CHAPTER III
PROCEDURES

3.1 Modeling of Gas Separation Process

The important step in HEN design is data extraction. In this work, the design data of PTT gas separation plant I was used for the analysis. Unfortunately, some of the important data, for example, enthalpy, heat capacity, is not available. To fill the missing data, the simulation is employed. Before doing the simulation, the process model has to be set up. In this work, the steps in process modeling are:

1) Collect the data for using in process modeling which include the operating condition for each unit operation; the stream data such as flow rate, composition, temperature and pressure; and the connectivity of the streams to the unit operation as appears in the process flow-sheet.

2) Construct a model representing the plant, by using commercial process simulation program, Aspen Plus.

3) Input the data of feed streams and unit operations and then run the simulation. Compare the results with the design data to check the validity of the model.

Gas Separation Plant I (GSP I) of PTT Public Company Limited was chosen for the study. The main unit operations of this process are demethanizer, deethanizer and depropanizer column. The functions of each unit operations are as follows:

Demethanizer: The first unit in the fractionating sequence to separate the methane out of natural gas, with methane leaving at overhead and ethane and the heavier components leaving at the bottom of the fractionators.

Deethanizer: The second unit in the processing sequence to separate ethane out of the demethanizer bottom stream, with ethane leaving at overhead and propane and the heavier components leaving at the bottom of the deethanizer.

Depropanizer: The last fractionation unit to separate propane from butane and the heavier components. Propane leave at overhead and butane and the heavier components leave from the bottom of the fractionator as natural gasoline. It has a side-drawn stream for producing Liquefied Petroleum Gas (LPG), as well.

The process flow diagram of GSP I is illustrated in Figure 3.1. The demethanizer column was designed to use chimney tray, which does not allow the liquid to flow through them. Three chimney trays are installed in this column at stage 15, 20 and 29. Therefore, the model of this column has to be modeled by using four distillation columns connected in series. The schematic diagram for the demethanizer model is shown in Figure 3.2.

For the deethanizer column and depropanizer column, the conventional distillation columns are used for modeling these two columns as shown in Figure 3.3 and 3.4, respectively. The Peng-Robinson property package is chosen for this simulation. This package is suitable for gas separation process as recommended by Aspen Plus user guide.

3.1.1 Distillation column modeling

Distillation column modeling was done by using RADFRAC model of Aspen Plus simulator. In modeling, the column specification; tray efficiency, condenser and reboiler duties were calculated in order to match the simulation values with the design values. The product specifications for design case are shown in Table 3.1.

3.1.2 Overall process modeling

Process model was designed to integrate with other unit operations such as shell and tube heat exchangers, LNG heat exchangers, flash drums and compressors with expanders. This aims to construct the model that represent the existing plant and reach the desired product quality and temperature.

3.2 Pinch analysis

There are five main steps for doing Pinch Analysis

1. Predicting minimum energy consumption
2. Design Heat Exchanger Networks
3. Changing process to save energy
4. State of the art improvement
5. Overall retrofit strategy

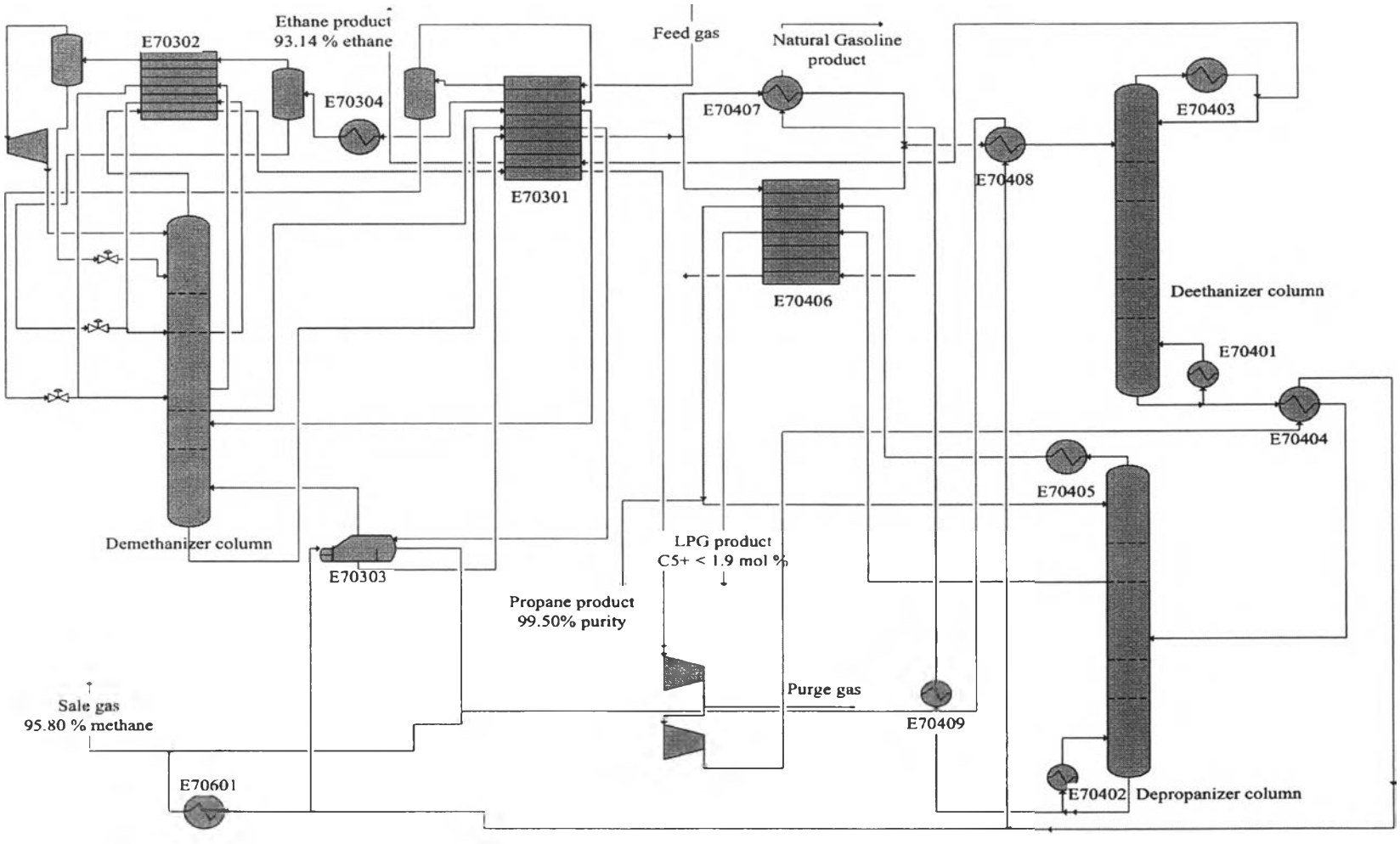

Figure 3.1 Process flow diagram of Gas Separation Plant Unit I.

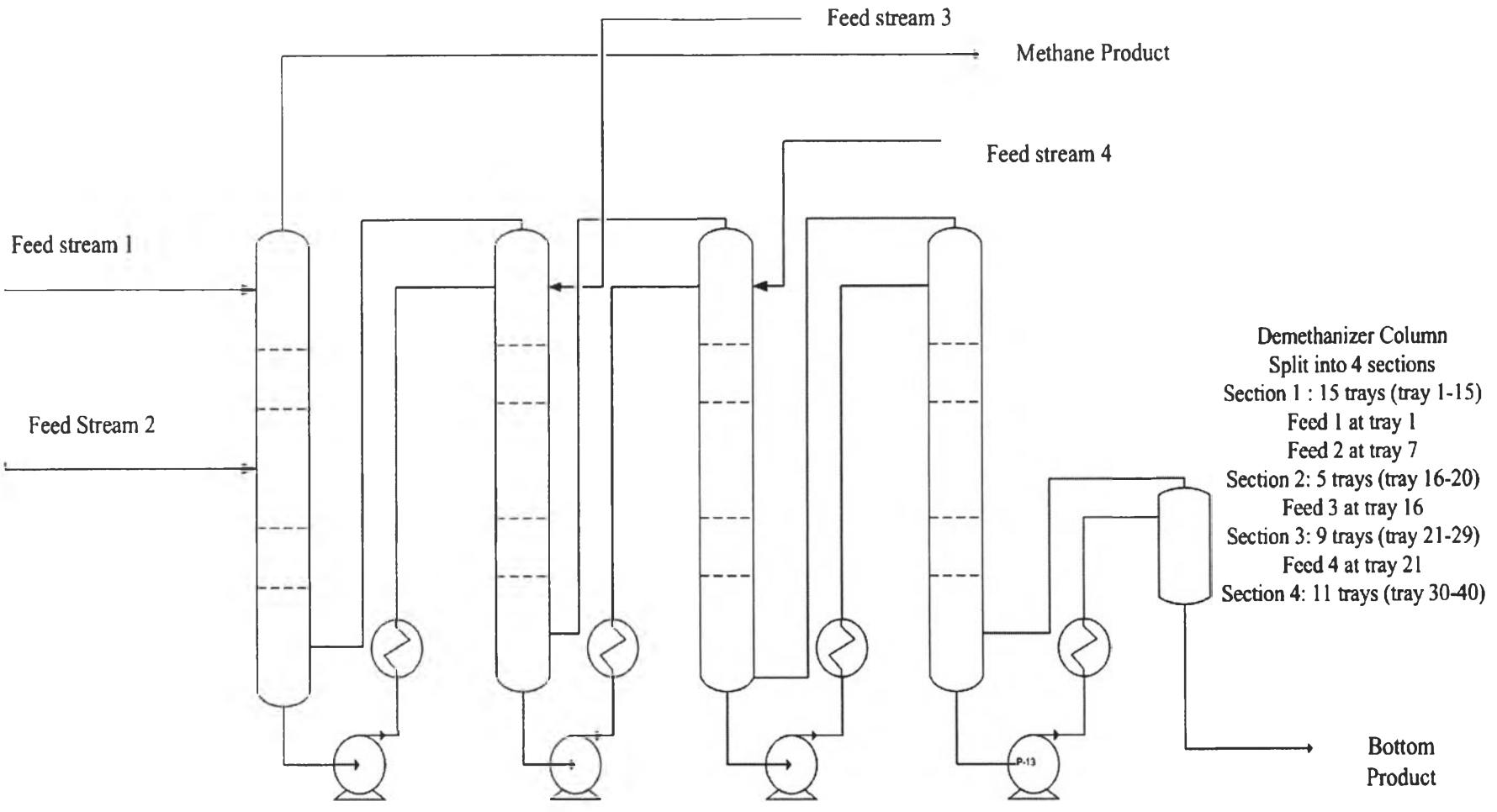

Figure 3.2 Schematic diagram of demethanizer column.

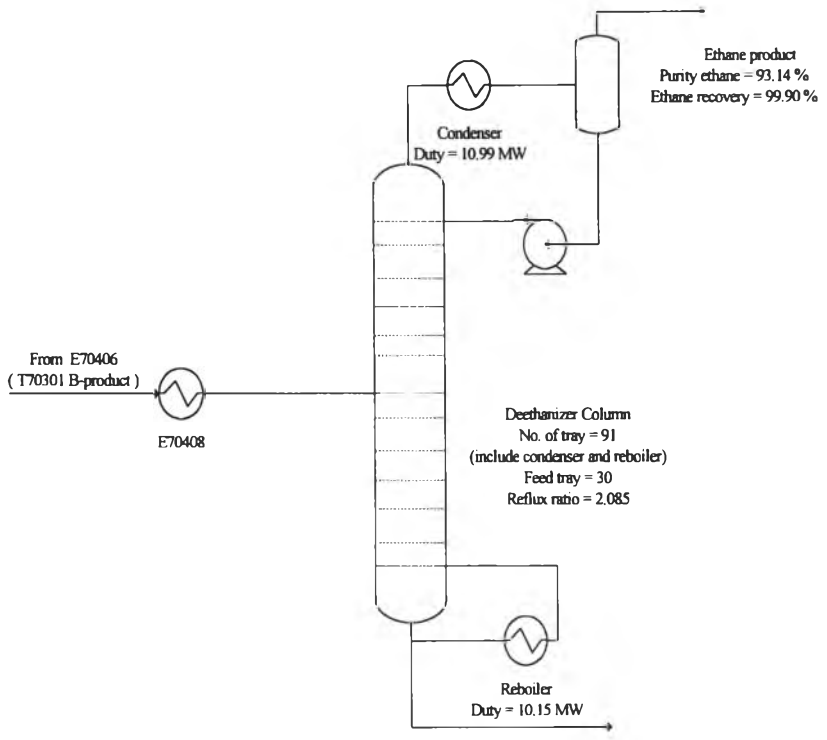

Figure 3.3 Schematic diagram of deethanizer column.

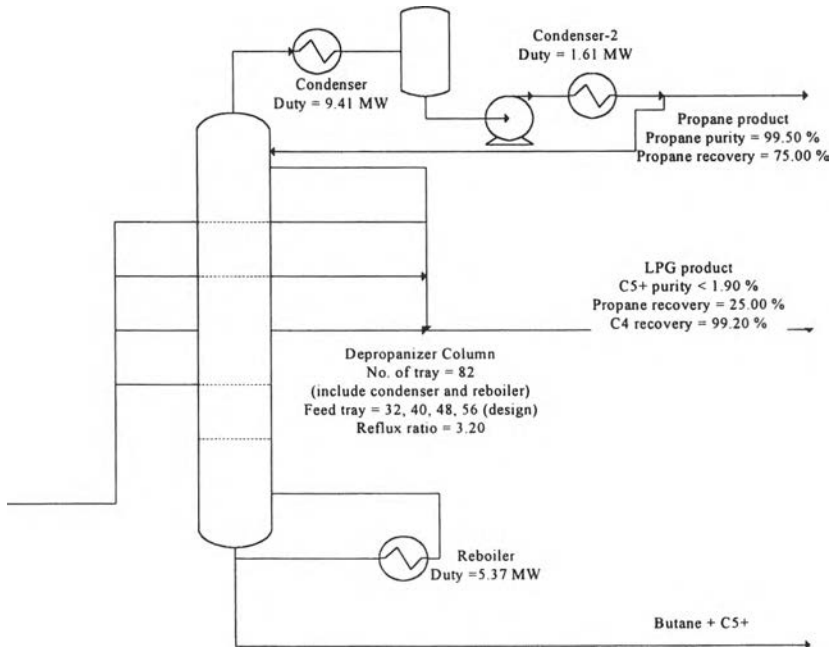

Figure 3.4 Schematic of depropanizer column.

Table 3.1 Product stream composition and flow rate of the design data

Component (mole fraction)	Methane product	Ethane Product	Propane product	LPG product
N_2	0.020	0.000	0.000	0.000
CH_4	0.957	0.019	0.000	0.000
C_2H_6	0.019	0.931	0.002	0.000
C_3H_8	0.000	0.015	0.995	0.362
i-C_4H_{10}	0.000	0.000	0.003	0.336
n-C_4H_{10}	0.000	0.000	0.000	0.295
i-C_5H_{12}	0.000	0.000	0.000	0.005
n-C_5H_{12}	0.000	0.000	0.000	0.001
n-C_6H_{14}	0.000	0.000	0.000	0.000
C 7 plus	0.000	0.000	0.000	0.000
CO_2	0.004	0.035	0.000	0.000
Flow rate (Mol/sec)	3395.156	402.680	172.760	158.141
Temperature (K)	171.590	273.300	300.000	349.710
Pressure (barg)	15.000	27.700	16.500	16.500

In this work, the algorithm for doing pinch analysis is shown in Figure 3.5. The detail of each step is explained as follows:

3.2.1 Stand-alone Column Modifications

Since column modifications have an impact on the process conditions. Thus, in order to obtain the correct results from pinch analysis, the column modification should be done before the pinch analysis.

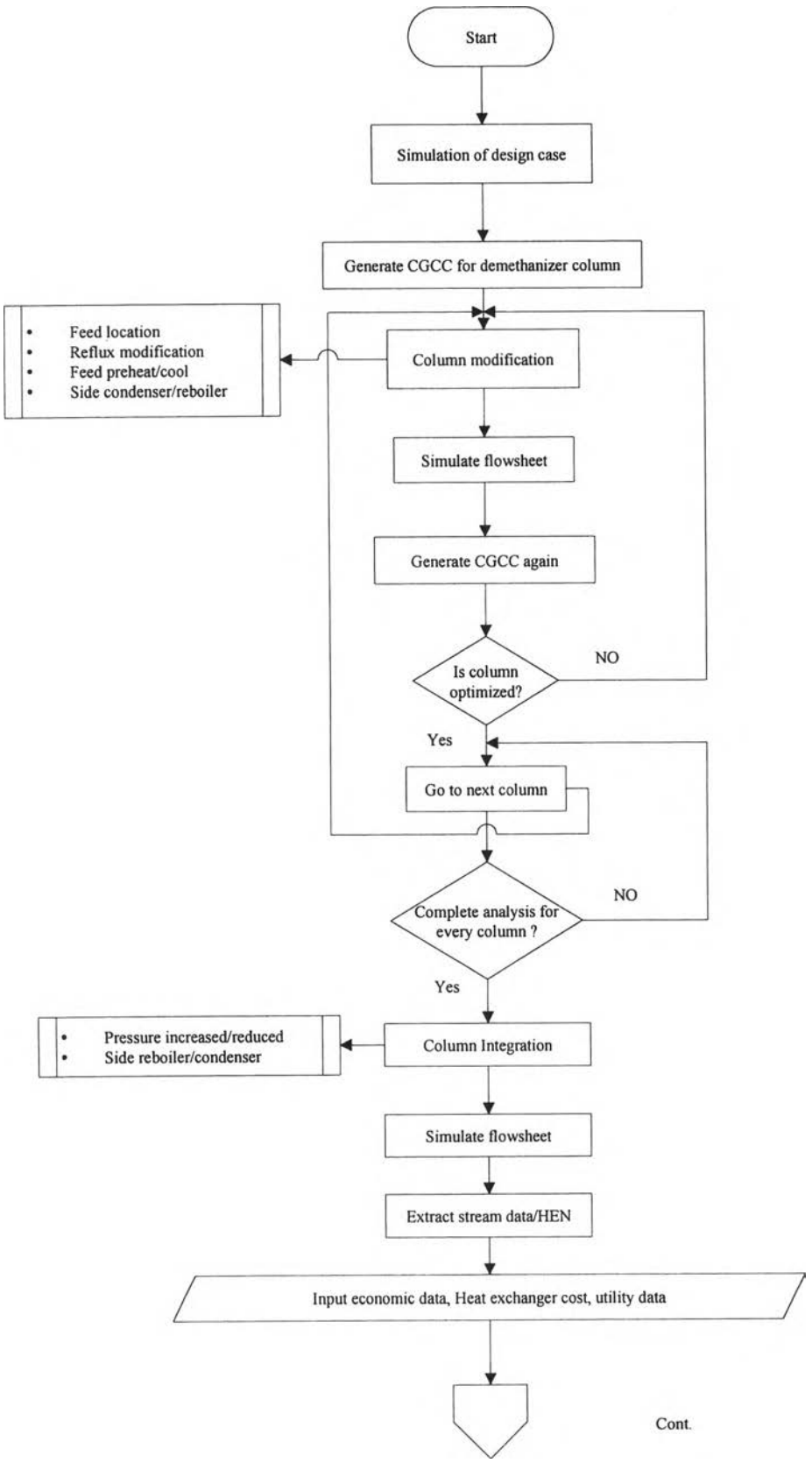

Figure 3.5 Flow-diagram for pinch analysis.

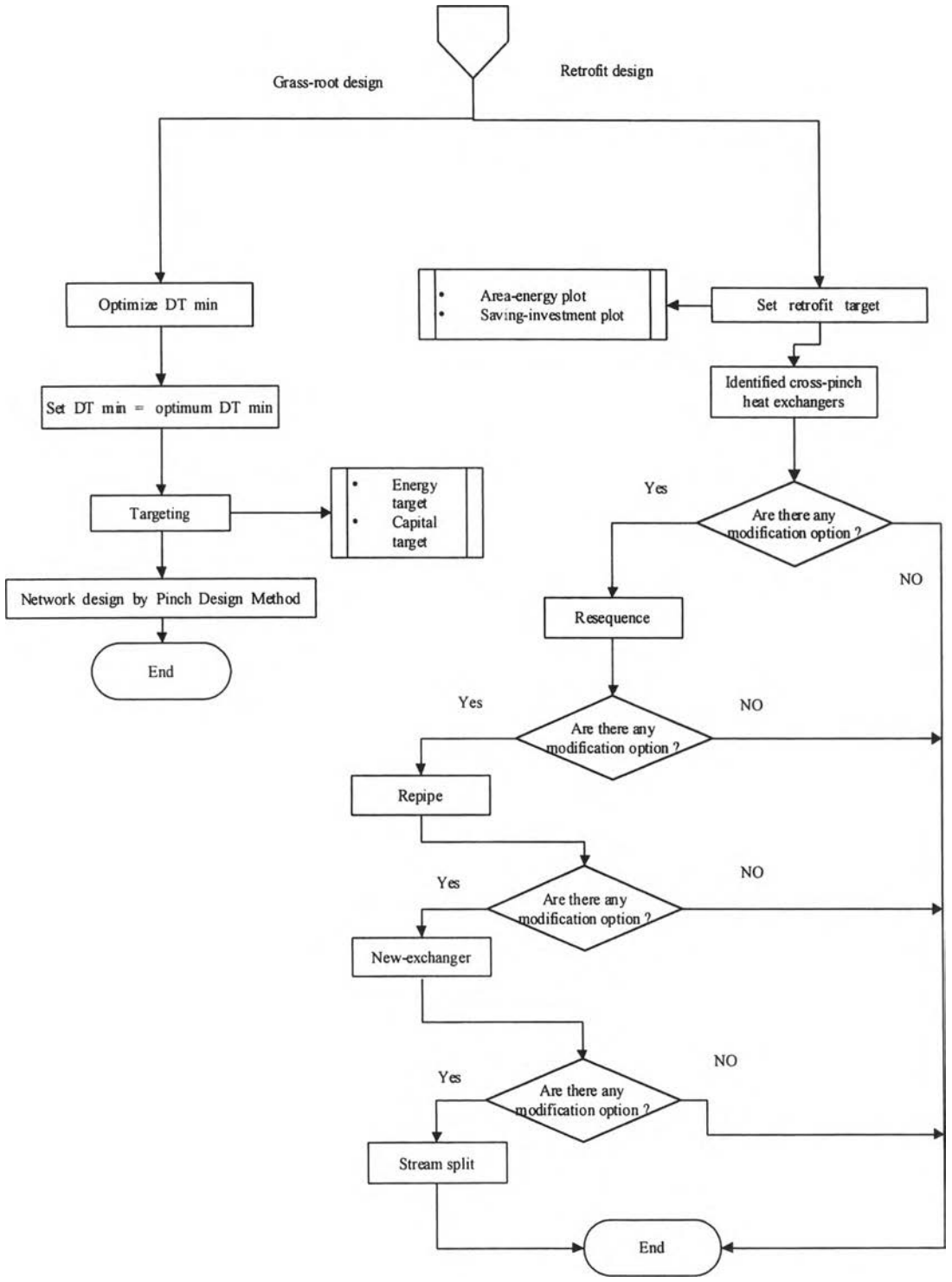

Figure 3.5 (Continued) Flow-diagram for pinch analysis.

The CGCCs of three distillation columns were generated by using Aspen Plus steady-state simulation. Aspen Plus generated CGCCs based on the Practical Near Minimum Thermodynamic Condition (PNMTC) approach (Dhole and Linnhoff, 1993). The resulting CGCCs were validated by comparing their condenser and reboiler duties with the values from simulation. The difference between these values should not be greater than 5 percent. After the CGCCs were validated, the stand-alone column modifications were done. The column modifications were implemented follows the guidelines (Dhole and Linnhoff, 1993).

3.2.2 Column integration

After the stand-alone column modifications were completed. Next step, the energy saving opportunity would then be investigated by column integration. The CGCC for each column was plotted together on the same temperature-enthalpy (T-H) diagram. The CGCCs were then used as a tool for identifying the potential for column integration. Increasing or decreasing column operating pressure and side condensing/reboiling were employed in order to enhance the column integration opportunity.

3.2.3 Process heat integration

The data for background process streams will be used to generate the GCC for a specified ΔT_{min}. The value of ΔT_{min} used in this work will be obtained after optimization over a range of ΔT_{min} as described in section 3.2.4.1. The value of optimum ΔT_{min} will be used to generate GCC. The optimization and generation of GCC will be done with Aspen Pinch program. The energy saving opportunity was investigated more by integrating distillation columns with the background process. As described in Chapter II, the appropriate placement of distillation columns must lie in either above or below the pinch temperature of background process. Again, three CGCCs are plotted together with grand composite curve of the background process to see the potential for heat integration between process and distillation columns.

After column modifications and integration were completed. The process condition was optimized. Therefore, the data extraction was done in the next step. In this work, the pinch analysis was done by using Aspen Pinch program. The data required for supplying the Aspen Pinch program are

1) Streams and Heat exchanger network data.
2) Heat transfer coefficient for each streams
3) Utility and economic data

3.2.4.1 Streams and Heat Exchanger Network Data

Once the column modifications and integration had been completed, the operating conditions of streams and heat exchanger network data were known. Aspen Pinch program provides a powerful interface between the Aspen Plus simulator and Aspen Pinch to import the streams and heat exchanger network data. Data transfer was done by selecting File/Import/Aspen Plus on Aspen Pinch menu bar.

3.2.4.2 Stream heat transfer coefficient

Heat transfer coefficient is another important data supplied to the Aspen Pinch program. The values are calculated based on the correlation and heat exchanger geometry (Seider *et al.*, 1999). The correlation for the heat transfer coefficient calculation is shown below:

For shell side without phase change, heat transfer coefficient can be calculated by Donohue equation as shown in equation 3.1.

$$Nu=\left(\frac{hD_o}{k}\right)=0.33\left(\frac{D_o v\rho}{\mu}\right)^{0.6}\left(\frac{C_p\mu}{k}\right)^{\frac{1}{3}} \qquad (3.1)$$

For tube side, Colburn equation as shown in equation 3.2 is used to calculate this value.

$$Nu = \left(\frac{hD_i}{k}\right) = 0.023\left(\frac{D_i v\rho}{\mu}\right)^{0.8}\left(\frac{C_p\mu}{k}\right)^{\frac{1}{3}} \qquad (3.2)$$

where,

Nu = Nusselt number

h = heat transfer coefficient

D_o = outside diameter of tube

D_i = inside diameter of tube

k = thermal conductivity of tube

ρ = fluid density

μ = fluid viscosity

C_p = heat capacity of fluid

3.2.4.3 Utility and Economic Data

The utility data is the next required input to the program. In this work, the utility data and their associated cost are summarized in Table 3.2.

Table 3.2 Utility data for GSP I

Utility	Type	Inlet Temp (K)	Outlet Temp (K)	h (W/m^2-K)	Price (US$/unit)	Unit
Refrigerant	Cold	230.95	230.95	2029.31	0.0355	kW-hr
CW*	Cold	308.15	318.15	499.22	0.0060	m^3
MPS†	Hot	478.15	478.15	15000.00	8.0000	Ton
LPS‡	Hot	416.15	416.15	7500.00	6.5000	Ton

* Cooling Water

† Medium Pressure Steam

‡ Low Pressure Steam

The economic data is used for conducting an economic analysis for the retrofit project. The economic data using in this work is summarized in Table 3.3.

Table 3.3 Economic data for GSP I

Economic parameter	Value
Hours on streams (hours/year)	8000
Plant lifetime (years)	10
Interest rate (%)	15
Required rate of return (%)	15
Payback time (years)	2

The heat exchanger cost is also an important parameter in calculating the capital cost of the project. In this work the cost equation for carbon steel, shell and tube heat exchanger in equation 3.3 was used (Polley and Haslego, 2002).

$$C = 7600 + 140\ A^{0.6} \tag{3.3}$$

where,

C = purchase cost of heat exchanger (US$)

A = heat exchanger surface area (m^2)

The installation factor of 3.5 is used in this work.

3.2.5 Grass-root Heat Exchanger Network Design

Heat exchanger network design was done on a grass-root basis first. The grass-root heat exchanger network would be the best network for a set of process streams. The steps in grass-root heat exchanger network design are as follows:

3.2.5.1 Optimization of ΔT_{min}

The value of minimum temperature difference (ΔT_{min}) is very important in pinch analysis. As described in Chapter II, the lower the value ΔT_{min},

the lower energy consumption, however, the capital investment is increased, as shown in Figure 3.6. Therefore, the value of ΔT_{min} should be optimized before performing heat exchanger network analysis. The optimization was done by calculating the operating cost (from energy targeting) and capital cost over a range of ΔT_{min}. The value of ΔT_{min} that produced the optimum network, i.e. lowest total cost, would be chosen for pinch analysis.

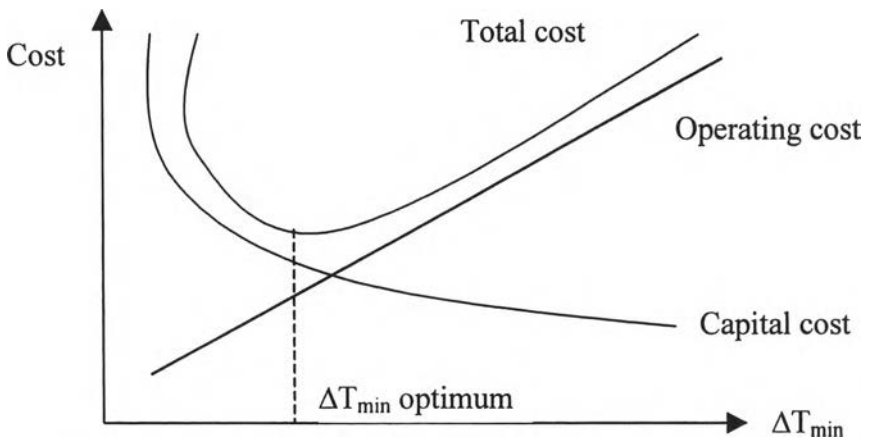

Figure 3.6 Optimization of ΔT_{min} by minimizing total cost.
(Linnhoff and Hindmarsh, 1983)

3.2.5.2 Setting performance targets

After the optimum value of ΔT_{min} was obtained, the performance targets were set. The targets involve energy and capital target. The energy target was set by generating composite curve for predicting minimum energy consumption of the process. The capital target was set by determining the minimum number of units and surface area required for heat exchanger network. These values were put into heat exchanger cost equation in order to estimate the required capital investment for heat exchanger network.

3.2.5.3 Heat exchanger network design

After the targeting stage was completed, the next step was the heat exchanger network design. In Aspen Pinch, the network design will be done on a grid diagram. To activate the network design window, select Tools on menu bar and select Network design. The corresponding grid diagram for the process will be shown. In that window the heat exchangers, multi-stream heat exchangers can be inserted into the network. For the retrofit, the cross-pinch heat exchanger will be identified in the grid diagram and then modified to minimize the cross-pinch heat transfer. After the network design in grid diagram is completed, the simulation will be implemented to see the effect of process changing.

3.2.6 Heat exchanger network retrofits

The heat exchanger network retrofit is unlike the grass-root design. Since the heat exchangers have been invested into the process, therefore, the retrofit project would involve the enhancement of network performance for the existing units. The steps in retrofit heat exchanger network design are as follows:

3.2.6.1 Retrofit targeting

The Aspen Pinch can help the user to set the retrofit target by using the area efficiency approach (Tjoe and Linnhoff, 1986). The area/energy plot as well as Saving/Investment plot was generated. By setting the payback time, the energy saving opportunity and its corresponding investment and ΔT_{min} will be identified.

3.2.6.2 Heat exchanger network modifications

After the saving opportunity was identified, the existing heat exchanger network would be modified to achieve the target. The step starts with generating a grid diagram for base case process at a value of ΔT_{min} obtained from the previous step. The network was investigated for cross-pinch heat exchangers. If there were cross-pinch heat exchangers, the process modification would be implemented to minimize the cross-pinch heat transfer.

3.3 Second law efficiency calculation

The reference state is one of the most important factors in exergy analysis. In this work, the reference state in exergy calculation was set based on the recommendation of Szargut *et al.* (1988), which are 298.15 K and 101.325 kPa for reference temperature and pressure, respectively.

The stream exergy composes of two exergy types. One is thermal exergy and the other is chemical exergy.

The thermal exergy can be calculated by using Equation 3.4 (Szargut *et al.*, 1988):

$$\psi = (h-h_o) + T_o(s-s_o) \qquad (3.4)$$

where ψ = stream thermal exergy

h = specific enthalpy at T, P

h_o = specific enthalpy at T_o, P_o

T_o = reference temperature (298.15 K)

s = specific entropy at T, P

s_o = specific entropy at T_o, P_o

P_o = reference pressure (101.325 kPa)

The chemical exergy can be calculated using a molar average of chemical exergy for each component. The chemical exergy at any state is assumed to be the same as the standard chemical exergy. This assumption is valid for the process in the absence of chemical reaction. The standard chemical exergy for each component in GSP I is shown in Table 3.4

Therefore, the stream exergy is calculated by summing the thermal and chemical exergy at the temperature and pressure of stream as shown in Equation 3.5 (Szargut *et al.*, 1988).

$$\text{Stream exergy} = \text{thermal exergy} + \text{chemical exergy} \qquad (3.5)$$

Table 3.4 Standard chemical exergy for chemical substances in GSP I (Szargut *et al.*, 1988)

Component	Standard chemical exergy (kJ/mol)
Nitrogen	0.720
Methane	831.650
Ethane	1495.840
Propane	2154.000
iso-butane	2711.540
n-butane	2805.000
iso-pentane	3369.840
n-pentane	3463.300
n-hexane	4118.500
n-heptane	4761.700
n-octane	5413.100
n-nonane	6064.900
n-decane	6716.800
Carbon dioxide	19.870
Propylene	2003.900

The process will be checked for the thermal efficiency by using the second law efficiency. The second law efficiency (η) is defined in Equation 3.6 (Szargut *et al.*, 1988).

$$\eta = \frac{\text{W useful}}{\text{W supply}} \times 100\ \% \qquad (3.6)$$

where

W useful = useful work (W)

W supply = shaft work supply to the process (W)

Useful work (W useful) can be calculated by the difference in the exergy of the product streams and feed streams. The supplied work can be calculated by adding the useful work with the summation of loss work from all equipment. Equipment loss work is determined from the exergy balance as shown in Equation 3.7 (Szargut *et al.*, 1988).

$$LW = \sum_{\text{products}} \psi - \sum_{\text{feeds}} \psi - \sum_{\text{net}} Q\left(1 - \frac{T_o}{T}\right) - \sum_{\text{net}} W_s \qquad (3.7)$$

where

LW = loss work (W)

ψ = stream exergy (W)

Q = amount of heat transfer from (to) heat reservoir (sink) (W)

T = absolute temperature of heat reservoir (sink) (K)

W_s = Shaft work. (W)

For heat exchangers, the exergy loss is calculated by Equation 3.8 (Szargut *et al.*, 1988).

$$\text{Exergy loss} = Q\left[\frac{T_{hm} - T_{cm}}{T_{hm} T_{cm}}\right] + RT_o\left[n_h \ln\left(\frac{p_{in,h}}{p_{in,h} - \Delta p_h}\right) + n_c \ln\left(\frac{p_{in,c}}{p_{in,c} - \Delta p_c}\right)\right] \qquad (3.8)$$

where

$\dot{Q}$ = Amount of heat exchanged

T_{hm} = Mean thermodynamic hot temperature

$$= \frac{h_{h,in} - h_{h,out}}{s_{h,in} - s_{h,out}}$$

T_{cm} = Mean thermodynamic cold temperature

$$= \frac{h_{c,in} - h_{c,out}}{s_{c,in} - s_{c,out}}$$

R = Gas constant

T_o = Standard temperature (298.15 K)

n_h = mole flowrate of hot stream

n_c = mole flowrate of cold stream

$p_{in,\,h}$ = inlet pressure of hot side

Δp_h = pressure drop of hot side

$p_{in,c}$ = inlet pressure of cold side

Δp_c = pressure drop of cold side

The second law efficiency will be calculated twice. The first calculation is done before modification for the existing performance. The other calculation will be done after modification to see the improvement in thermal performance.