage in the designed process and is performed using HEN method. Heat integration was performed using the GAMS program with a stage-wise model (Yee and Grossmann, 1990). HEN was used on the base-case processes which was the process without heat integration. GAMS program was run using a constant heat capacity mode. In order to ensure the data from GAMS, the validation between conceptual design (constant heat capacity mode) by GAMS and actual design (inconstant heat capacity mode) was neccessary.

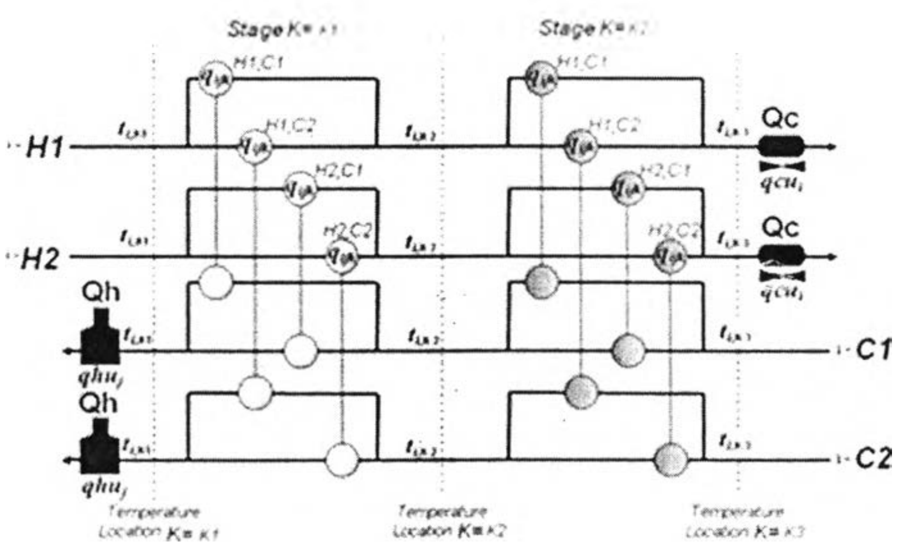

Figure 3.4 Stage-wise model for HEN (Yee and Grossmann, 1990).

3.5 Economic Evaluation

The economic analysis in this project consists of two parts; capital investments, and total production cost. The details of each part were described in follows Hassan *et al.*, (2007).

3.5.1 Capital Investment Cost

Capital investment can be divided into two categories namely direct and indirect costs.

3.5.1.1 Direct Costs

3.5.1.1.1 Purchased equipment

The cost of purchased equipment is the basis of estimating the capital investment. This includes all equipment listed on the complete flowsheet, spare parts and non-installed equipment spares, surplus equipment, supplies, equipment allowance, inflation cost allowance, freight charges, taxes, insurance, duties, and allowance for modification during startup. Sources of equipment prices, methods of adjusting equipment prices for capacity, and methods of estimating auxiliary process equipment are therefore essential to the estimator in making reliable cost estimates. This part is calculated by Aspen Process Economic Analyzer V8.4. The cost basis of the version are estimated in first quarter of 2013 and then converted in 2014 by chemical engineering plant cost index (CEPCI)(www.chemengonline.com).

3.5.1.1.2 Purchased-equipment installation

The installation of equipment involves costs for labor, foundations, structural supports, platforms, construction expenses, insulation, paint and other factors; directly related to the erection of purchased equipment. Depending upon the complexity of the equipment and type of the plant in which the equipment is installed, the installation costs for equipment are estimated from 25 to 55 percent of the purchased equipment cost.

3.5.1.1.3 Instrumentation and controls

This cost includes the costs for instrument, installation-labor, calibration, and expenses for auxiliary equipment and materials required for instrumentation. Total instrumentation costs depend on the amount of control required and may amount 6 to 30 percent of the purchased costs for all equipment. Depending on the complexity of the instruments and the service, additional charges for installation and accessories may amount to 50 to 70 percent of the purchased cost, with the installation charges being approximately equal to the cost for accessories.

3.5.1.1.4 Piping

The cost for piping covers the process pipe, labour, valves, pipe hangers, fittings, pipe, supports, insulation for piping and other items involved in the complete erection of all piping used directly in the process. This kind of cost can vary depending on the type of the chemical processes, which can be divided into solid process, solid-fluid process, and fluid process. The process plant piping can run as high as 80 percent of purchased equipment cost or 20 percent of fixed capital investment. Material and labour for pipe insulation is estimated to vary from 15 to 25 percent of the total installed cost of the piping.

3.5.1.1.5 Electrical installations

The electrical installation consists of four major components, namely, power wiring, lighting, transformation and services, and instrument and control wiring. The cost for electrical installations consists primarily of electrical equipment, materials and labor. In ordinary chemical plants, electrical installations cost amounts 10 to 15 percent of the value of all purchased equipment. The electrical installation cost is generally estimated between 3 to 10 percent of the fixed-capital investment. Building (including services) This cost consists of labour, materials, and supplies involved in all building connected to the plant.

3.5.1.1.6 Yard improvements

Yard improvement cost includes costs for fencing, site clearing, grading, road, walkways, railroad, fences, parking area, wharves and piers, and landscaping. Yard improvement cost for a chemical process is approximately 10 to 20 percent of the purchased equipment cost or 2 to 5 percent of the fixed capital investment.

3.5.1.1.7 Service facilities

Utilities for supplying steam, water, power, compressed air, and fuel are part of the service facilities of an industrial plant. Waste disposal, fire protection, and miscellaneous service items, such as shop, first aid, and cafeteria equipment and facilities, require capital investment, which are included under the general heading of service facilities cost. The total cost for service facilities in chemical plants generally ranges from 30 to 80 percent of the purchased equipment cost.

3.5.1.1.8 Land

The land cost for the plants is approximately 4 to 8 percent of the purchased equipment cost or 1 to 2 percent of the total capital investment.

3.5.1.2 Indirect Costs

3.5.1.2.1 Engineering and supervision

The cost for engineering and supervision includes the costs for construction design and engineering, drafting, purchasing, accounting, construction and cost engineering, travel, reproductions, communications, and home office expense. Generally, it is approximately 30 percent of the purchased equipment cost or 8 percent of the total direct costs of the process plant.

3.5.1.2.2 Construction expenses

The construction or field expense includes temporary construction and operation, construction tools and rentals, home office personnel located at the construction site, construction payroll, travel and living, taxes and insurance, and other construction overhead. For ordinary chemical plant, the construction expense is approximately 10 percent of the total direct cost of the plant.

3.5.1.2.3 Contractor's fee

The contractor's fee varies for different situations, but it can be estimated to be 2 to 8 percent of the direct plant cost or 1.5 to 6 percent of the fixed capital investment.

3.5.1.2.4 Contingency

Contingency factor is usually included in an estimate of capital investment to compensate for unpredictable events, such as storms, floods, strikes, price changes, small design changes, errors in estimation, and other unforeseen expenses. Contingency factor ranging from 5 to 15 percent of the direct and indirect plant costs are commonly used.

3.5.2 Estimation of Total Product Cost

Capital investment is only one part of a complete cost estimate. Another equally important part is the estimation of costs for operating the plant and selling the products which can be grouped under the heading of total product cost. This cost can be divided into two categories of manufacturing costs and general expenses. Manufacturing costs are also known as operating or production costs.

3.5.2.1 Manufacturing Costs

The manufacturing costs associated with all expenses directly connected with the manufacturing operation or the physical equipment of the process plant. These expenses can be divided into three classifications as given below.

3.5.2.1.1 Direct production cost

This cost includes the expenses directly associated with the manufacturing operation. These types of cost involve expenditures for:

i. Raw materials
ii. Operating labor
iii. Operating supervision
iv. Power and Utilities (Steam, electricity, fuel, refrigeration, and water)
v. Maintenance and repairs
vi. Operating supplies
vii. Laboratory charges

3.5.2.1.2 Fixed charges

Fixed charges are the expenses which do not vary with the change in production rate. They involve:

i. Depreciation
ii. Property taxes
iii. Insurance
iv. Rent

3.5.2.1.3 Plant overhead costs

These costs are similar to the fixed charges in that they do not vary with the change of the production rate. They consist of:

i. Medical expenses
ii. Safety and protection
iii. General plant overhead
iv. Payroll overhead
v. Packaging
vi. Restaurant
vii. Recreation
viii. Salvage
ix. Control laboratories
x. Plant superintendence
xi. Storage facilities

3.5.2.2 General Expenses

In addition to the manufacturing cost, the general expenses are involved in every plant's operation. The general expenses may be classified as:

i. Administrative expenses include costs for executive and clerical wages, office supplies, engineering and legal expenses, upkeep on office buildings, and general communications.
ii. Distribution and marketing expenses are costs incurred in the process of selling and distributing the various products. These costs include expenditure for materials handling, containers, shipping, sales offices, sales man, technical sale services and advertising.
iii. Research and development expenses are the costs for any progressive concern which wishes to remain in a competitive industrial position.

iv. Financing (interest) expenses include the extra costs involved in procuring the money necessary for the capital investments.

Table 3.4 Total Capital Investment (TCI) Summary table of economic evaluation factor (Hassan *et al.*, 2007)

Manufacturing Fixed-Capital Investment (Direct Cost)	**Fraction of Purchased Equipment Cost for Fluid Processing Plant**
Purchased Equipment Installation	0.25-0.55
Instrumentation and Controls (installed)	0.06-0.3
Additional charges for installation and accessories	0.5-0.7
Piping (installed)	0.8
Material and labor for pipe insulation	0.12-0.2
Electrical installations	0.1-0.15
Yard Improvement	0.1-0.2
Service Facilities (installed)	0.3-0.8
Land	0.04-0.08
Non-Manufacturing Fixed-Capital Investment (Indirect Cost)	**Fraction of Direct Cost for Fluid Processing Plant**
Engineering and Supervision	0.08
Construction Expenses	0.1
Contractor's Fees	0.02-0.08