

Superstructure Optimization Approach for Optimal Design of a Petroleum Refinery Topology with Heat Integration

by

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(9448)

Dissertation submitted in partial fulfilment of
the requirements for the
Bachelor of Engineering (Hons)
(Chemical Engineering)

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CERTIFICATION OF APPROVAL

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A project dissertation submitted to the
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Approved by,

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July 2010

CERTIFICATION OF ORIGINALITY

This is to certify that I am responsible for the work submitted in this project, that the original work is my own except as specified in the references and acknowledgements, and that the original work contained herein have not been undertaken or done by unspecified sources or persons.

SITI SAHIRAH NOORDIN

ABSTRACT

Designing petroleum refineries that satisfies multiple economics, operations, and environmental constraints is a highly complex task. The objective of this project is to obtain a mathematically viable model to determine the optimal topology for a petroleum refinery with incorporation of heat integration. Naphtha produced exiting from Atmospheric Distillation Unit (ADU) is chosen as the superstructure, meanwhile Expanded Linear Programming (LP) Transshipment Model and Mix-Integer Linear Programming (MILP) Transshipment Model are used as the energy constraints subsequently with linear yield-based material balances to generate the optimal refinery topology with its associated optimal design parameters that achieve the maximum profit and least energy consumption. Implementing heat integration features in a refinery design model will enable us to achieve an optimal topology that incorporates the best alternatives that offers minimum operating cost in terms of minimum utility cost as well as minimum capital cost.

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LIST OF NOTATIONS AND ABBREVIATIONS

i	hot process stream
j	cold process stream
k	temperature interval
m	hot utility
n	cold utility
H_k	{ i hot stream i supplies heat to interval k }
C_k	{ j cold stream j demands heat from interval k }
S_k	{ m hot utility m supplies heat to interval k }, (S indicates steam as a representative hot utility)
W_k	{ n cold utility n extracts heat from interval k } (W indicates cooling water as a representative cold utility)
H'_k	{ i hot stream i present at interval k or at higher interval}
S'_k	{ m hot stream m present at interval k or at higher interval}
Q_n^W	heat load of cold utility n
Q_m^S	heat load of hot utility m
$Q_{i,k}^H, Q_{i,k}^C$	heat content of hot stream i and cold stream j in interval k
c_m	cost coefficient for hot utility m
c_n	cost coefficient for cold utility n
$U_{i,j}$	upper bound for maximum heat exchange between hot stream i and cold stream j
CP_i	heat capacities for hot streams
$Q_{i,j,k}$	exchange of heat of hot stream i and cold stream j at interval k ,
$Q_{m,j,k}$	cold process stream
$Q_{i,n,k}$	exchange of heat of hot stream i and cold utility n at interval k
$R_{i,k}$	heat residual of hot stream i exiting interval k
$R_{m,k}$	heat residual of hot utility m exiting interval k
$y_{i,j,q}$	hot stream i and cold stream j exchange heat at subnetwork q
T_{in}	inlet temperatures
T_{out}	outlet temperatures
f_1	heat capacity flowrate C1
$t_{1,in}, t_{1,out}$	inlet and outlet temperatures for stream C1
f_2	heat capacity flowrate C2
$t_{2,in}, t_{2,out}$	inlet and outlet temperatures for stream C2
$c_1, c_2, \text{ and } \beta$	cost parameters.
$U_{1,1}, U_{1,2}$	overall heat transfer coefficients for the two exchangers.
HP	hot streams, represented by index i
CP	cold streams, represented by index j
HU, CU	correspond to the heating and cooling duties
F	heat capacity flow rate,
CCU	unit cost for cold utility,
CF	fixed charge for exchangers,
$C_{i,CU}$	area cost coefficient for heat coolers,
β	exponent for area cost,

Ω	upper bound for heat exchange,
U	overall heat transfer coefficient,
CHU	unit cost for hot utility,
$C_{i,j}$	area cost coefficient for heat exchangers,
$C_{HU,j}$	area cost coefficient for heaters,
NOK	total number of stages,
Γ	upper bound for temperature difference
$dt_{i,j,k}$	temperature approach for match (i,j) at temperature location k ,
$dtcu_i$	temperature approach for the match of hot stream i and cold utility,
$dthu_i$	temperature approach for the match of cold stream j and hot utility,
$q_{i,j,k}$	heat exchanged between hot process stream i and cold process stream j in stage k ,
qcu_i	heat exchanged between hot stream i and cold utility,
qhu_j	heat exchanged between hot utility and cold stream j ,
$t_{i,k}$	temperature of hot stream i at hot end of stage k ,
$t_{j,k}$	temperature of cold stream j at hot end of stage k ,
$z_{i,j,k}$	binary variable to denote existence of match (i,j) in stage k ,
zcu_i	binary variable to denote that cold utility exchanges heat with stream i ,
zhu_j	binary variable to denote that hot utility exchanges heat with stream j .

CHAPTER 1

INTRODUCTION

1.1 BACKGROUND OF STUDY

Process synthesis can be defined as the selection, arrangement and operation of processing unit so as to create optimal scheme. This task is combinatorial and open-ended in nature and has received great deal of attention over past 20 years. In order to formulate the synthesis problem as mathematical problem, a superstructure must be postulated which include many alternative designs from which the optimal process will be selected. The superstructure has proved an effective tool for the synthesis of chemical-engineering process flowsheets. In this way, unit operations, process streams, utility units, and utility streams can be embedded in such a way that all the process synthesis alternatives can be realized.

In process synthesis, there are two major approaches to determine the optimal configuration of a flowsheet and its operating condition. First approach, the problem can be solved in sequential form, by decomposition, fixing some elements in the flowsheet, and then using heuristic rules to determine changes in the flowsheet that may lead to an improved solution. The heuristic and evolutionary approach and thermodynamic targets and physical insight approach are purely driven by the designers experience and creativity. A disadvantage of heuristic approach proposed by Douglas, (1988) is the solution's quality cannot be determined through any reasonable or scientific method. While the thermodynamics approach does not consider the capital cost properly into its solution and the solution also requires a lot of trial-and-error from the designer. The second strategy that can be applied to solve a process synthesis problem is based on simultaneous optimization using mathematical programming (Grossmann, 1996). The algorithm approach on the other hand is based upon mathematical programming which is backed by strong and proven theoretical

background. This allows the designer to propose an optimal superstructure which encounters the weaknesses in the first two methods.

1.2 RESEARCH MOTIVATION

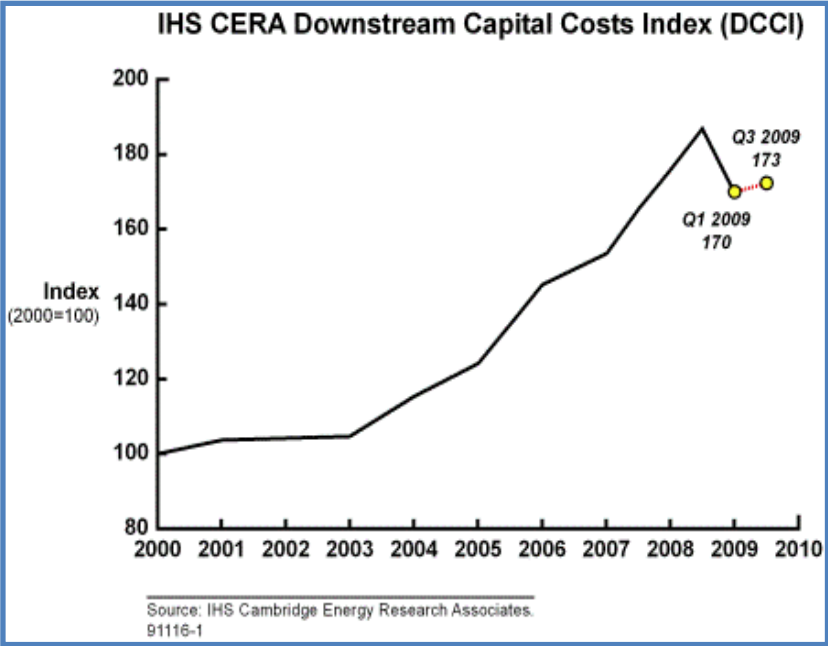


Figure 1: IHS CERA Downstream Capital Cost Index as of December 2009

Figure 1 above show the costs for designing and constructing downstream refining and petrochemical projects rose 1.5 percent in the past six months after bottoming out at 9 percent below peak 2008 price levels, according to the latest edition of the IHS CERA Downstream Capital Costs Index (DCCI). The current DCCI rose from 170 to 172.5 over the past 6 months. The values are indexed to the year 2000, meaning that a project that cost \$USD100 in 2000 would cost \$USD172.50 today. The turnaround was driven by construction labor costs, which rose over 5 percent, costs of equipment, facilities, materials, and personnel (both skilled and unskilled) used in the construction of a geographically diversified portfolio of more than thirty refining and petrochemical construction projects.

Despite the currently poor economics, the bulk of new downstream construction planned for regions such as China and the Middle East are expected to eventually proceed, fueled by forecasts of growing regional demand and often by economic support from local governments, the study finds. The IHS CERA DCCI concludes that slight increases in downstream capital costs should be expected in the near term as demand for materials rise, but not to the point where it will stretch the market's ability to supply. Thus factor as discussed above motivate this research project to further accomplish.

One of major components in a chemical processing system is the heat exchanger network, because it determines to a large extent the energy efficiency of the process. The heat exchanger network has the task of integrating the hot and the cold process streams in a process in order to reduce the amount of synthesizing optimal network configuration (Floudas, Ciric and Grossmann, 1986). Another drive aspect that arises to this project is when considering a process flowsheet, energy is not the only costs. According to Biegler, Grossmann, and Westerberg(1997), in fact the dominant cost item is usually raw materials. However, certain designs which are proven optimal in flowrates and unit selection will end up having more energy consumptions. Choosing a design with minimal energy requirements will probably give an infeasible process flowsheet. A natural question that then arises is how to determine the proper trade-off between the two. Work based on the simultaneous approach solve the problem without any decomposition, and can explicitly handle the trade-offs between the capital and operational cost of networks.

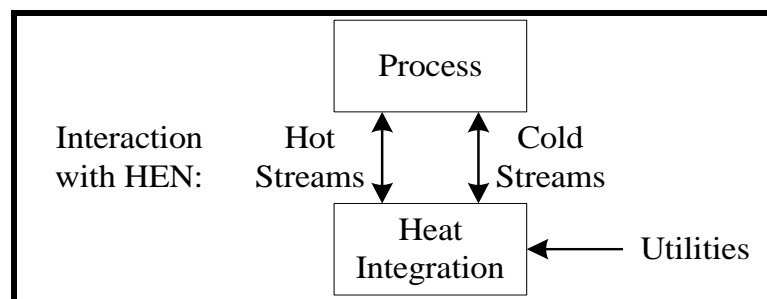


Figure 2: **Interaction between process flowsheet and heat integration**

1.3 PROBLEM STATEMENT

Designing petroleum refineries that satisfies multiple economics, operations, and environmental constraints is a highly complex task. The questions that we are interested to answer in this research concern the optimal design of the topology or configuration of a refinery with heat integration that addresses the following aspects:

- i. the selection of the process units (tasks) and material streams (states) in terms of the types of the units as well as the number of the units and streams;
- ii. the sequence of the interconnections among the units and the streams;
- iii. the level of production as given by the stream flowrates.

This research project will be undertaken using the optimization approach of mixed integer linear programming (MILP).

1.4 OBJECTIVES

The research's main objective is to obtain a mathematically viable model to determine the optimal topology for a petroleum refinery with incorporation of heat integration. The variable in concern are the process unit to be selected, the number of these selected units and the interconnection or sequence between the selected units. In order to achieve the main objective, the following sub-objectives are form:

- i. To develop a superstructure representation for a refinery network topology with a suitable level of detail and abstraction by incorporating heat integration features;
- ii. To construct an optimization model based on the superstructure representation that includes: (a) mass balances (linear), (b) energy balances,

and (c) logical constraints enforcing the design specifications and the interconnectivity relationships among the units and the streams for the selection of the alternative routes;

- iii. To apply heat integration technique into the optimization model;
- iv. To solve the mixed-integer programming optimization model using the modeling language GAMS (General Algebraic Modeling System).

1.5 SCOPE OF STUDY

The scope for this project in the present semester is to understand the refinery topology superstructure that has been formulated by a previous student which is on naphtha processing from atmospheric distillation unit (ADU) in an oil refinery. There are two different types of formulations for naphtha processing in an oil refinery with heat integration which are:

- i. MILP based on Papoulias and Grossmann (1983a, b, c) for simultaneous optimization of flowsheet and heat integration, in which the heat integration optimization is performed sequentially and exclude isothermal streams

CHAPTER 2

LITERITURE REVIEW

2.1 REFINING PROCESS: NAPHTA PRODUCED FROM ATMOSPHERIC DISTILLATION UNIT

2.1.1 Atmospheric Distillation Unit (ADU)

The atmospheric distillation unit (ADU) is the first unit in which the crude oil is processed. The main function of this unit is to separate crude oil to fractions based on the boiling point of each product so that the subsequent downstream units have feedstock that meets their specifications. The feed is prepared for separation by preheating the crude oil to 120°C by a series of heat exchangers. Then, the crude is sent to the desalters before being heated to 280°C in which light gases are separated in flash drum before the crude oil enters the furnace where it is heated to 360°C (Gary and Handwerk, 2001) then crude oil enters the atmospheric distillation unit wherein several naphtha products are withdrawn from the side of the column.

2.1.2 Hydrotreatment Unit (HDT)

Hydrotreating is the process of catalytically stabilized petroleum products or remove objectionable from products or feedstock by reacting them with hydrogen. Stabilization is usually involved converting unsaturated hydrocarbons such as olefins and gum forming diolefins to paraffin. Objectionable elements that removed by hydrotreating is including sulphur, nitrogen, oxygen, halides and trace metals (Gary and Handwerk, 2001). Naphtha separated from crude oil in the ADU is sent to hydrotreatment unit (HDT) to remove sulphur as well as other unwanted compounds, e.g. unsaturated hydrocarbons, nitrogen from refinery process streams, so that it will not poison the reformer catalyst. HDT feed is heated to 300°C, and compressed to 10 bar, then is fed to reactor then the products are cooled down to 40°C. Then reactor product stream is separated in fractionators and each stream is cooled down.

2.1.3 Catalytic Reformer Unit (REF)

The hydrotreated naphtha is sent to catalytic reformer unit where the main function of reformer unit is restructuring the naphtha to increase the octane number so that it can be used in vehicles. Cyclization and isomerization reactions must occur so the paraffins and naphthenes will be converted to high octane component. Naphtha sent from HDT is heated to 500°C then it is fed to reactor and reactor is cooled down to 38°C, then fed to unit fractionator where Naphtha is separated to several products..

2.1.4 Sulfur Recovery Unit (SRU)

The hydrogen sulfide generated from HDT unit is sent to Sulfer recovery unit (SRU) to recover elemental sulfur to minimize the atmospheric pollution by sulfur dioxide. The feed of this unit is heated up to 350°C and fed to 3 stage reactors where then the reactor product is cooled and condensed and the liquid sulfur is separated and the elemental sulfur is sold to generate additional revenue.

2.1.5 Isomerization Unit (ISO)

The paraffins of light straight run naphtha can be converted to isomers by increasing of octane number. The feed to Isomerization unit is heated to 200°C-285°C then it is fed to unit reactor and the product is cooled down and fed to the unit fractionators.

2.2 OPTIMIZATION APPROACHES FOR PERFORMING HEAT INTEGRATION

Heat exchanger networks have been the subject of numerous investigations in the past because of their impact in the energy recovery of industrial plants. Two major methodologies have been proposed for the synthesis of heat exchanger network problems, namely the sequential and the simultaneous approach

2.2.1 Sequential Approach for Performing Heat Integration

One of the most-widely known sequential approaches is the pinch design method (Linnhoff and Hindmarsh, 1983), in which targets for the minimum utility requirement, the minimum number of exchanger units and the minimum capital cost of the network are obtained sequentially. Several heuristic rules are then used to synthesize a network that approaches these targets. These methods typically involve partitioning of the HENS problem into a number of intervals, which is usually accomplished by dividing the temperature range of the problem into temperature intervals. There is also the concept of super targeting for determining the optimal minimum approach temperature (ΔT_{\min} or heat recovery approach temperature HRAT) used in partitioning of the problem into temperature intervals because the minimum capital cost of the network is a function of this parameter.

In particular, an optimal or near optimal heat exchanger network exhibits the characteristics of minimum utility cost, minimum number of units and minimum investment cost. In sequential approach, these objectives are achieved chronologically.

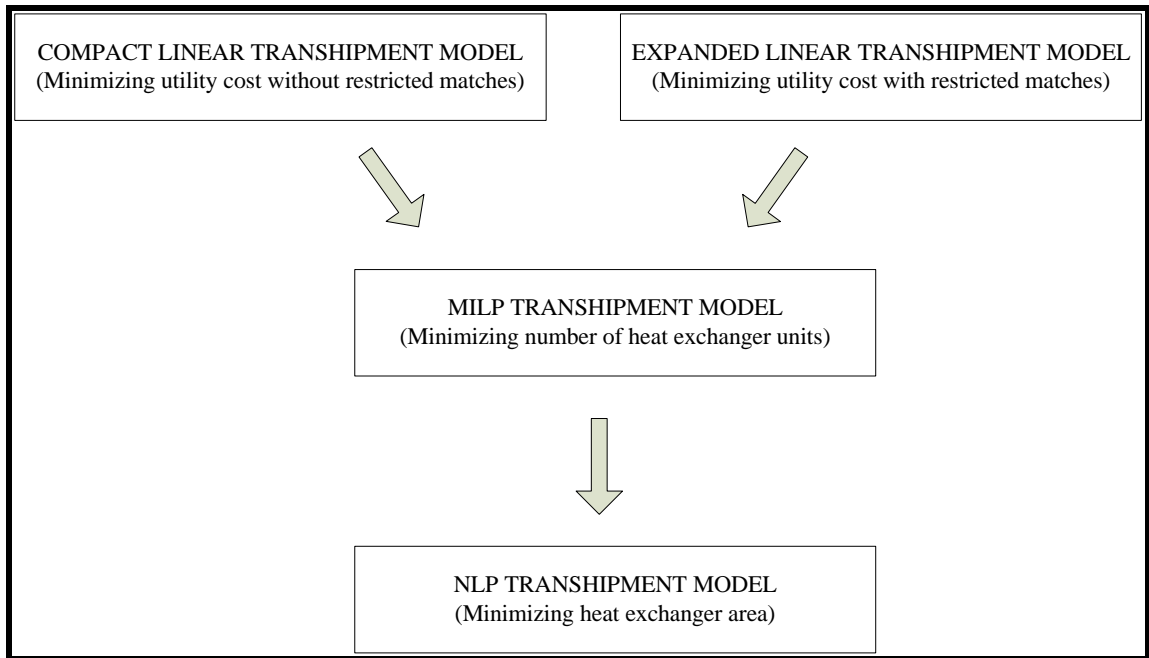


Figure 3: Summarization of heat integration sequential synthesis

2.2.2 Simultaneous Mixed-Integer Nonlinear Programming (MINLP) Model for Heat Integration

The disadvantage of using the sequential method is that the trade-offs between energy, number of units and area are not rigorously taken into account. The simultaneous approach by Yee and Grossman (1990) used the mixed integer nonlinear programming to derive for the minimum utility, number of units and area concurrently and is approximated by a problem that conceptually can be stated as follows.

$$\begin{array}{ll}
 \min & \text{area cost} \\
 \text{s.t.} & \min. \quad \text{number of units} \\
 & \text{s.t.} \quad \text{minimum utility cost}
 \end{array}$$

The proposed MINLP model for heat integration is based on the stage-wise superstructure representation proposed by Yee et al. (1990). The representation allows for different possibilities and sequences for matching streams. The superstructure for the problem is shown in figure below.

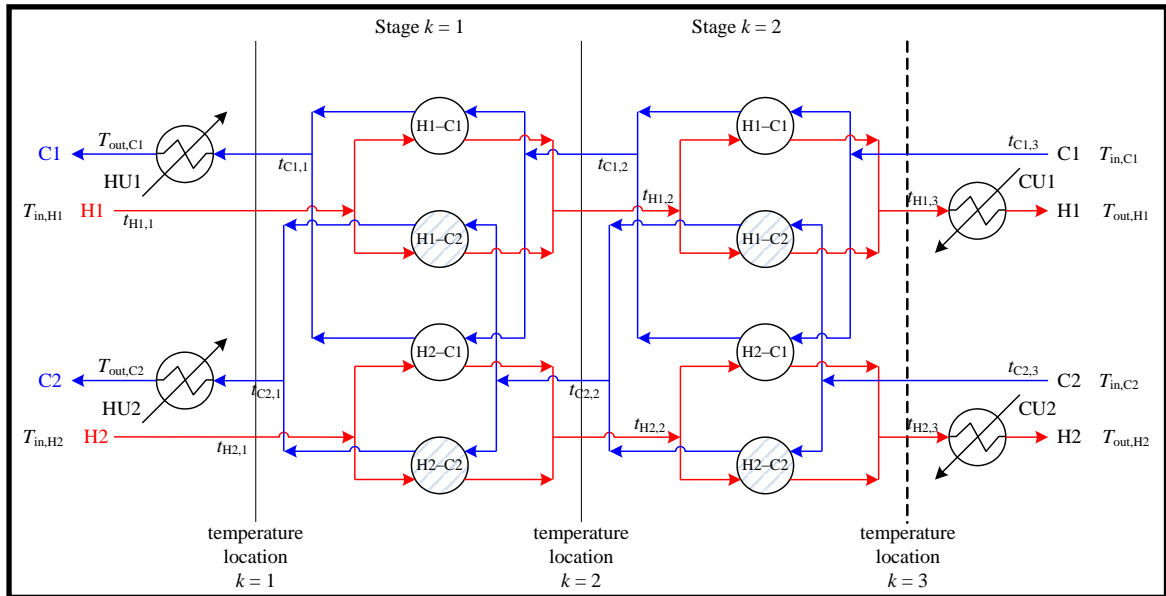


Figure 4: Two-stage superstructure for the MINLP model of Yee and Grossmann (1990)

Within each stage of the superstructure, potential exchanges between any pair of hot and cold streams can occur. In each stage, the corresponding process stream is split and directed to an exchanger for a potential match between each hot stream and each cold stream. It is assumed that the outlets of the exchangers are isothermally mixed (i.e., the outlets are mixed at the same temperature), which simplifies the calculation of the stream temperature for the next stage, since no information of flows is needed in the model.

2.2.3. Comparison between Sequential and Simultaneous Heat Exchanger Network Synthesis

The main advantage in the sequential synthesis approach is that the problem is made more manageable by solving a sequence of smaller problems. Clearly, targets are essential for setting up these smaller problems, as was the case of the minimum utility cost, minimum area, and minimum number of units' targets. On the other hand, the advantage of the simultaneous approach is that the trade-offs are all taken simultaneously into account, thus increasing the possibility of determining improved solutions. However, the computational requirements are greatly increased; for this reason, it motivates simplifications such as the one that was presented on isothermal mixing for the MINLP model. One important aspect, though, that is offered by simultaneous optimization models is that they do not rely on heuristics.

2.3. OPTIMIZATION APPROACHES FOR FLOWSHEET OPTIMIZATION WITH HEAT INTEGRATION

2.3.1 Simultaneous Mixed Integer Linear Optimization Approach for Flowsheet Optimization and Heat Integration

Simultaneous flowsheet optimization and heat integration approach is introduced by Papoulias and Grossmann (1983). The main objective of this approach is model a mixed-integer programming model that solves for the minimum utility cost and can handle restricted matches and multiple utilities by applying the transshipment models with fixed temperature intervals.

In the simultaneous strategy, on the other hand, we will perform the heat integration of the streams while we optimize the process. To avoid the problem of synthesizing a heat exchanger network (HEN) for each process condition that is generated throughout the

optimization (Yee et al., 1990), we will consider only the utility cost for maximum heat integration. For example, objective function = minimize cost of flowsheet together to minimize utility cost (without minimizing heat exchange area and heat exchange units). consider the case when the units in a process flowsheet are described by linear equations given that fixed pressure and temperature levels are assumed, the formulation is described below:

2.3.2 Simultaneous Mixed Integer Non-Linear Model Optimization Approach for Flowsheet Optimization and Heat Integration

This approach is apply when considering Simultaneous mixed integer nonlinear optimization approach is introduced by Yee and Grossmann (1990). This approach has several objective functions that can be solved for;

- Minimum area cost and energy consumption
- Minimum annual cost
- Optimal process and heat exchanger design

To solve for minimum area cost, energy consumption, and minimum annual cost require a given fixed flows, inlet and outlet temperatures. To solve for optimal process and heat exchanger design flows, inlet and outlet temperature is considered as variable. With the following assumptions are made:

- Constant heat capacities
- Constant heat transfer coefficients
- Countercurrent heat exchangers

CHAPTER 3 METHODOLOGY

3.1 PROJECT METHODOLOGY

This work consists of two major subproblems: first, the flowsheet optimization problem and second, the heat integration subproblem. The procedure below briefly summarizes the proposed strategies involved in those two subproblems

- Step 1.** Develop a superstructure representation for a refinery network topology with a suitable level of detail and abstraction. (Note that in this work, we adopt the superstructure for the problem reported in Loh (2008)).
- Step 2.** Identify hot streams and cold streams to incorporate heat integration into the optimization model formulation.
- Step 3.** Develop the temperature intervals based on the identified inlet, highest and lowest temperature of hot streams and cold streams.
- Step 4.** Formulate the corresponding optimization model for the flowsheet superstructure without heat integration by developing constraints on:
- linear material balances with constant yields;
 - logical constraints on design specifications (binary 0–1 variables);
 - logical constraints structural specifications (binary 0–1 variables);
 - Big-M logical constraints.
- Step 5.** Develop energy (heat) balances for the optimization model formulated in Step 4 to incorporate heat integration features.
- Two model formulations are considered for incorporating heat integration in the optimization framework for determining the optimal refinery topology:
- model (HI1): expanded linear programming (LP) transshipment model for profit maximization with constrained matches;
 - model (HI2): mixed-integer linear programming (MILP) transshipment model for prediction of matches for minimum number of heat exchanger units.
- Step 6.** Solve the optimization model (MILP1) that considers simultaneous

flowsheet optimization and heat integration based on model (HI1).

It is worth mentioning that by the simultaneous optimization of the flowsheet superstructure and the heat integration for minimum utility cost, we are considering the optimal heat integration network that eliminates or modifies the bottlenecks presented by the pinch points if we had only considered the heat integration model alone with a fixed structure of the flowsheet (as mentioned by Papoulias and Grossmann (1983b)).

- Step 7.** Solve the optimization model (MILP2) that considers sequential flowsheet optimization and heat integration based on model (HI2). Note that this is considered as a sequential approach for handling flowsheet optimization and heat integration because model (HI2) uses the solution for heat loads of the heating and cooling utilities from model (HI1) in order to determine the minimum number of heat exchange matches (in which we further assume that each match gives rise to one heat exchanger unit).

The simplified methodology is represented in **Figure 5** below:

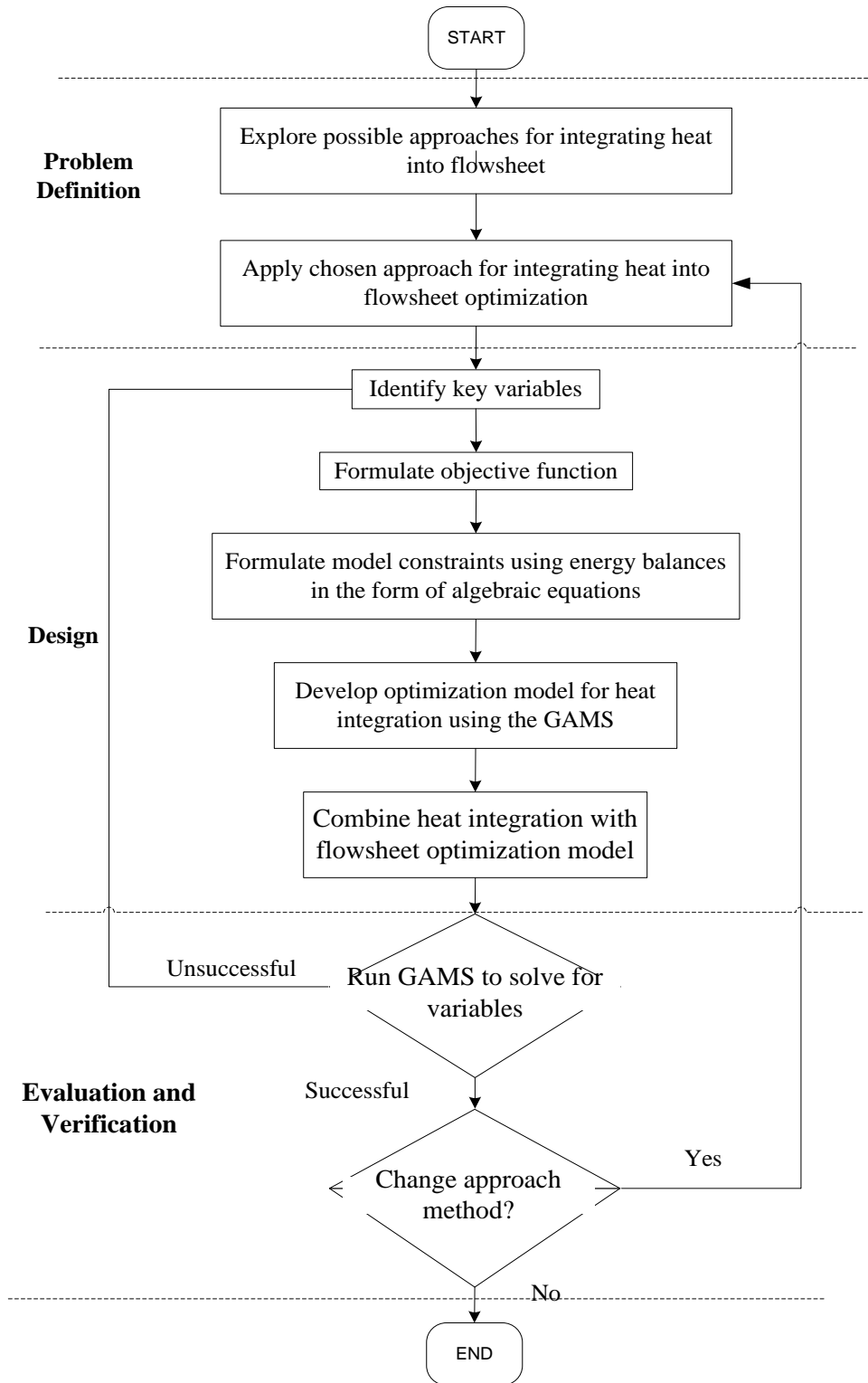


Figure 5: **Flowchart of the proposed methodology for model formulation to carry out the thesis research**

3.2 SUPERSTRUCTURE REPRESENTATION (STEP 1)

For this project, various naphtha states exiting ADU are chosen which mainly light, heavy and undifferentiated naphtha.

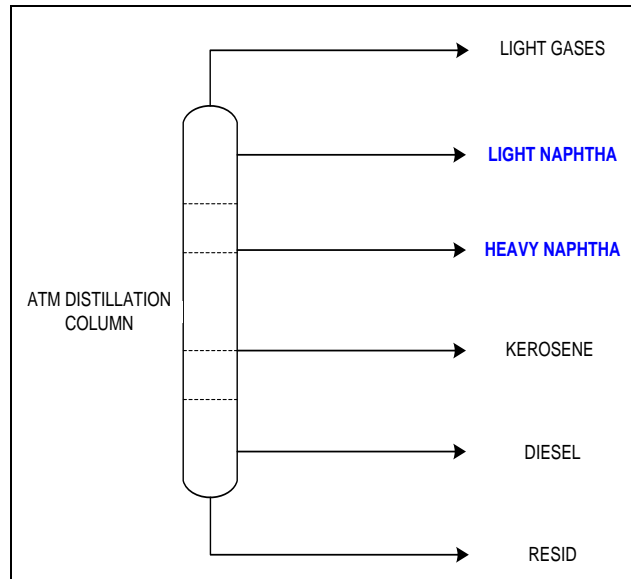


Figure 6: Fractions from crude distillation

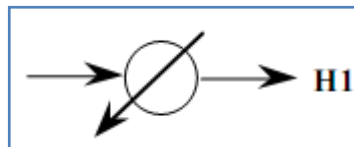
3.2.1 Short descriptions of each process units used in the superstructure

- i. Atmospheric Distillation Unit (ADU) - Atmospheric Distillation Unit perform the initial separation of crude oil into raw products, namely Gas, Naphtha, Kerosene, Diesel and Residue (Atmospheric Bottoms).
- ii. Naphtha Hydrotreater (HDT) - Naphtha Hydrotreater unit uses hydrogen to desulfurize naphtha from atmospheric distillation. The naphtha must be hydrotreated before sending to a Catalytic Reformer unit.
- iii. Catalytic Reformer (REF) - Catalytic Reformer unit is used to convert the naphtha-boiling range molecules into higher octane reformate (reformer product). The reformate has higher content of aromatics and cyclic hydrocarbons). An important byproduct of a reformer is hydrogen released during the catalyst reaction. The hydrogen is used either in the hydrotreaters or the hydrocracker.

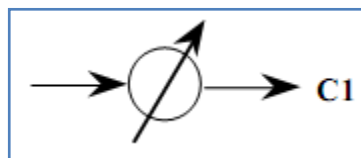
- iv. Fluid Catalytic Cracker (FCC) - Fluid Catalytic Cracker unit upgrades heavier fractions into lighter, more valuable products.
- v. Hydrocracker (HCR) - Hydrocracker unit uses hydrogen to upgrade heavier fractions into lighter, more valuable products.
- vi. Visbreaking unit (VIS) - Visbreaking unit upgrades heavy residual oils by thermally cracking them into lighter, more valuable reduced viscosity products.
- vii. Coking unit (COK) - Coking units (delayed coking, fluid coker, and flexicoker) process very heavy residual oils into gasoline and diesel fuel, leaving petroleum coke as a residual product.
- viii. Isomerization unit (ISO) - Isomerization unit converts linear molecules to higher-octane branched molecules for blending into gasoline or feed to alkylation units.

3.3 IDENTIFICATION OF HOT STREAMS AND COLD STREAMS(STEP 2)

Hot stream - is a stream that needs to be cooled, $T_{out} < T_{in}$
 (Example: overhead vapor in a distillation column).



Cold stream - is a stream that needs to be heated, $T_{out} > T_{in}$
 (Example: bottom liquid in a distillation column).



We consider the superstructure reported in Loh (2008) for the general model formulation.

3.4 OPTIMIZATION MODEL FORMULATION FOR HEAT INTEGRATION (STEP 4,5,6,7)

In this section, both optimization model formulations for naphtha produced from atmospheric distillation unit incorporated with heat integration which is sequential and simultaneous approach with respect to heat integration are being further discussed.

3.4.1 Sequential Approach for Heat Integration

3.4.1.1 Development of Temperature Intervals

Using LP Transshipment Model, temperature intervals are developed using the following approach as proposed by Biegler, Grossmann, and Westerberg (1997):

1. First, partition the entire temperature into temperature intervals based on the: (1) inlet temperatures of the process streams, (2) the highest and lowest stream temperatures
2. Consider that we have K temperature intervals with (3) the intermediate utilities whose inlet temperatures fall within the range of the temperatures of the interval K .
3. Intervals are numbered from the top to the bottom.

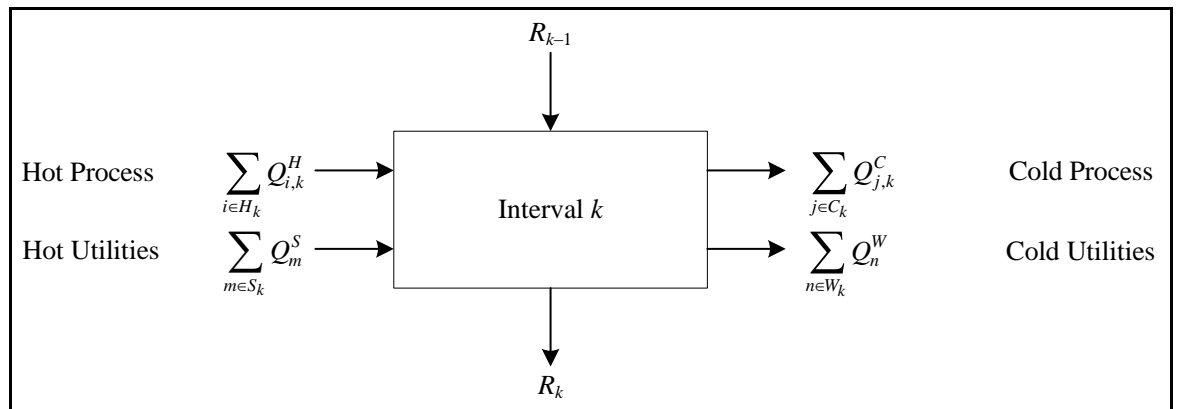


Figure 7: Heat flows in interval k

$$RHu(m, k) - RHu(m, k-1) + \sum_{c \in YC(k, c)} Q(m, c, k) = Q(m) \quad \forall (k, m) \in YHu3(k, m)$$

$$RHu(m, k) - RHu(m, k-1) + \sum_{c \in YC(k, c)} Q(m, c, k) = 0 \quad \forall (k, m) \in YHu2(k, m)$$

- iii. for the cold process streams at the destination node C that relate the heat content and heat exchanges:

$$\sum_{i \in H_k} Q(h, c, k) + \sum_{m \in S_k} Q(m, c, k) = F(c) \cdot C_p(c) \cdot \Delta T(k, c), \quad j \in C_k$$

- iv. for the cold utility streams at the destination node D that relate the heat content and heat exchanges

$$\sum_{i \in H_k} Q(h, n, k) = QCu(n) \Rightarrow \sum_{i \in H_k} Q(h, n, k) - QCu(n) = 0, \quad n \in W_k$$

- ii. additional constraints:

$$R(h, k_0) = R(i, k_K) = 0$$

- v. no heat residual from the previous higher temperature interval compared to the highest temperature interval at which hot stream h is present at:

$$R(h, k-1) = 0, \quad k = \text{highest temperature interval at which hot stream } h \text{ is present at}$$

$$RHu(st, k-1) = 0, \quad k = \text{highest temperature interval at which hot utility } st \text{ is present at}$$

3.4.1.3 Objective Function Minimization of Flowsheet Optimization and Utilities Requirement

According to Biegler, Grossmann, and Westerberg (1997), the problem of simultaneous optimization and heat integration can be formulated as a linear program (LP) as follows:

$$\begin{aligned}
\min \quad & C = c^T x + \underbrace{c_S Q_S}_{\text{cost of hot utility}} + \underbrace{c_W Q_W}_{\text{cost of cold utility}} \\
\text{s.t.} \quad & Ax = a \\
& Bx \leq a \\
& s(x) = 0 \\
& R_k - R_{k-1} - Q_S + Q_W = \sum_{i \in H_k} F_i \Delta T_{i,k} - \sum_{j \in C_k} f_j \Delta t_{j,k}, \quad k=1, \dots, K \quad \textbf{(P1)} \\
& x, Q_S, Q_W \geq 0 \\
& R_k \geq 0, \quad k=1, \dots, K-1 \\
& R_0 = R_K = 0, \\
& F_i \geq 0, \quad i=1, \dots, n_H \\
& f_j \geq 0, \quad j=1, \dots, n_C
\end{aligned}$$

The objective function involves the linear cost $c^T x$ in terms of equipment sizes and flows, and the cost of heating and cooling utility. This formulation will consider for the optimization that the required utility loads Q_S and Q_W correspond to the maximum heat integration of the process streams for any given values of the flow rates of the streams.

Extension of the model **(P1)** for the case of multiple utilities and unrestricted matches are presented in the following as model **(P2)**:

$$\begin{aligned}
\max \quad & P = p_{\text{product}} F_{\text{product}} - \underbrace{c_{\text{capital}}^T y_{\text{unit}}}_{\text{capital cost}} + \underbrace{c_{\text{operating}}^T F_{\text{unit}}}_{\text{operating cost}} + \underbrace{\sum c_m Q_m^S}_{\text{cost of hot utility}} + \underbrace{c_n Q_n^W}_{\text{cost of cold utility}} \\
& \qquad \qquad \qquad \underbrace{\hspace{10em}}_{\text{flowsheet optimization problem}} \qquad \qquad \qquad \underbrace{\hspace{10em}}_{\text{heat integration problem}} \\
\text{s.t.} \quad & Ax = a \\
& Bx \leq a \\
& s(x) = 0 \\
& R_k - R_{k-1} - \sum_{m \in HU_k} Q_{S,m} + \sum_{n \in CU_k} Q_{W,n} = \sum_{i \in H_k} F_i \Delta T_{i,k} - \sum_{j \in C_k} f_j \Delta t_{j,k}, \quad k \in K \quad \textbf{(P2)} \\
& x, Q_S, Q_W \geq 0 \\
& R_k \geq 0, \quad k = 1, \dots, K-1 \\
& R_0 = R_K = 0, \\
& F_i \geq 0, \quad i = 1, \dots, n_H \\
& f_j \geq 0, \quad j = 1, \dots, n_C
\end{aligned}$$

in which the additional variables compared to **(P1)** are $Q_{m,S}$ and $Q_{n,W}$, the heat load of hot utility m and cold utility n , respectively.

Extension of the model **(P2)** to the case of multiple utilities and restricted matches are as follows:

$$\begin{aligned}
\max \quad & P = p_{\text{product}} F_{\text{product}} - \underbrace{c_{\text{capital}}^T y_{\text{unit}}}_{\text{capital cost}} + \underbrace{c_{\text{operating}}^T F_{\text{unit}}}_{\text{operating cost}} + \underbrace{\sum c_m Q_m^S + c_n Q_n^W}_{\substack{\text{cost of} \\ \text{hot utility} \quad \text{cost of} \\ \text{cold utility}}} \\
& \qquad \qquad \qquad \text{flowsheet optimization} \qquad \qquad \qquad \text{heat integration} \\
& \qquad \qquad \qquad \text{problem} \qquad \qquad \qquad \text{problem} \\
\text{s.t.} \quad & Ax = a \\
& Bx \leq a \\
& s(x) = 0 \\
& R_{i,k} - R_{i,k-1} + \sum_{j \in C_k} Q_{i,j,k} + \sum_{n \in W_k} Q_{i,n,k} = Q_{i,k}^H, \quad i \in H'_k \\
& R_{m,k} - R_{m,k-1} + \sum_{j \in C_k} Q_{m,j,k} + Q_m^S = 0, \quad m \in S'_k \\
& \sum_{i \in H_k} Q_{i,j,k} + \sum_{m \in S_k} Q_{m,j,k} = Q_{j,k}^c \quad j \in S'_k \\
& \sum_{i \in H_k} Q_{i,n,k} - Q_n^W = 0 \quad n \in W_k = k = 1, \dots, K \\
& x, Q_m^S, Q_n^W, Q_{m,j,k}, Q_{i,j,k} \geq 0 \\
& R_{i,k}, R_{m,k} \geq 0, \quad k = 1, \dots, K-1 \\
& R_{i,0} = R_{i,K} = 0
\end{aligned} \tag{P3}$$

For the case when we want to impose a given match, we can do this by specifying that its total heat exchange, which is the sum of $Q_{i,j,k}$ over all intervals, must lie within some specified lower and upper bounds, that is given by;

$$Q_{i,j}^L \leq \sum_{k=1}^K Q_{i,j,k} \leq Q_{i,j}^U$$

3.4.1.4 Objective Function Minimization of Number of Heat Exchangers Unit with Fixed Optimal Flowsheet and Utilities Load

The model (P3) can be extended further to predict rigorously the actual number of fewest units, as well as the stream matches that are involved in each unit, and the amount of heat that they must exchange.

For each predicted matches by the binary variables with a value of one, is associate to a single heat exchanger unit. The objective function then can be expressed as:

$$\min \sum_{i \in H} \sum_{j \in C} y_{ij}^q$$

The heat balances at each node discussed before will remain as the constraint. Since the heat content of the utility streams is known, the associated constraints can be simplified as below:

$$\begin{aligned} R_{ik} - R_{i,k-1} + \sum_{j \in C_k} Q_{ijk} &= Q_{ik}^H & i \in H'_k & \quad k = 1, \dots, K_q \\ \sum_{i \in H_k} Q_{ijk} &= Q_{jk}^C & j \in C_k & \\ R_{ik}, Q_{ijk} &\geq 0 & & \end{aligned}$$

There is also the need to express a logical constraint that states that if the binary variable is zero, the associated continuous variable must also be zero. The constraint can be written as:

$$\sum_{k=1}^{K_q} Q_{ijk} - U_{ij} y_{ij}^q \leq 0$$

The upper bound, U_{ij} will be given by the smallest of the heat contents of the streams. This set of constraint, can solve independently over all the sub networks q (as implied above) or simultaneously over all the sub networks. The solution to this problem then will indicate the following:

- Matches that take place ($y_{ij}=1$)

- Heat exchange at each match Q_{ijk}

Consider that we have K temperature intervals that are based on the: (1) inlet temperatures of the process streams, (2) the highest and lowest stream temperatures, and (3) of the intermediate utilities whose inlet temperatures fall within the range of the temperatures of the process streams. Assume, as in the above example, that the intervals are numbered from the top to the bottom. When we consider a given temperature interval k , we will have the following known parameters and variables:

- known parameters : $Q_{i,k}^H, Q_{i,k}^C, c_m, c_n$
- variables : Q_m^S, Q_n^W, R_k

The minimum utility cost for a given set of hot and cold processing streams can then be formulated as the following LP (Biegler, Grossmann, and Westerberg(1997)):

$$\begin{aligned}
 \min \quad & Z = \sum_{m \in S} c_m Q_m^S + \sum_{n \in W} c_n Q_n^W \\
 \text{s.t.} \quad & R_k - R_{k-1} - \sum_{m \in S_k} Q_m^S + \sum_{n \in W_k} Q_n^W = \sum_{i \in H_k} Q_{i,k}^H - \sum_{j \in C_k} Q_{j,k}^C, \quad \underbrace{k=1, \dots, K}_{k \in KK} \\
 & Q_m^S \geq 0, Q_n^W \geq 0, R_k \geq 0, \quad \underbrace{k=1, \dots, K-1}_{k \in KK} \\
 & R_0 = 0, R_K = 0
 \end{aligned}$$

3.4.2 Simultaneous Approach for Flowsheet Optimization and Heat Integration

3.4.2.1 Development of Heat Energy Balance

Overall Heat Balance for Each Stream

The overall heat balances are stipulated to ensure sufficient heating or cooling for each cold and hot process stream, respectively. The constraints enforce that the overall heat

transfer is equal to the summation of the heat exchanged with other process streams at each stage and of the heat exchanged with the available utilities.

$$\begin{aligned} (T_{in,i} - T_{out,i}) f_i cp_i &= \sum_{k \in ST} \sum_{j \in CP} q_{i,j,k} + qcu_i, & i \in HP = \{H1, H2, \dots, H10\} \\ (T_{out,j} - T_{in,j}) f_j cp_j &= \sum_{k \in ST} \sum_{i \in HP} q_{i,j,k} + qhu_j, & j \in CP = \{C1, C2, \dots, C10\} \end{aligned}$$

Heat Balances at Each Stage

The model involves ten (10) hot streams and 12 cold streams. The heat balance at each stage of the superstructure is needed to determine the intermediate temperatures of the streams at each stage.

$$\begin{aligned} (t_{i,k} - t_{i,k+1}) f_i cp_i &= \sum_{j \in CP} q_{i,j,k} & i \in HP, k \in ST \\ (t_{j,k} - t_{j,k+1}) f_j cp_j &= \sum_{i \in HP} q_{i,j,k} & j \in CP, k \in ST \end{aligned}$$

Assignment of Superstructure Inlet Temperatures

For the hot streams and cold streams

$$\begin{aligned} T_{in,i} &= t_{i,1}, & i \in HP \\ T_{in,j} &= t_{j,NOK+1}; & j \in CP \end{aligned}$$

Thermodynamic Feasibility of Temperatures (Bounds for the Heat-Integrated Streams)

This constraint enforces a requirement for utility load if a heat-integrated stream does not reach its desired outlet temperature.

$$t_{i,k} \geq t_{i,k+1}, \quad k \in ST, i \in HP$$

$$t_{j,k} \geq t_{j,k+1}, \quad k \in ST, j \in CP$$

$$T_{out,i} \leq t_{i,NOK+1}, \quad i \in HP$$

$$T_{out,j} \geq t_{j,1}, \quad j \in CP$$

Hot and Cold Utility Load

If the heat-integrated streams do not achieve their desired temperatures, the remaining heat requirements are obtained from the utilities. The corresponding heat load requirements are given by the following energy balances, in which for the hot streams, the cooling utility duty is given by:

$$(t_{i,NOK+1} - t_{out,i}) f_{i,cp_i} = qcu_i, \quad i \in HP$$

For cold streams the heating utility duty is given by:

$$(t_{out,j} - t_{j,1}) f_{j,cp_j} = qhu_j, \quad j \in CP$$

Logical Constraints

Logical constraints are needed to determine the existence of a process match (i,j) in stage k and also any match involving utility streams. They ensure that if a match does not exist, then the corresponding heat exchange is equals to zero.

$$\begin{aligned}
q_{i,j,k} &\leq \Omega z_{i,j,k} \leq 0 & i \in HP, j \in CP, k \in ST \\
qcu_i &\leq \Omega zcu_i & i \in HP \\
qhu_j &\leq \Omega zhu_j & j \in CP \\
z_{i,j,k}, zcu_i, zhu_j &\in \{0,1\} \\
z_{i,j,k} &= \begin{cases} 1, & \text{heat exchange exists between } i \text{ and } j \\ 0, & \text{otherwise} \end{cases} \\
zhu_j &= \begin{cases} 1, & \text{heat exchange exists between hot utility and } j \\ 0, & \text{otherwise} \end{cases} \\
zcu_i &= \begin{cases} 1, & \text{heat exchange exists between cold utility and } i \\ 0, & \text{otherwise} \end{cases}
\end{aligned}$$

Calculation of Approach Temperatures

The following constraints ensure feasible temperature driving forces in the selected stream matches. The upper bound Γ is the lowest allowable value for the exchanger minimum approach temperature (EMAT).

$$\begin{aligned}
dt_{i,j,k} &\leq t_{i,k} - t_{j,k} + \Gamma(1 - z_{i,j,k}), & i \in HP, j \in CP, k \in ST \\
dt_{i,j,k+1} &\leq t_{i,k+1} - t_{j,k+1} + \Gamma(1 - z_{i,j,k}), & i \in HP, j \in CP, k \in ST \\
dtku_{i,1} &\leq t_{i,NOK+1} - T_{OUT,CU} + \Gamma(1 - zcu_i), & i \in HP \\
dtku_{i,2} &\leq t_{out,i} - T_{IN,CU} + \Gamma(1 - zcu_i), & i \in HP \\
dthu_{j,1} &\leq T_{OUT,HU} - t_{j,1} + \Gamma(1 - zhu_j), & j \in CP \\
dthu_{j,2} &\leq T_{IN,HU} - t_{out,j} + \Gamma(1 - zhu_j), & j \in CP \\
dt_{i,j,k}, dtku_i, dthu_j &\geq EMAT, & k \in ST, i \in HP, j \in CP
\end{aligned}$$

Stream Matching at Each Stage

$$\begin{aligned}
\sum_{i \in HP} z_{i,j,k} &\leq 1, & k \in ST, j \in CP \\
\sum_{j \in CP} z_{i,j,k} &\leq 1, & k \in ST, i \in HP \\
z_i, z_j &\in \{0,1\}
\end{aligned}$$

Binary variables z_i and z_j are used to enforce streams that are activated (or deactivated) in the optimal solution.

3.4.2.2 Objective Function Minimization of Heat Exchanger Area, Heat Exchanger Units and Utility Requirement

$$\begin{aligned}
\min \quad & \underbrace{F(w, x)}_{\text{cost of flowsheet optimization}} + \underbrace{\sum_{i \in HP} (CCU) qcu_i}_{\text{cost of cold utility}} + \underbrace{\sum_{j \in CP} (CHU) qhu_j}_{\text{cost of hot utility}} \\
& + \underbrace{\sum_{i \in HP} \sum_{j \in CP} \sum_{k \in ST} (CF_{i,j}) z_{i,j,k}}_{\text{exchanger cost for match between hot stream - cold stream}} + \underbrace{\sum_{i \in HP} (CF_{i,CU}) zcu_i}_{\text{exchanger cost for match between hot stream - cold utility}} + \underbrace{\sum_{j \in CP} (CF_{j,HU}) zhu_j}_{\text{exchanger cost for match between hot utility - cold stream}} \\
& \underbrace{\hspace{15em}}_{\text{fixed charges for exchangers}} \\
& + \sum_{i \in HP} \sum_{j \in CP} \sum_{k \in ST} \underbrace{C_{i,j}}_{\substack{\text{area} \\ \text{cost} \\ \text{coefficient}}} \left[\frac{q_{i,j,k}}{U_{i,j} \left[(dt_{i,j,k} dt_{i,j,k+1}) \left(\frac{dt_{i,j,k} + dt_{i,j,k+1}}{2} \right) \right]^{1/3}} \right]^{\beta_{i,j}} \\
& \underbrace{\hspace{15em}}_{\text{area of exchanger for match between hot stream - cold stream}} \\
& + \sum_{i \in HP} C_{i,CU} \left[\frac{qcu_i}{U_{i,CU} \left[(dtku_i (T_{OUT_i} - T_{IN_{CU}})) \left(\frac{dtku_i + (T_{OUT_i} - T_{IN_{CU}})}{2} \right) \right]^{1/3}} \right]^{\beta_{i,CU}} \\
& \underbrace{\hspace{15em}}_{\text{area of exchanger for match between hot stream - cold utility}} \\
& + \sum_{j \in CP} C_{HU,j} \left[\frac{qhu_j}{U_{HU,j} \left[(dthu_j (T_{IN_{HU}} - T_{OUT_j})) \left(\frac{dthu_j + (T_{IN_{HU}} - T_{OUT_j})}{2} \right) \right]^{1/3}} \right]^{\beta_{HU,j}} \\
& \underbrace{\hspace{15em}}_{\text{area of exchanger for match between hot utility - cold stream}}
\end{aligned}$$

where $\frac{1}{U_{i,j}} = \frac{1}{h_i} + \frac{1}{h_j}$; $\frac{1}{U_{i,CU}} = \frac{1}{h_i} + \frac{1}{h_{CU}}$; $\frac{1}{U_{HU,j}} = \frac{1}{h_{HU}} + \frac{1}{h_j}$.

3.5 PROJECT GANTT CHART

No.	DETAIL	WEEK							MID-SEM BREAK	WEEK								
		1	2	3	4	5	6	7		8	9	10	11	12	13	14		
1	Selection of Project Topic	█	█															
2	Preliminary Research Work		█	█	█													
	Problem Statement		█	█	█													
	Objectives		█	█	█													
	Scope of Research		█	█	█													
3	Literature Review (Part 1)																	
3.1	Optimization Approach for Perfoming Heat Integration				█	█												
	Sequential				█	█												
3.2	Optimization Approach for Flowsheet Optimization with Heat Integration							█		█								
	Simultaneous MILP							█		█								
	Simultaneous MINLP							█		█								
	Simultaneous by Pinch Point Location Method							█		█								
3.3.	Modelling Framewok							█	█									
	State Task Network							█	█									
	State Equipment Network							█	█									
4	Methodology																	
5	Submission of Progress Report																	
6	Literature Review (Part 2)																	
6..1	Isothermal Streams																	
	MILP										█	█						
	MINLP										█	█						
6.1	Optimization Approach for Perfoming Heat Integration												█	█				
	Simultaneous (Yee and Grossmann 1990 a,b,c)												█	█				
7	GAMS Exercise																	█
8	Submission of Interim Report																	█
9	Oral Presentation																	█

Figure 9a: FYP I Project Gantt chart

No	Work Progress	Weeks																
		1	2	3	4	5	6	7	MIDDLE SEMESTER BREAK	8	9	10	11	12	13	14	15	
1	GAMS Model Development																	
1.1	Superstructure Flowsheet Optimization	█																
1.2	Simultaneous Flowsheet and Sequential Heat Integration Optimization		█	█														
1.3	Simultaneous Flowsheet and Heat Integration Optimization				█	█												
2	Progress Report 1					█												
3	Continuation of Model Development						█	█		█								
4	Poster Presentation Preparation										█	█	█	█				
5	Pre-Engineering Design Exhibition (EDX)													█				
6	Engineering Design Exhibition (EDX)													█	█			
7	Report Writin : Final Dissertation													█	█	█	█	█
8	Final Oral Presentation																	█

Figure 9b: FYP II Project Gantt chart

CHAPTER 4

RESULTS AND DISCUSSION

4.1. NUMERICAL EXAMPLES

Case Study 1: Simultaneous optimization of MILP flowsheet problem without heat integration

Case Study 2: Simultaneous optimization of MILP flowsheet problem and minimum utilities problem (LP based on Papoulias and Grossmann (1983)) incorporated with heat integration.

4.1.1. Problem Data

Table 2: Hot streams data

Hot Stream	Supply temperature (°C)	Target temperature (°C)	Heat capacity (kJ/kg·°C)
LSRN1	88	40	236
HSRN2h	420	40	240
LSRN2	88	40	236
LSRN3	88	40	236
HSRN5h	400	40	240
REF	200	40	200
H2S1h	230	46	76
S	120	40	76
ISO	205	40	236

Table 3: Cold streams data

Cold Stream	Supply temperature (°C)	Target temperature (°C)	Heat capacity (kJ/kg·°C)
HSRN2c	179	370	240
NAP2	135	370	246
H2S1c	40	280	36
HSRN3	179	485	240
NAP4	135	485	246
HSRN4	179	485	240
NAP3	135	485	246
HSRN5c	179	505	240
H2	70	150	30
LSRN5	88	205	236

Table 4: Legend for modified state–task network superstructure representation

Symbols	Descriptions
CR	Crude oil
ADU	Atmospheric distillation unit
LSRN	Light straight run naphtha
HSRN	Heavy straight run naphtha
NAP	Naphtha
MIX	Mixer
SPLT	Splitter
VIS	Visbreaker
COK	Coker
FCC	Fluidized catalytic cracker
HCR	Hydrocracker
PCHN	Purchased naphtha
HDT	Hydrotreater
LPG	Liquefied petroleum gas
H2	Hydrogen
ISO	Isomerization unit
SRU	Sulfur recovery unit
REF	Reformer
S	Sulfur
FG	Fuel gas
BLND	Blending
FGH	Fuel gas header
GSLN	Gasoline
TG	Tail gas

4.1.2 Base Data

- i. Input data from user (the input values are in brackets):
 - a. Production requirement of gasoline (100,000kg/d)
 - b. Crude API gravity (44.6)
 - c. Crude oil cost (RM 120.0 per bbl)
 - d. Naphtha cost (RM 0.524 per kg)

- ii. Nelson–Farrar Refinery Construction Index (NFRCI) (Maples, 2000, p. 388; EU-OPEC Roundtable on Energy Policies, 2008):
 - a. Jan 1991 : 1241.7
 - b. Dec 2008 : 2067.2

- iii. Assumptions:
 - a. Refinery operates 330 days per year
 - b. Crude charge is fixed to be between 100 000 bbl/d to 150 000 bbl/d
 - c. Gasoline requirement of at least 100 000 kg/d

- d. Maximum capacity of each unit = 1×10^8 kg
- e. Total capital investment
= Fixed capital investment + Working capital
= Total equipment base cost + Working capital
- f. Total operating cost
= Fixed operating costs + Variable operating costs + General expenses
- g. Total cost
= Total capital investment + Total operating cost
- h. Revenues = Cost price for each product x Each product amount

iv. Utilities cost:

Table 5: Utilities cost per unit (www.mida.gov.my)(2008)

Utilities Cost per Unit (RM/unit)	
Electricity (per kWh)	0.1980
Fuel (per MJ)	0.1018
HP Steam (per kg)	0.0050
CW (per m ³)	0.8400

v. Base Capacity, Base Cost and Utilities Consumption of Major Unit Operations:

Table 6: Base cost and utilities consumption of major unit operations (Maples, 2000, p.386)

Process	Jan '91 (mil RM)	Dec '08 (mil RM)	Electricity (MWh/kg)	Fuel (kJ/kg)	Steam (kg/kg)	CW (m ³ /kg)
ADU	137	228	0.0039	0.0826	0.0888	0.0000
VIS	86	144	0.0039	0.0660	0.1776	0.0000
COK	166	276	0.0282	0.0991	0.1421	0.0000
FCC	310	515	0.0078	0.0660	0.0710	0.0119
HCR	342	569	0.1402	0.2766	0.0000	0.0000
HDT	58	96	0.0157	0.0248	0.0533	0.0000
REF	162	270	0.0078	0.2477	0.1421	0.0030
ISO	25	42	0.0078	0.0083	0.1279	0.0000
SRU (per tonne)	18	30	0.3132	0.0000	2.6636	0.1482

4.2. Case Study 1

4.2.1. Superstructure for Flowsheet Optimization

Figure 10 shows a state–task network (STN)-based superstructure representation that is sufficiently rich to embed all possible alternative topologies for the subsystem of naphtha produced from the atmospheric distillation unit (ADU) of a refinery. Constant-yield material balances are employed to represent the process units, mainly in order to preserve the model linearity (for an MILP formulation).

Description of Superstructure

The first processing step in petroleum refining is crude distillation, in which crude oil (CR) is distilled into oil fractions with respect to its boiling points. Naphtha constitutes the lighter fractions that are obtained from this process. Depending on the crude distillation column design and the refining economics, the ADU can produce: (a) light straight run naphtha (LSRN–1) and heavy straight run naphtha (HSRN–1), or (b) an undifferentiated class of naphtha, typically termed as “wild naphtha” (NAP–1), for which, the 0–1 structural variables of z_i are used to represent these three possible states of naphtha.

In the first case, LSRN–1 is mixed with purchased naphtha (PCHN–2) and LSRN–2 from the hydrotreater HDT–1 in a mixer (MIX–3). The output from MIX–3, i.e., LSRN–4, can undergo two processes: (a) it is used as a feedstock for the isomerization unit (ISO), and (b) it is sold as a final product. Isomerization yields isomerate (ISO), one of the blending components for gasoline (GSLN). Meanwhile, HSRN–1 is mixed with naphtha from the cracking of heavier fractions in MIX–1 before being sent to HDT–1 to be desulfurized. HDT–1 produces hydrogen sulfide gas (H₂S–1), liquefied petroleum gas (LPG–1), desulfurized naphtha (LSRN–2, HSRN–3, NAP–4), and fuel gas (FG–1). H₂S–1 is sent to the sulfur recovery unit (SRU) where sulfur (S) is extracted and finally sold. All LPG (LPG–1, –2, –3) are sent to MIX–6 and subsequently to the LPG recovery unit (LPG), from which treated LPG (LPG–5) is sold. Similar to the ADU outputs, the desulfurized naphtha from HDT–1 can be classified as light (LSRN–2) and heavy (HSRN–3) or wild (NAP–4). HSRN–3 is sent to a mixer (MIX–4), possibly with purchased naphtha

(PCHN-3-1) *and/or* naphtha from the hydrocracker (HCR-3). The output of MIX-4 (HSRN-5) is the feedstock for the reformer (REF). FG-1 goes to the fuel gas header (FGH), supplying fuel gas (FG-5) to the entire refinery. In the case that NAP-4 is produced from HDT-1, it is also mixed with purchased naphtha (PCHN-3-2) *and/or* naphtha from the hydrocracker (HCR-4) in MIX-5, whose output of NAP-5 is sent to the reformer. The products from the reformer are hydrogen gas (H₂), fuel gas (FG-3), LPG (LPG-2), and reformate (REFs). H₂ is a feed to the HDTs while reformate is used as a gasoline blending component. FG-3 is sent to the FGH.

In the second case involving NAP-1 exiting ADU, the processing route is similar to the first case in that NAP-1 is mixed with naphtha from cracking processes in MIX-2 before being hydrotreated in HDT-2. The products from HDT-2 are H₂S-2, LPG-3, desulfurized naphtha of LSRN-3, HSRN-4, and NAP-3, and FG-2. Each product has the exact same route as the products from HDT-1. Other than distillation, naphtha is also produced from the cracking of distillation bottoms in the visbreaker (VIS), coker (COK), catalytic cracker (FCC), hydrocracker (HCR). VIS has the lowest severity while COK has the highest

4.2.2. Non Heat-Integrated Superstructure

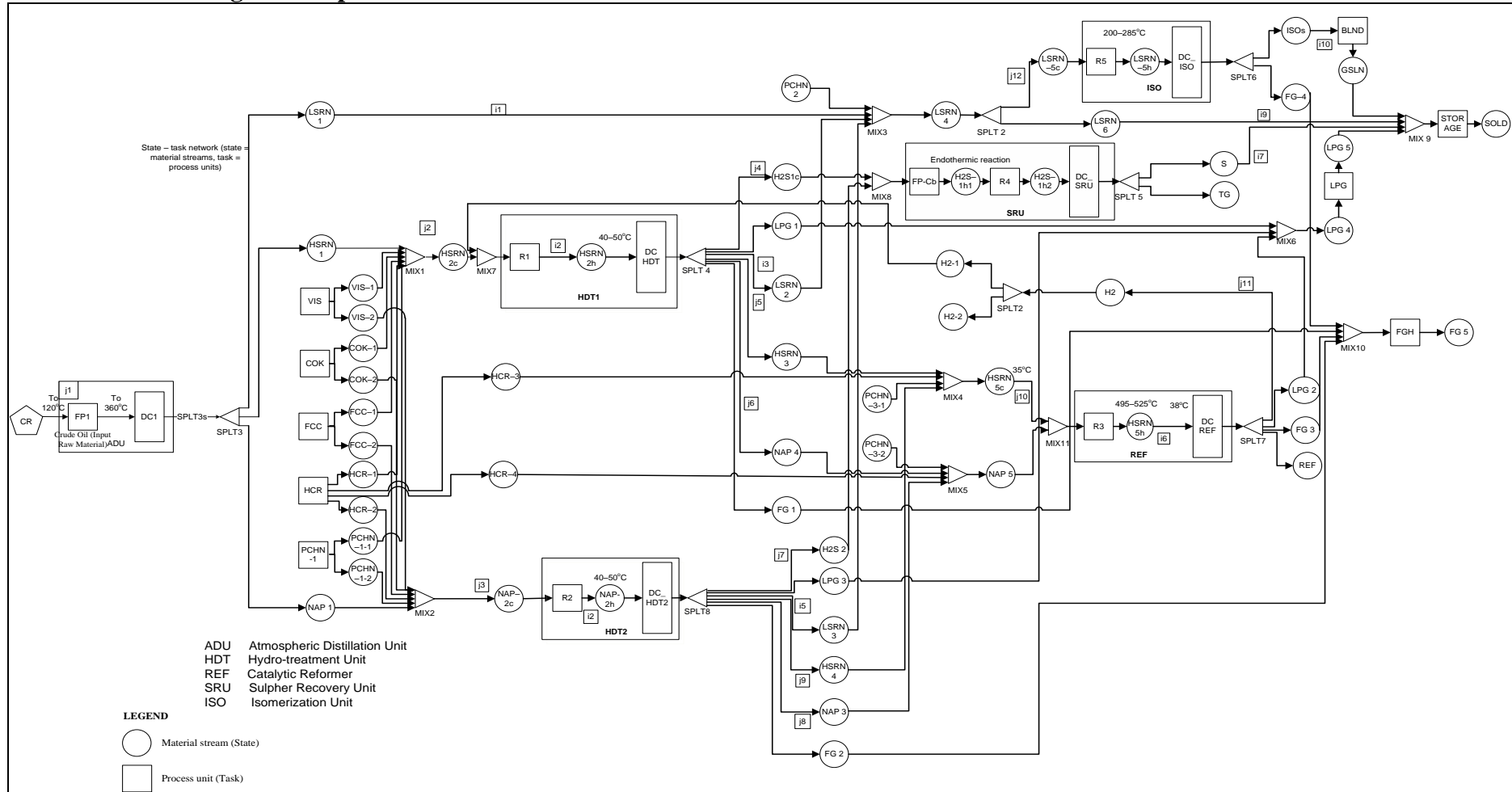


Figure 10: Modified state–task network (STN) superstructure representation for the naphtha produced from the atmospheric distillation unit (ADU)

Table 7: Optimum Flowrate for Case Study 1

Stream	Flowrate(kg/d)	Stream	Flowrate(kg/d)	Stream	Flowrate(kg/d)
COK	2000000.000	HSRN3	7.211114E+7	LSRN6	3247412.628
FCC	2000000.000	HSRN4	0	NAP1	1.044000E+7
FG1	1090000.000	HSRN5c	7.211214E+7	NAP2	0
FG2	0	ISO	2.893445E+7	NAP3	0
FG3	2668149.280	LPG1	580000.000	NAP4	0
FG4	292267.137	LPG2	5624747.131	NAP5	0
FG5	4050416.417	LPG3	0	PCHN1	8.125241E+7
GSLN	9.044610E+7	LPG4	6204747.131	PCHN2	6375268.983
H2	2307588.567	LPG5	6204747.131	PCHN3	1000.000
H2S1c	120000.000	LSRN1	0	REF	6.151166E+7
H2S1h	120000.000	LSRN2	2.609886E+7	S	101736.000
HCR	2000000.000	LSRN3	0	SOLD	1.000000E+8
HSRN1	0	LSRN4	3.247413E+7	TG	18264.000
HSRN2hs	1.000000E+8	LSRN5	2.922671E+7	VIS	0
HSRN2cs	9.769241E+7	HSRN5hs	7.211214E+7		

4.3 Case Study 2

Table 8: Legend for stream colors

Red	Hot stream: stream that requires cooling
Blue	Hot stream: stream that requires heating
Green	Stream that do not requires cooling or heating

4.3.1 Heat Integrated Flowsheet Superstructure

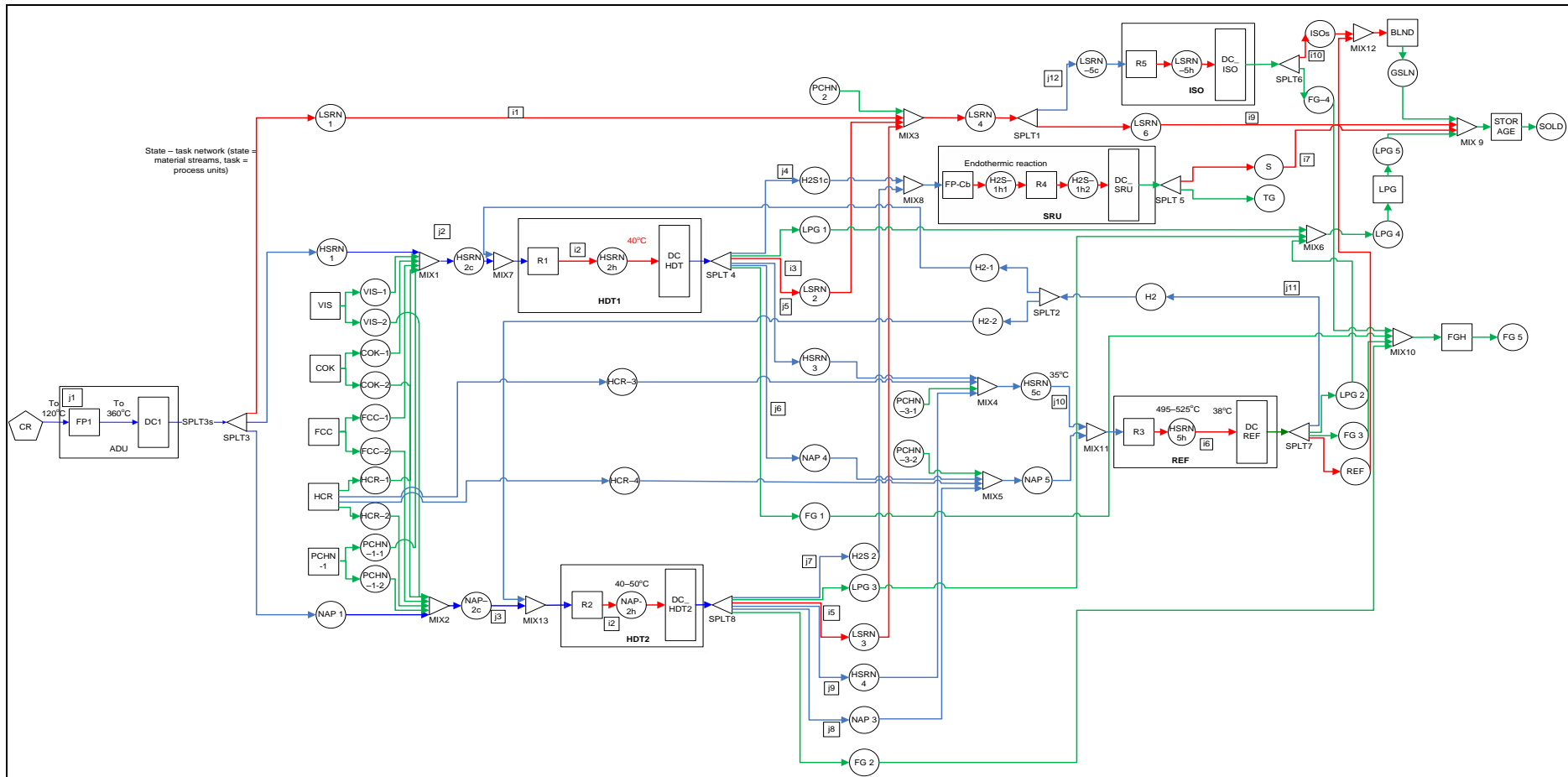


Figure 11: Modified state-task network (STN) superstructure representation for the naphtha produced from the atmospheric distillation unit (ADU) with identified hot and cold streams.

4.3.2. Heat-Integrated Flowsheet Optimization

The two models (MILP1) and (MILP2) are implemented on GAMS Integrated Development Environment (IDE) version 2.0.19.0 for Windows platform with the associated computational statistics as reported in Table 7. The model is solved using a branch and bound algorithm (with the inclusion of cutting planes) as executed in CPLEX with GAMS 22.3 (32-bit version). The CPU times are as reported by GAMS/CPLEX on the computing platform of 1.40 GHz Intel® Pentium® processor with 1GB of RAM computer running on Windows XP platform. The constraint satisfaction tolerance is specified to be 10^{-5} . The relative termination tolerance criterion is set at the GAMS default value of OPTCR = 0.1 while the absolute termination tolerance criterion assumes the GAMS default value of OPTCA = 0.0.

Table 10: Computational statistics of the model

Platform	GAMS 22.3 (32-bit version)
Computing systems	1.40 GHz Intel® Pentium® processor on an Acer Aspire 4736Z laptop with 1 GB of RAM computer running on Windows platform
Solver	CPLEX
No. of single continuous variables	2513
No. of binary variables	152
No of constraints	304
CPU time	0.047

4.3.3 Flowrates and Total Cost

Previously, similar problem but without the objective function of minimizing utility load (Loh, 2008) was solved to minimize plant's investment and operating costs. In this work, the change in the optimal topology and streams flowrates will be reported when introducing the LP transshipment model to simultaneously minimize plant's investment, operating cost and utility load. The optimum for flowrates and total cost for the plant is given in Table 8 and Table 9 respectively. The optimal topology obtained is shown in Figure 12.

Table 11: Optimum Flowrate for Case Study 2

Stream	Flowrate(kg/d)	Stream	Flowrate(kg/d)	Stream	Flowrate(kg/d)
COK	0	HSRN3	0	LSRN6	3247412.628
FCC	2000000.000	HSRN4	2.609886E+7	NAP1	5.00E+7
FG1	0	HSRN5c	7.211214E+7	NAP2	0
FG2	0	ISO	2.893445E+7	NAP3	0
FG3	2668149.280	LPG1	0	NAP4	0
FG4	292267.137	LPG2	5624747.131	NAP5	7.211214E+7
FG5	4050416.417	LPG3	580000.000	PCHN1	0
GSLN	9.044610E+7	LPG4	6204747.131	PCHN2	6375268.983
H2	2307588.567	LPG5	6204747.131	PCHN3	4.51E+7
H2S1c	0	LSRN1	0	REF	6.151166E+7
H2S2	120000.000	LSRN2	0	S	101736.000
HCR	0	LSRN3	2.609886E+7	SOLD	1.000000E+8
HSRN1	0	LSRN4	3.247413E+7	TG	18264.000
HSRN2h	0	LSRN5	2.922671E+7	VIS	0
H2S1h	120000.000	HSRN2c	0	HSRN5h	7.211214E+7

Table 12: Comparison of results on product flowrates and cost components in the objective function for Case Study 1 and Case Study 2

Details	Million \$ / year		Improvement
	Case Study 1	Case Study 2	
Product Revenues	2481.202	2481.202	
Total Capital Investment	0.001731	0.001731	0.00%
Total Operating Cost	5.9694792E+01	5.96961180E+01	0.0022%
Total Utilities	0.001005937	0.002031023	101.90%

The heating utility and cooling utility are only included in the model that correspond to minimum utility load. From the results, by employing the simultaneous flowsheet optimization with heat integration approach, we achieve a reduction in the overall total cost for the optimal refinery topology

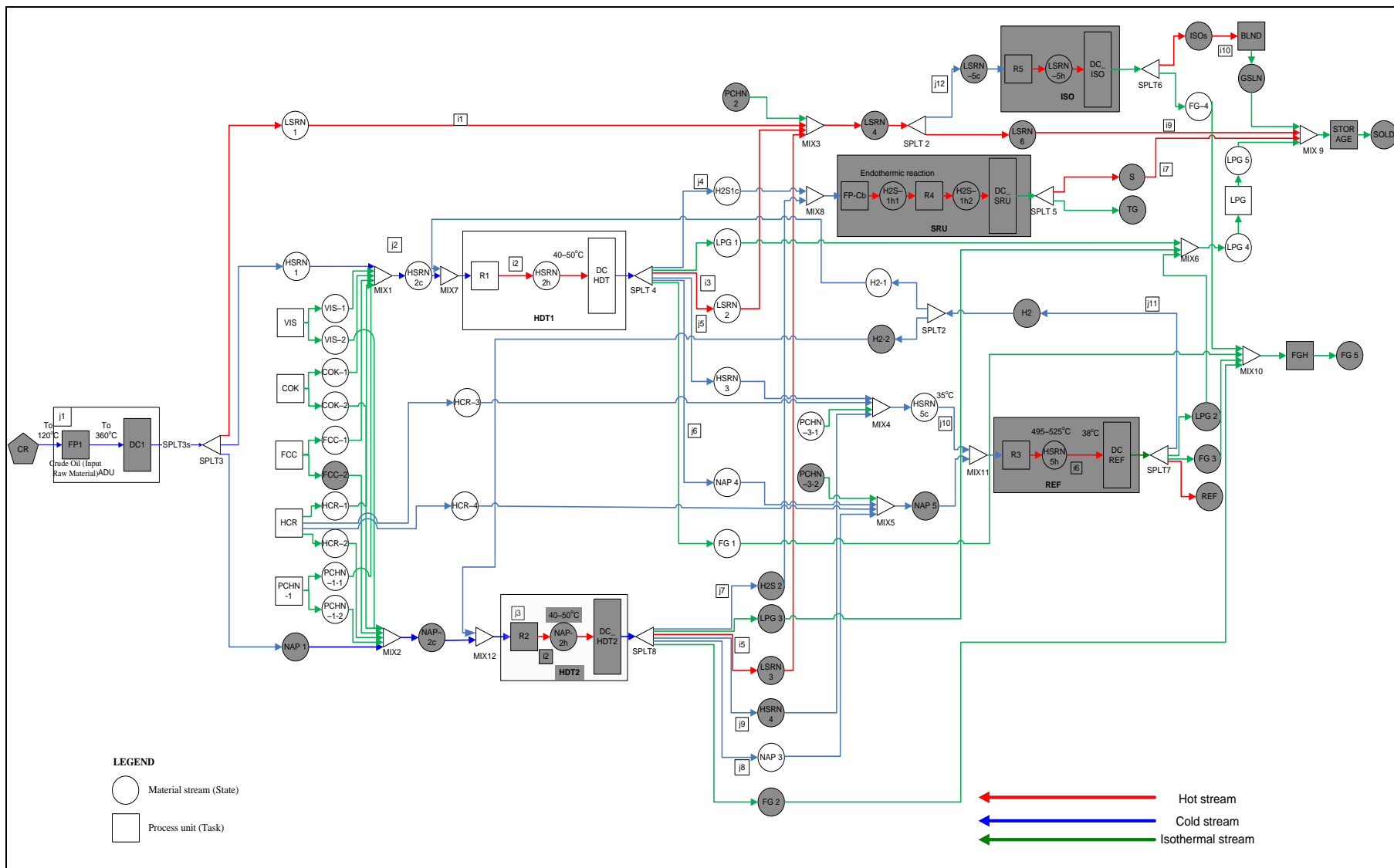


Figure 12a: Optimal selection of states and tasks for naphtha exiting the atmospheric distillation unit with heavy crude charge

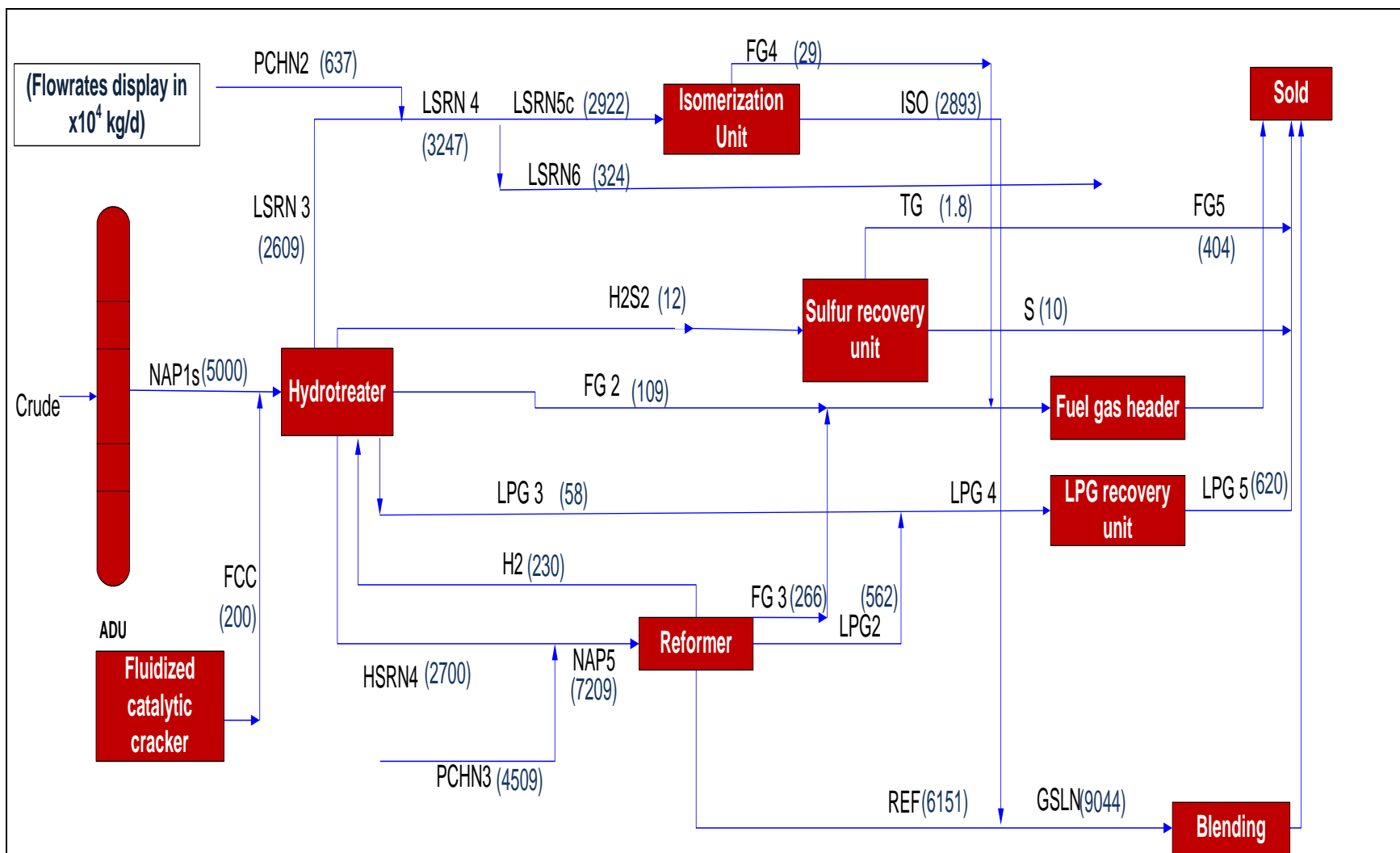


Figure 12b: Optimal flowsheet and heat integration for naphtha exiting the atmospheric distillation unit with heavy crude charge.

4.3.4 Utility Load & Cost

The minimum approach temperature required at all points of the network is specified at 10°C. In the absence of any restricted matches, the minimum utility cost is determined using the linear programming transshipment model formulation, consists of fourteen temperature intervals. The pinch location for this problem is at interval 9 corresponding to temperatures 120–110°C.

The total utilities load and cost is calculated and shown in Table 10

Table 13: Hot and cold utilities load and annual cost

Types of utilities	Total Load (MJ/yr)	Cost (million \$/year)
Fuel	7810290	843.51132
HP	7785600	38.92799699
MP	7703080	23.10924
LP	1453.458	0.002180187
CW	15102400	12.68601963

4.3.5 Heat Matches

The (MILP1) model, which incorporates heat integration via the LP transshipment network, solves for the minimum utility load and minimum plant investment and operating cost. The model will optimally increase the heat matches between the hot and cold streams to concurrently minimize the utility load. The heat matches determined in each interval are not representing the actual heat exchanger units.

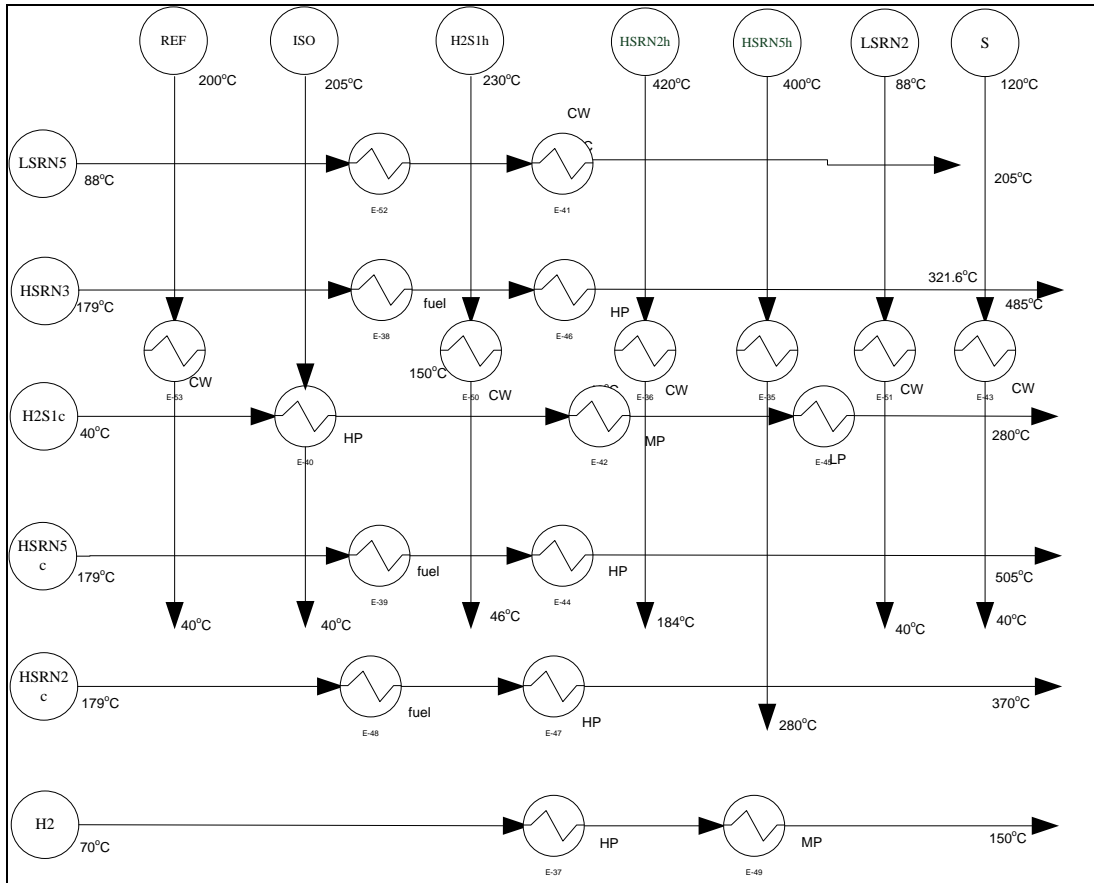


Figure 13: Optimal heat recovery network

CHAPTER 5

CONCLUSION

Result between Case Study 1 and Case Study 2 which mean comparison between heat integrated and non-heat integrated plant has been completely discussed. A huge reduction in the total utility cost has been seen as a result of adding heat integration features into the optimization model formulation. A superstructure representation embedding all feasible alternatives for naphtha produced from atmospheric distillation unit is developed with a suitable level of detail. Logical constraints on design and structural specifications for processing alternatives are developed.

Implementing heat integration in superstructure optimization will lead to an optimal refinery configuration that has a minimum heat utility cost. Such a project will reduce the designing cost and time which will have impact on petroleum industry.

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