CHAPTER II
BACKGROUND AND LITERATURE REVIEW

2.1 Crude Oil

Crude oil is a naturally occurred product made of the fossil remains of plants and animals. Crude oil is found in the pores of rocks either deep down into the surface of the earth and in the sea. Crude oil needs to be refined to become usable petroleum products such as gasoline, diesel, and various petrochemical feed stocks. Crude oil is ranging in viscosity and can vary in color to various shades of black and yellow depending on its commensurate hydrocarbon composition. Thus, that is why the chemical compositions of crude oils are surprisingly inconsistent and their physical characteristics vary widely.

Even though crude oil has a variety of physical property, Golovko *et al.*(2012) indicated that there are 30 structural types of the hydrocarbon with up to 43 carbon atoms. The series of C_{43} are specific only for the hydrocarbon types with no more than three rings in the molecule. Moreover, they showed that carbonate strata in the basin that under their investigation, independent on the depth of reservoir and the age of the host deposits. Nevertheless, the commensurate composition of crude oil usually is within the ranges as roughly showed below:

Table 2.1 Composition ranges of crude oil

Element	**Percent by weight**
Carbon	85 - 87
Hydrogen	11 - 14
Sulfur	0 - 2
Nitrogen	0.01 - 0.2
Oxygen	0.15 - 0.45

The group elements of carbon and hydrogen in crude oil are known as hydrocarbons. Crude oil can be categorized by its hydrocarbon types as follows:

- Paraffins: the general formula is C_nH_{2n+2} (where n is a whole number, usually from 1 to 20). Paraffinc hydrocarbons are mostly straight- or branched chain molecules and can be gasses or liquids at room temperature depending upon the molecules (for examples: methane, ethane, propane, butane, iso-butane, pentane, hexane, and etc.).

- Aromatics: the general formula is C_6H_5 - Y (where Y is a longer, straight molecule that connects to the benzene ring). Aromatic hydrocarbons are ringed structures with one or more rings, contain six carbon atoms, with alternating double and single bounds between the carbons and they are typically liquids (for examples: benzene and napthalene).

- Napthenes or Cycloalkanes: the general formula is C_nH_{2n} (where n is a whole number usually from 1 to 20). Naphthenic hydrocarbons are ringed structures with one or more ring that contain only single bounds between the carbon atoms. They are typically liquids at room temperature (for examples: cyclohexane, and methyl cyclopentane).

- Other hydrocarbons: Other types of hydrocarbons are Alkenes. The general formula is C_nH_{2n} (where n is a whole number, usually from 1 to 20). Alkenes are linear or branched chain molecules containing one carbon-carbon double-bond and can be liquid or gas (for examples: ethylene, butene, and iso-butene). The rest of hydrocarbons are Dienes and Alkynes, whose general formula is C_nH_{2n-2} (where n is a whole number, usually from 1 to 20). Dienes are linear or branched chain molecules containing two carbon-carbon double bond, whereas alkynes contain one carbon-carbon triple bond. These compounds can be either liquid or gas, for examples: Acetylene, and butadienes.

2.2 Heat Integration

Heat integration has been a subject of significant research activity in industrial processes in the past decades. Two major methodologies have been proposed, namely the sequential and the simultaneous approaches. The former is the most-widely known as the pinch design method (Linnhoff *et al.*, 1983), which focused-on the minimum utility requirement, the minimum units number of heat exchanger and the minimum capital cost of the network. Several heuristic rules are used to synthesize a network by incorporation of thermodynamic properties. The main limitation of this technology is the high resolution times especially in the case of large networks, and, consequently, can make this method inappropriate for the aim. The latter methodology is based on a mathematical programming to sequentially or simultaneously synthesize the minimum utility requirements and determining the stream matches with the minimum number of units for a fixed utility cost. Examples of this methodology include the transportation problem formulation (Cerda *et al.*, 1983) and the transshipment model (Papoulias *et al.*, 1983).

2.3 State of the Arts for Heat Exchanger Network Synthesis

Heat integration and HEN synthesis, which is a heuristic approach to utilize energy efficiently and economically, has been widely used either in the petroleum or petrochemical industries. Likewise, there are many innovations, and a lot of research effort to develop the models for network synthesis problem.

2.3.1 HEN Configuration Design

Since the mathematical programming was developed in 1980, the approaches to solve the heat exchanger network synthesis problem have been classified as simultaneous and sequential techniques (Figure 2.1). For solving objective, these techniques consider the trade-off between operation and capital cost to find an optimal point or minimum total annual cost. Sequential technique decomposes the problem to determine first utility, number of unit and investment cost and then synthesize the network. Therefore, the main advantage of this approach

is based on the decomposition of the problem into simpler sub-problems which can be treated in a much easier fashion than the original single-task problem, but as a consequence it may not yield an optimal network.

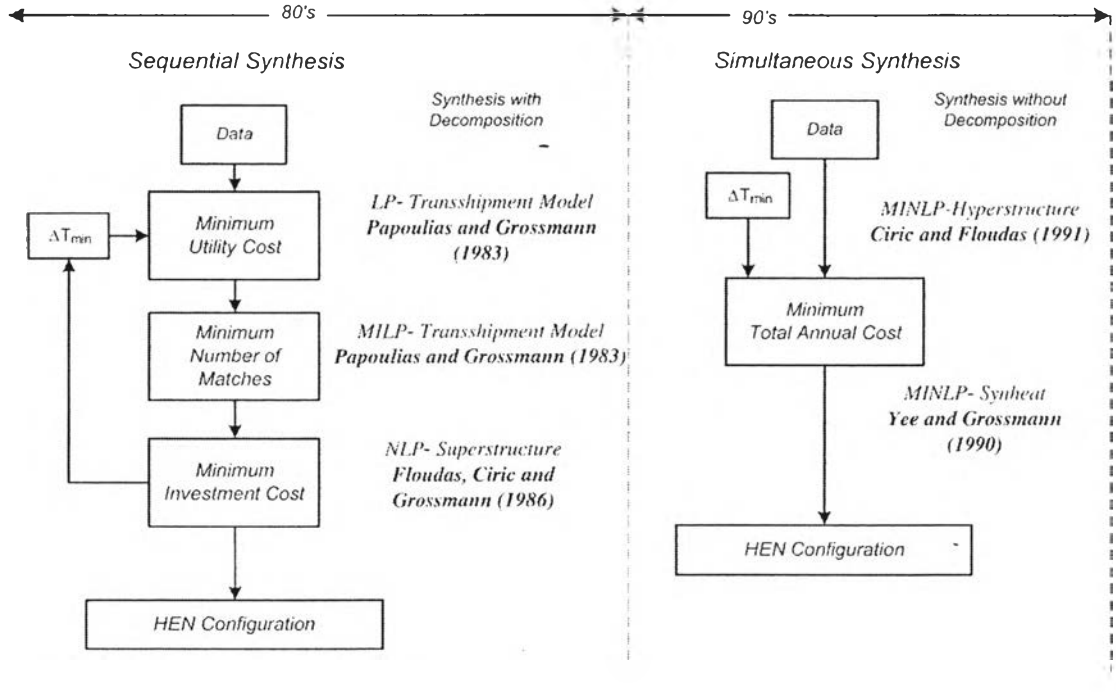


Figure 2.1. Classical HEN approaches over the last decades (Escobar *et al.*, 2013).

In the other hand simultaneous technique synthesize the network as a single task. The problems are usually formulated based on MINLP, however, MINLP techniques can result in a more complex MINLP problem (Escobar *et al.*, 2013).

Among the superstructure-based models for HEN design, the most popular one is a stage-wise superstructure approach (Figure 2.2) or SYNHEAT model that was proposed by Yee and Grossmann (1990). One interesting feature of the proposed superstructure is that all constraints are linear. It uses a superstructure in which the problem is decomposed into stages, and in each stage the corresponding steam is split and directed to a heat exchanger for each potential matching between hot and cold streams. The outlet temperature of each stage are mixed at the same temperature, i.e. isothermal mixing. The isothermal mixing assumption eliminates the requirement for non-linear heat balances around heat exchangers as well as non-linear heat mixing equations. In the stage-wise superstructure, the utility is located at

the extreme of superstructure. Although SYNHEAT is user-friendly and robust for trivial problems, it can result in more complex MINLP models when adding the area equations with complex and non-convex log mean temperature calculation.

Combination the aforementioned two-step approach of linear problem and non-linear problem into a single step by using an MINLP formulation to optimize the heat exchanger area, energy consumptions, and variety features of HEN (Ciric *et al.*, 1989; Ciric *et al.*, 1990). Some researchers provided a step by step interaction approach for a retrofit scenario by combining the Pinch technology and the mathematical programming (Asante *et al.*, 1996). Asante and Zhu introduced a scope of pinch technology that identified the smallest gap temperature approach of hot and cold streams in the composite curve. Once a topology is changed by adding a new heat exchanger, new splitting, or relocating an existing heat exchanger, then a new-topology is analyzed by a non-linear programming (NLP) method. The procedure is repeated till the network could not reach any better economical solution or identify any topological change.

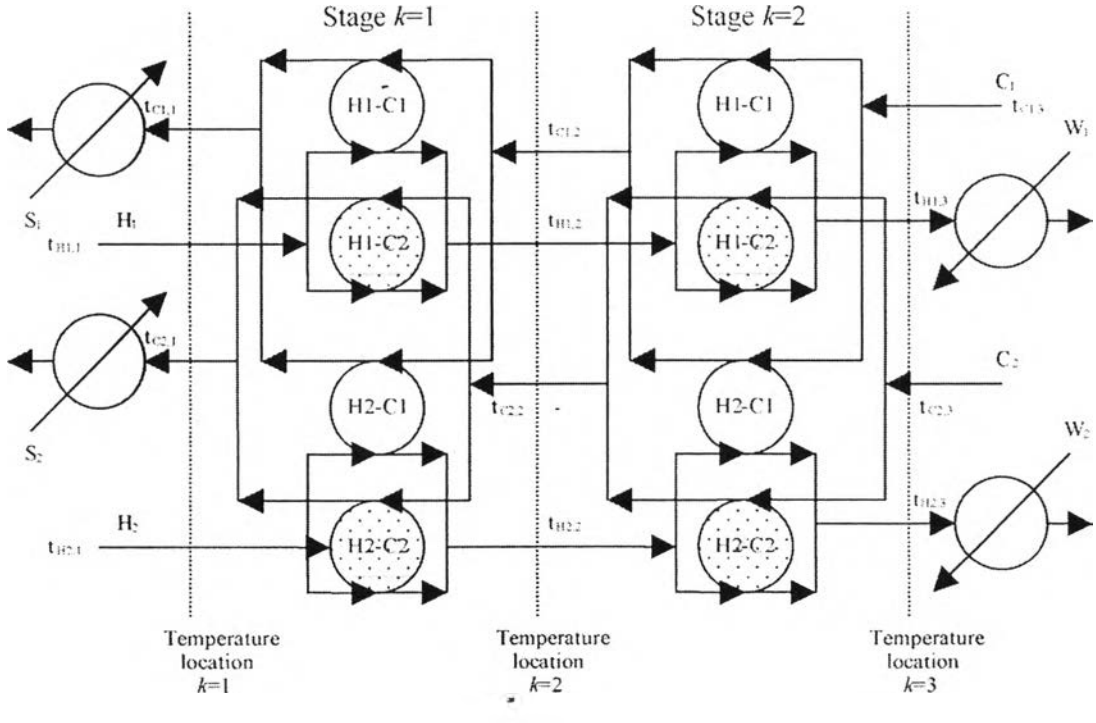


Figure 2.2 The two-stage superstructure (Yee *et al.*, 1990).

Figure 2.2 depicts a postulated stage-wise superstructure or SYNHEAT model with isothermal mixing that is the most well-known model and widely used in heat exchanger network synthesis. As it showed above the process streams are divided into two sets, HP for hot streams, declared by index i, and CP for cold streams declared by index j. The number of stage, N_T, is a total set of max[N_H,N_C], where N_H and N_C are the number of hot and cold streams, respectively. For each stage, k is used to denote the superstructure stage given by a set ST. The corresponding stream is split and directed to a heat exchanger for each potential matching between hot and cold streams. The outlet temperature of each stage are mixed and treated as variables in the formulation. Indices HU and CU represent the heating and cooling utilities, respectively. The following are parameters and variables that are used in the formulation:

2.3.1.1 Parameter Definition

TIN = inlet temperature of stream

TOUT = outlet temperature of stream

F = heat capacity flow rate

U = overall heat transfer coefficient

CCU = unit cost for cold utility

CHU = unit cost of hot utility

CF = fixed charge for exchangers

C = area cost coefficient

Ω = upper bound for heat exchange

NOK = total number of stages

CP = set of cold stream

HP = set of hot stream

EMAT = exchanger minimum approach temperature

Γ = upper bound for temperature different

β = exponent for area cost

2.3.1.2 Variable Definition

dt_{ijk} = temperature approach for matching (i,j) at temperature location k

$dtcu_i$ = temperature approach for the match of hot stream i with cold utility

$dthu_j$ = temperature approach for the match of cold stream j with hot utility

q_{ijk} = heat exchanged for the match of hot stream i with cold process stream j within stage k

qcu_i = heat exchanged between hot steam i and cold utility

qhu_i = 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 cold begin of stage k

z_{ijk} = binary variable for existence of match (i,j) in stake k

zcu_i = binary variable to denote that cold utility exchange heat with stream i

zhu_j = binary variable to denote that hot utility exchange heat with stream j

In the model formulation, an overall heat balance is needed to ensure sufficient heating or cooling of each process stream. At each stream, the overall heat transfer requirement of each stream is equal to the summation of the heat exchange with other streams.

$$\sum_{k\in ST}\sum_{j\in CP} q_{ij} + qcu_i = (\mathrm{TIN_i} - \mathrm{TOUT_i})\mathrm{F_i}\,, \mathrm{i} \in \mathrm{HP} \tag{2.1}$$

$$\sum_{k\in ST}\sum_{i\in CP} q_{ij} + qhu_j = (\mathrm{TOUT_j} - \mathrm{TIN_j})\mathrm{F_j}\,, \mathrm{j} \in \mathrm{CP} \tag{2.2}$$

To satisfy the energy balance of the system, the energy balance at each stage is also needed for the superstructure to evaluate the temperatures. Note that for the two-stage superstructure as shown in Figure 2.2, three temperatures, t, are required. In order to simplify the model, an isothermal mixing is assumed at each stage. The energy balances at the mixers are no longer needed and no variable for the flows. For every outlet temperature of the hot and cold stream leaving each stage is the same as the inlet temperature of the downstream stage. Thus the energy balance for each stage is linear:

$$\sum_{j\in CP} q_{ijk} = \left(\mathrm{T_{i,k}} - \mathrm{T_{i,k+1}}\right)\mathrm{F_i}\,, \mathrm{i} \in \mathrm{HP}, \mathrm{k} \in \mathrm{ST} \tag{2.3}$$

$$\sum_{i\in HP} q_{ijk} = \left(\mathrm{T_{j,k}} - \mathrm{T_{j,k+1}}\right)\mathrm{F_j}\,, \mathrm{j} \in \mathrm{CP}, \mathrm{k} \in \mathrm{ST} \tag{2.4}$$

Fixed supply temperatures (TIN) of the process streams are assigned as the inlet temperatures to the superstructure. In Figure 2.2, for hot streams the inlet temperature corresponds to the location k=1, while the inlet temperature corresponds to the location k = 3 for cold streams.

$$t_{i,1} = \mathrm{TIN_i}\,, \mathrm{i} \in \mathrm{HP} \tag{2.5}$$

$$t_{j,NOK+1} = \mathrm{TIN_j}\,, \mathrm{j} \in \mathrm{CP} \tag{2.6}$$

The temperature constraints are specified to ensure a monotonic decrease of temperature at each successive stage. A bound is settled for the outlet temperature. In addition, the outlet temperature of each stream at the last stage does

not necessarily match to the stream target temperature since the utility exchanges can occur at the outlet of the model.

$$t_{i,k} \geq t_{i,k+1}, i \in HP, k \in ST \quad (2.7)$$

$$t_{j,k} \geq t_{j,k+1}, j \in CP, k \in ST \quad (2.8)$$

$$TOUT_i \leq t_{i,NOK+1}, i \in HP \quad (2.9)$$

$$TOUT_j \geq t_{j,1}, j \in CP \quad (2.10)$$

The hot and cold utility load requirements are evaluated for each process stream from the outlet temperature of the last stage and the target temperature of each stream as follows:

$$qcu_i = \left(t_{i,NOK+1} - TOUT_i\right) F_i, i \in HP \quad (2.11)$$

$$qhu_j = \left(TOUT_j - t_{j,1}\right) F_j, j \in CP \quad (2.12)$$

Logical constraints and binary variables are needed to determine the existence of a match between a hot and a cold stream in stage k, namely z_{ijk} and matches between a process stream and utilities, namely zcu_i for the process and cold utility match, and zhu_j for the process and hot utility match. The upper bound constraints are needed to relate the existence of heat loads with the binary variables in the Equations 2.13, 2.14, and 2.15 where Ω is equal to the maximum possible number of heat load in the process. An integer value for any binary variable corresponding to the existence of heat load will be forced to unity, if the heat load at stage k of matching stream (i,j) is not zero. However, the objective function will force the binary variable to be zero in order to minimize the number of units.

$$q_{ijk} - \Omega z_{ijk} \leq 0, i \in HP, j \in CP, k \in ST \quad (2.13)$$

$$qcu_i - \Omega z_{ijk} \leq 0, i \in HP, j \in CP, k \in ST \quad (2.14)$$

$$qhu_j - \Omega z_{ijk} \leq 0, i \in HP, j \in CP, k \in ST \quad (2.15)$$

The area requirement of each match will be incorporated in the objective function. Calculation of the approach temperature is needed to be determined. To ensure feasible driving forces for exchangers that are selected in the optimization procedure, the binary variables used to identify the existence of heat loads are used to activate or deactivate the following constraints to determine the approach temperatures. The upper bound temperature difference is set as a constraint to calculate the temperature approach in Equations 2.16, 2.17, 2.18, and 2.19, where r is the maximum temperature difference of the process-process or the process-utility steams. If the heat load at stage k of matching stream (i,j) is zero, the equation is deactivated. That means that the temperature different between stream (i,j) is zero and dt_{ijk} is less than or equal to r.

$$dt_{ijk} \leq t_{ik} - t_{jk} + r(1 - z_{ijk}), i \in HP, j \in CP, k \in ST \quad (2.16)$$

$$dt_{ijk+1} \leq t_{ik+1} - t_{jk+1} + r(1 - z_{ijk}), i \in HP, j \in CP \quad (2.17)$$

$$dtcu_i \leq t_{i,NOK+1} - TOUT_{CU} + r(1 - z_{ijk}), i \in HP, j \in CP \quad (2.18)$$

$$dthu_j \leq TOUT_{HU} - t_{i,1} + r(1 - z_{ijk}), i \in HP, j \in CP \quad (2.19)$$

All the temperature differences are always positive. Then, one can specify a minimum approach temperature so that in the network, the temperature approach between the hot and cold stream at any exchanger will be at least equal to EMAT by adding the following constraints:

$$dt_{ijk} \geq EMAT \quad (2.20)$$

$$dtcu_i \geq EMAT \quad (2.21)$$

$$dthu_j \geq EMAT \quad (2.22)$$

Finally, the objective function can be defined as the trade-off between the investment and the operating costs. LMTD is the logarithmic mean temperature difference for each heat exchanger and is replaced by Chen approximation (Chen, 1987).

$$LMTD_{ijk} = \left[dt_{ijk} dt_{ijk+1} \frac{dt_{ijk}+dt_{ijk+1}}{2}\right]^{1/3}, \mathrm{i} \in \mathrm{HP}, \mathrm{j} \in \mathrm{CP} \quad (2.23)$$

$$LMTD_{CUi} = \left[dtcu_i\left(\mathrm{t_{i,NOK+1}} - \mathrm{TOUT_{i,}}\right) \frac{dtcu_i+\left(\mathrm{t_{i,NOK+1}}-\mathrm{TOUT_{i,}}\right)}{2}\right]^{1/3} \quad (2.24)$$

$$LMTD_{HUj} = \left[dthu_j\left(\mathrm{TOUT_j} - \mathrm{t_{j,1,}}\right) \frac{dthu_j+\left(\mathrm{TOUT_j}-\mathrm{t_{j,1,}}\right)}{2}\right]^{1/3} \quad (2.25)$$

LMTD approximation is to avoid the numerical difficulties of the LMTD equation when the approach temperatures (dt1, dt2) for both side of exchanger are zero, the driving force will be converted to zero. Area calculation of process-process heat exchangers can be calculated by the following equation:

$$q_{ijk} - A_{ijk}\mathrm{U_{ij}LMTD_{ijk}} \leq 0, \mathrm{i} \in \mathrm{HP}, \mathrm{j} \in \mathrm{CP}, \mathrm{k} \in \mathrm{ST} \quad (2.26)$$

$$q_{CUi} - A_{CUi}\mathrm{U_{iCU}LMTD_{CUi}} \leq 0, \mathrm{i} \in \mathrm{HP}, \mathrm{j} \in \mathrm{CP}, \mathrm{k} \in \mathrm{ST} \quad (2.27)$$

$$q_{HUj} - A_{HUj}\mathrm{U_{jHU}LMTD_{HUj}} \leq 0, \mathrm{i} \in \mathrm{HP}, \mathrm{j} \in \mathrm{CP}, \mathrm{k} \in \mathrm{ST} \quad (2.28)$$

Then, additional bounds of the variables are needed as follows:

$$TOUT_i \leq t_{i,k} \leq \mathrm{TIN_i}, \ \mathrm{i} \in \mathrm{HP} \quad (2.29)$$

$$TOUT_j \geq t_{j,k} \geq \mathrm{TIN_j}, \ \mathrm{j} \in \mathrm{CP} \quad (2.30)$$

$$0 \leq q_{ijk} \leq \min\left\{(\mathrm{TIN_i} - \mathrm{TOUT_i})\mathrm{F_i}, (\mathrm{TOUT_j} - \mathrm{TIN_j})\mathrm{F_j}\right\} \quad (2.31)$$

$$0 \leq q_{CUi} \leq (\mathrm{TIN_i} - \mathrm{TOUT_i})\mathrm{F_i}, \quad \mathrm{i} \in \mathrm{HP} \quad (2.32)$$

$$0 \leq q_{HUj} \leq (\mathrm{TOUT_j} - \mathrm{TIN_j})\mathrm{F_j}, \quad \mathrm{j} \in \mathrm{CP} \quad (2.33)$$

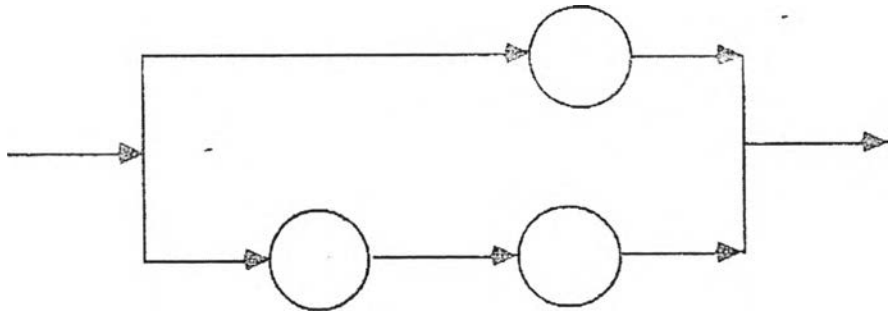
The objective function is defined as follows:

$$\min Cost = CCU \sum_{i\in HP} qcu_i + CHU \sum_{j\in CP} qhu_j + CF_{ij} \sum_{i\in HP}\sum_{j\in CP}\sum_{k\in ST} z_{ijk} + \sum_{i\in HP} CF_{i,CU} zcu_i + \sum_{j\in CP} CF_{j,hU} zhu_j + C\sum_{i\in HP}\sum_{j\in CP}\sum_{k\in ST} A_{ijk}^{\beta} + C\sum_{i\in HP} A_{cui}^{\beta} + C\sum_{j\in CP} A_{huj}^{\beta} \quad (2.34)$$

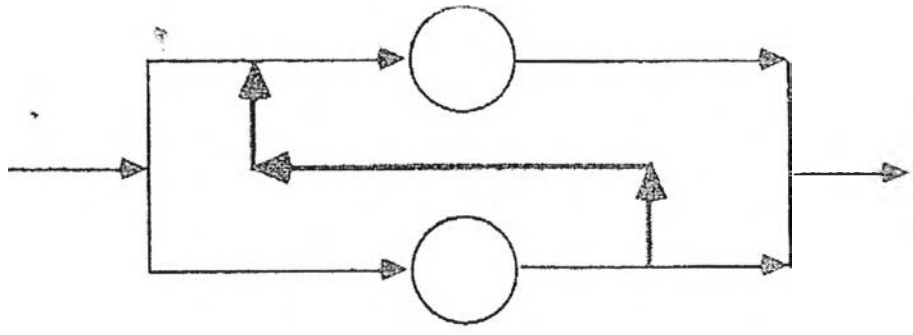
where,

$$\frac{1}{U_{ij}} = \frac{1}{\mathrm{h_i}} + \frac{1}{\mathrm{h_j}}; \ \frac{1}{U_{i,CU}} = \frac{1}{\mathrm{h_i}} + \frac{1}{\mathrm{h_{CU}}}; \ \frac{1}{U_{j,hU}} = \frac{1}{\mathrm{h_j}} + \frac{1}{\mathrm{h_{HU}}} \quad (2.35)$$

The main proposed MINLP model for the synthesis problem consists of the objective function in Eq.(2.34) subject to the feasible values defined by Eq.(2.1) to Eq.(33). The continuous variables (t, q, qhu, qcu, dt, dtcu, and dthu) are non-negative and the values of discrete variables (z, zcu, zhu) are 0 and 1. However, there are nonlinearities in the objective function because Eq.(2.23) to Eq.(2.25) may reach to more than one optimal solution due to their non-convex nature. Likewise, from the mathematical algorithm, it is noted that there are certain alternatives in the network configuration. Specifically, the superstructure does not include case of branch stream which contains two or more exchangers in the series and the case of stream bypasses, as shown in Figure 2.3 In general, the effect of the stream bypasses has been disregarded as a significant limitation because these are usually not required and also not favorable. Although decreasing the number of units may be done by the use of stream bypass, it resulted in an increase in the heat exchanger area. On the other hand, the more important network, which is neglected in the superstructure, is the case where a split stream contains more than one heat exchanger in series. In this regard, there is not much flexibility in selecting structures. Therefore, this limitation may cause the global optimal being excluded in HEN.



a) A split stream going through exchangers in series



b) A stream by-pass

Figure 2.3 Limitations of superstructure (Yee *et al.*, 1990).

Due to the fact that the nature of MINLP is non-convex, the global optimization of non-convex MINLP problem that contains bilinearities was proposed (Faria *et al.*, 2011). Débora *et al.* (2011) presented a special method, which contracts the bounds of one variable at a time and allowed a reduction of the gap between a linear lower and upper bounds. The authors concentrated on the linearization of Chen's approximation equation, and modified the logarithmic mean temperature equation by applying the temperature differences equation to reduce the number of variables is in the equations.

Finally, an important point of this application of the proposed model is the selection of the number of stages. A simple alternative set of the number of stages is equal to the maximum number of hot or cold streams. Albeit this alternative is often adequate, there is a possibility that the maximum heat recovery network is excluded. From that reason, preliminary screening procedure for selecting the number of stages, and eliminating units in the superstructure are proposed (Daichendt *et al.*, 1994), to guarantee the maximum heat recovery networks and, consequently, this procedure can greatly reduce the size of the MINLP. Thus, a recommended choice is to set the number of stages equal to the number of temperature intervals with EMAT.

In industries, stream splitting and mixing are not preferable in the design of HEN, because it is not only difficult to solve the model, but also hard to control the process. Therefore, a global optimization approach for the heat exchanger

network synthesis with no stream splits was investigated (Zamora *et al.*, 1997). Solving for the solutions of the mathematical model in HEN synthesis is not straightforward due to the non-convex terms in the MINLP model and gives rise to a number of numerical complications. The proposed algorithm is able to handle the non-convexities, which are introduced by the LMTD. To become a convex MINLP model, a lot of effort has been done to develop a class of bounding that is used to predict the lower bounds for the minimum total annual cost of HEN, namely HENS-LB model. This method can simplify the HENS-LB because all constraints are linear. This model can slightly reduce the annual cost; however, more than double of the heat transfer area was obtained at the global optimum and the model was inconsistent. From their aforementioned results, the authors then proposed a new approach relying on the use of two different sets of convex to underestimate the heat transfer area (Zamora *et al.*, 1998). Their results demonstrated that even though the sub-optimal network consumes less energy than the global optimal solution, the penalty for the limited number of branches or no stream splits resulted in higher utilities, and a higher total heat transfer area.

In 2001, Ji and Bagajewicz introduced a rigorous procedure for the design of conventional atmospheric crude fractionation units. First they aimed to find the best network of a multipurpose crude distillation unit that can handle various type of crude oil. To obtain an optimal scheme, heat demand-supply diagrams were used as a guide instead of using the composite curves. Therefore, the total energy consumption from streams, heaters and coolers clearly showed that this process can easily reach optimal. Later, Soto and Bagajewicz (2001) proposed the multi-purpose heat exchanger network, which can process variety of crude. In order to overcome the small gap between hot and cold stream line in the composite curves, the minimum heat recovery approximation temperature (HRAT) and the exchanger minimum approach temperature (EMAT) of models were generated and fixed. After that they attempted to establish a model for determining a heat exchanger network above and below the desalter with only two branches. The total annualized costs, utility cost and capital cost, of the solution are limited to a two branches that are compared with the four branches. Also, in this part, the model was based on a

transshipment model and the vertical heat exchanger constraints combined with the HRAT/EMAT. Furthermore, their investment cost was not controlled in this model but indirectly controlled by the minimum number of units. The less number of units simultaneously causes the minimum capital cost and energy consumption.

Generally the grass-root design of heat exchanger network synthesis problem is classified into two tasks: minimum utility, and the selection of the number of stream matches configuration. Combining the tasks into a single optimization problem, all of the solution provides simultaneously the optimal energy consumption, matching and network configuration (Ciric *et al.*, 1991) by performing several optimization loops to determine more optimal networks. Babaro and Bagajewicz (2005) established a new rigorous heat exchanger network synthesis using a mixed integer linear programming (MILP) which was capable in many real-world scenarios. Their methodology dose neither rely on traditional super-targeting network design by the pinch technology, nor is a nonlinear model, the model is linearized by dividing the energy balance of each stream, which is based on data and using multi-variable management. Moreover, they can combine many tasks; i.e. incorporating various costs for exchanger area including additional and reduction area of existing shell, adding area as a new shell, and passing heat exchange.

2.3.2 Designed and Modified Mathematical Algorithm

New evolution of mathematical algorithm is one strategy to generate a good solution in HEN synthesis for large scale energy integration systems. Therefore, researchers have put effort to develop new approach for solving such problems with fast convergence and better results.

Genetic algorithm, namely GA/SA (genetic algorithm/simulated annealing) (Yu *et al.*, 2000) is famous one. The key success of this method was how to diversify a number of variables/parameters properly, and reduce the number of optimization variables. In some applications, the algorithm, which based on GAs, was developed to avoid the convergence difficulties associated with the introduction of non-convex equations. The use of two GAs for the optimization of the network were classified to a binary GA for the structural optimization and a continuous GA

for optimizing the heat loads (Ponce-Ortega *et al.*, 2008). However this strategy did not effectively keep the diversification in a population. Thus, a hybrid genetic algorithm combining the local optimization and the structure control strategy, was developed (Luo *et al.*, 2009). The results obtained from this algorithm indicated that the genetic algorithm would be suitable for a complex process design. Although the genetic algorithm does not use the gradient information of the objective function, the mathematical model can be built up in a more practical manner.

To achieve a difficult class of the optimization problems as in the case of maximum energy recovery heat exchanger network (MER) based on heuristic methods, the Deterministic Algorithm was proposed (Errico *et al.*, 2007). Although this method can design a HEN with equal or minor number of exchangers by applying the Pinch method or Genetic Algorithms, it did not consider the configuration of the network. The introduction of this method excluded the objective function, which was the most non-linearity part, due to the LMTD term in the heat transfer area calculations. Thus, an additional objective function that is considered only the energy targeting without the effect of multiple objective functions can cause more complexity and tightness to the model.

Disjunctive optimization model is the application of logic disjunctions to the explicit model. Grossmann and Yeomans (1998) presented a new disjunctive model for simultaneous process optimization and heat integration that can rigorously handle both isothermal and non-isothermal process. An MINLP problem and logic relations, which is based on the heat cascade and applied to the pinch location method. However this strategy avoided the use of smoothing functions, and gave rise to a serious difficult problem when dealing with the non-isothermal case. Albeit the proposed MINLP model can be reduced to an MILP problem by assuming only relevant isothermal streams. Hence, this formulation guaranteed a global optimum solution (Grossmann *et al.*, 1998). Because the MINLP model required solving several NLP and MILP problems, the tightness of this strategy was reflected in the small or non-existent nodes in the branch and bound search. In addition, there were also some possibilities that the solutions reach the sub-optimal solution by the NLP model.

Björk and Westerlund (2002) proposed a global optimization method for synthesing HEN problems to show the effect of with and without isothermal mixing by using modified mathmitical algorithm. In their work, they modified area equations (Eqs 2.36-2.38) that are nonlinear constraints in the optimization model:

$$\frac{q_{i,j,k}}{A_{i,j,k}^{\frac{1}{\beta_{i,j}}}} - \frac{2}{3}U_{i,j}dt_{i,j,k}^{\frac{1}{2}}dt_{i,j,k+1}^{\frac{1}{2}} - \frac{1}{6}U_{i,j}dt_{i,j,k} - \frac{1}{6}U_{i,j}dt_{i,j,k+1} \leq 0,$$

$$\forall\, i \in HP, j \in CP, k \in ST \qquad (2.36)$$

$$\frac{qcu_i}{Acu_i^{\frac{1}{\beta_{i,cu}}}} - \frac{2}{3}U_{i,cu}dtcu_i^{\frac{1}{2}}dtcup_i^{\frac{1}{2}} - \frac{1}{6}U_{i,cu}dtcu_i - \frac{1}{6}U_{i,cu}dtcup_i \leq 0,$$

$$\forall\, i \in HP \qquad (2.37)$$

$$\frac{qhu_j}{Ahu_j^{\frac{1}{\beta_{j,hu}}}} - \frac{2}{3}U_{j,hu}dthu_j^{\frac{1}{2}}dthup_j^{\frac{1}{2}} - \frac{1}{6}U_{j,hu}dthu_j - \frac{1}{6}U_{j,hu}dthup_j \leq 0,$$

$$\forall\, j \in CP \qquad (2.38)$$

$$\min Cost = CCU \sum_{i \in HP} qcu_i + CHU \sum_{j \in CP} qhu_j + CF_{ij} \sum_{i \in HP} \sum_{j \in CP} \sum_{k \in ST} z_{ijk} + \sum_{i \in HP} CF_{i,CU} zcu_i + \sum_{j \in CP} CF_{j,hU} zhu_j$$

$$+C \sum_{i \in HP} \sum_{j \in CP} \sum_{k \in ST} A_{i,j,k} + C \sum_{i \in HP} Acu_i + C \sum_{j \in CP} Ahu_j \qquad (2.39)$$

The main difference is found in the constraint, the non-convex terms are ones of the form $q/A^{1/\beta}$ and the rest of the terms are convex. They showed that the constsaints can be relaxed in this way, while the areas are minimized by objective function which are linearized (Eq 2.39). In the optimization of the Synheat model, the objective is to convexify the term $q/A^{1/\beta}$. The replaced the non-convex term by transformation of the variable q to Q according to $q = \exp(Q)$. They prove that $\exp(Q)/A^{1/\beta}$ is convex on R^+ by using the Hessian-matrix of $f(x,y) = y^{-k} \exp(x)$, where, k is a constant and x, y, $k \geq 0$, is convex. The constraint $q = \exp(Q)$ is also convex, but the concave relationship in the equation can be approximated with a piece-wise linear function (Figure 2.4). If this method is applied on $Q = \ln(q)$, the model will be convex. But the disadvantage of this methos is that the variable Q will

always be underestimated due to the piece-wise linear approximation. Therefore, this procedure leads to a relaxation of the feasible region of their model.

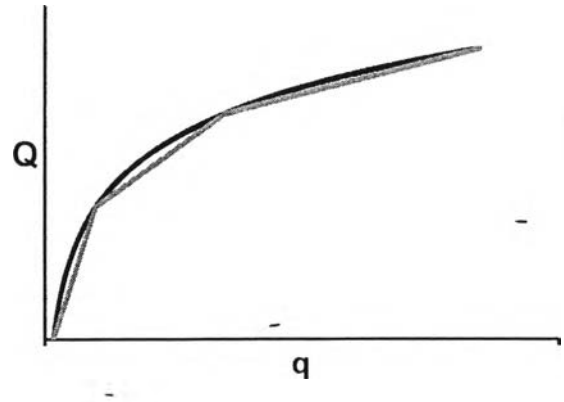


Figure 2.4 A piece-wise linear approximation of the relationship Q = ln(q) in three steps (Björk *et al.*, 2002).

In addition, because of Q = ln(q), q cannot take the value of 0, since Q would then need to have an infinite value, expecailly, the heat balance equations. They then overcome this problem and kept the heat balances as equality constraints by defining the range of q instead from a small ε-value with additional the binary variable z. For example, the heat balance equation could be written as Eq.2.40. Althought these techeniques can relax the feasible region and solve the model much more easier but it causes the model not to yield a better solution in case of large problems.

$$\sum_{j\in CP}\sum_{k\in ST} q_{i,j,k} + qcu_i + \sum_{j\in CP}\sum_{k\in ST}\left(z_{i,j,k}\varepsilon - \varepsilon\right) + zcu_i\varepsilon - \varepsilon = F_i\left(T_{i,in} - T_{i,out}\right), \quad \forall i \in HP \tag{2.40}$$

Huang and Karimi (2012) proposed superior HENs using a stage-wise superstructure with non-isothermal mixing and improved temperature bounds (Figure 2.5) with logical constraint. Their work also show effect of including stage bypass variable and constraints to obtain more feasible solution quality and efficienctly.

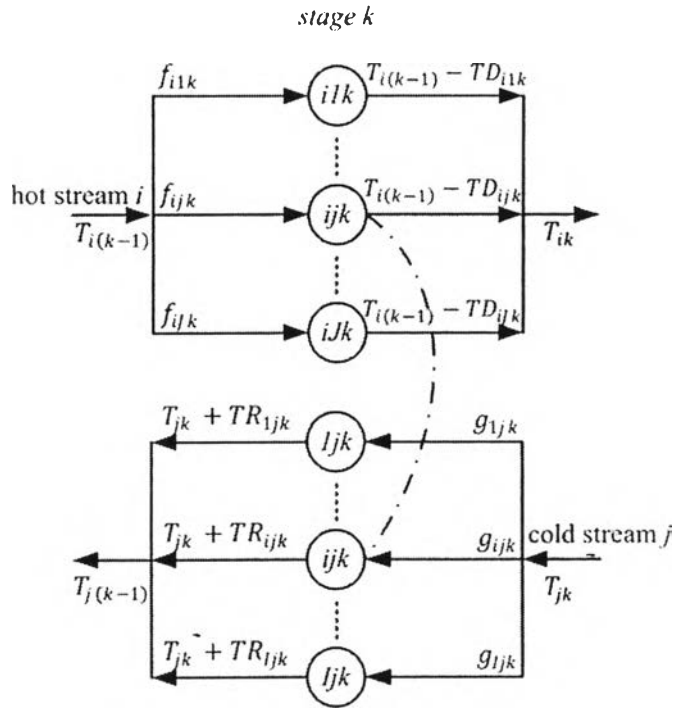


Figure 2.5 Additional variables for non-isothermal mixing at stage k (Huang *et al.*, 2012).

As shown in Figure 2.5, they introduced the constraint variables $TD_{i,j,k}$ as the temperature drop for hot stream i and $TR_{i,j,k}$ as the temperature rise for cold stream j. From this technique, they applied these variable constraints into their model as relaxed equations as follows:

$$TD_{ijk}^{U} = TR_{ijk}^{U} = \Delta T_{ijk}^{U} = \max\{0, TIN_i - TIN_j - EMAT\} \quad (2.41)$$

$$Q_{ijk}^{U} = \min\{F_i(TIN_i - TOUT_i), F_j(TOUT_j - TIN_j), \Delta T_{ijk}^{U} \min\{F_i, F_j\}\} \quad (2.42)$$

$$TD_{ijk} \leq x_{ijk} \Delta T_{ijk}^{U} \quad (2.43)$$

$$TR_{ijk} \leq x_{ijk} \Delta T_{ijk}^{U} \quad (2.44)$$

$$Q_{ijk} \leq x_{ijk} Q_{ijk}^{U} \quad (2.45)$$

$$Q_{ijk} \leq f_{ijk} F_i TD_{ijk} \quad (2.46)$$

$$Q_{ijk} \leq g_{ijk} F_j TR_{ijk} \quad (2.47)$$

Where f_{ijk}, and g_{ijk} are fractional flow of hot and cold stream respectively.

Eqs 2.46-2.47 involve bilinear terms. Therefore, they use the bounds on TD_{ijk}, TR_{ijk}, f_{ijk}, and g_{ijk} and wrote the following convex and concave estimators as below:

$$Q_{ijk} \geq F_i[TD_{ijk} + (f_{ijk} - 1)\Delta T_{ijk}^U] \tag{2.48}$$

$$Q_{ijk} \geq F_j[TR_{ijk} + (g_{ijk} - 1)\Delta T_{ijk}^U] \tag{2.49}$$

$$Q_{ijk} \leq F_i TD_{ijk} \tag{2.50}$$

$$Q_{ijk} \leq F_j TR_{ijk} \tag{2.51}$$

$$Q_{ijk} \leq f_{ijk} F_i \Delta T_{ijk}^U \tag{2.52}$$

$$Q_{ijk} \leq g_{ijk} F_j \Delta T_{ijk}^U \tag{2.53}$$

In contrast to isothermal mixing, the temperature approaches at the hot and cold ends of HE_{ijk} are rearranged by:

$$EMAT \leq TAH_{ijk} \leq TIN_i - TR_{ijk} + T_{jk} + \Gamma_{ijk}(1 - x_{ijk}) \tag{2.54}$$

$$EMAT \leq TAH_{ijk} \leq T_{i(k-1)} - TR_{ijk} + T_{jk} + \Gamma_{ijk}(1 - x_{ijk}) \tag{2.55}$$

$$EMAT \leq TAC_{ijk} \leq TIN_i - TD_{ijk} + T_{jk} + \Gamma_{ijk}(1 - x_{ijk}) \tag{2.56}$$

$$EMAT \leq TAC_{ijk} \leq T_{i(k-1)} - TD_{ijk} + T_{jk} + \Gamma_{ijk}(1 - x_{ijk}) \tag{2.57}$$

Where TAH_{ijk} and TAC_{ijk} are hot and cold side temperature respectively.

$$\Gamma_{ijk} = \begin{cases} TIN_i - TIN_j, & \text{if } TIN_i \geq TIN_j + EMAT \\ abs\{TIN_i - TIN_j\} + EMAT, & \text{Otherwise} \end{cases}$$

Moreover, in term of LMTD, they added a constraint (Eq.2.58) to guarantee that it cannot exceed the arithmetic mean.

$$LMTD_{ijk} \leq \frac{1}{2}(TAH_{ijk} - TAC_{ijk}) \tag{2.58}$$

From Huang and Karimi strategies, their new modified stage-wise superstructure model can yield better solution than the original one, especially, in term of non-isothermal mixing result. Their model can include the case of sub-stream that its temperature can be cooled(heated) lower(higher) than its final temperature. All existing HENS models (Yee *et al.*, 1990; Björk et al., 2002), to our knowledge, limit all the sub-stream temperatures for everywhere in a HEN to be within the initial and final temperatures of their parent stream. Therefore, the existing HENS formulations may yield sub-optimal and cannot valid possibly optimal HENs. But because their strategy solve problems without any feasible initial point, then, as in case of having more than one feasible solution at a same bound variables, their model may miss another possibly solution.

2.3.3 Development of Heuristic Approach in Objective Function and Variables

HEN synthesis with simultaneous approach objective functions, is one of the great strategic and widely used methods to drastically reduce the annual cost of the original stage-wise superstructure model (Yee *et al.*, 1990). An attempt was done to synthesize the heat and power integrated HENs using an MINLP model (Soršak *et al.*, 1999). The proposed method was employed to obtain feasible networks with optimal trade-offs between investment, utility, and power consumption caused by pressure drops. To simplify and implement the model, the assumptions were accommodated below:

- The buffle spacing (l_b)is equal to 20% of the internal shell diameter (D_s),
- The pitch between the tubes is 25% greater than the external tube diameter(D_z),
- The effective shell side diameter is defined by external tube diameter. An effective diameter coefficient C_{ef} is specified (C_{ef} = $6.25\pi/\pi$),

- The tube side convective heat transfer coefficient is calculated by Dittus-Boelter's equation,
- The shell side convective heat transfer coeffcient is calculated by Kern's method.
- During the heat transfer the aggregation of the streams does not change.
- The film and fouling transfer coefficients(R) can thus differ significantly from the actual ones in the final exchanger design.

From the assumptions above, Equation (35) is rearranged:

$$U = \left[R + \frac{D_z}{2\lambda_{tu}} \ln\left[\frac{D_z}{D_z - 2.\delta}\right] + \left[\frac{\lambda_s}{D_z C_{ef}} \begin{Bmatrix} 0.36\left(\frac{V_x D_z C_{ef}}{V_x}\right)^{0.55} \\ Pr_x^{\left(\frac{1}{3}\right)} \end{Bmatrix}\right]^{-1} + \left(\frac{D_z}{D_z C_{ef}}\right).\left(R_r + \begin{Bmatrix} \frac{0.023}{D_z - 2\delta}\left[\frac{(D_z - 2\delta).V_i}{V_i}\right]^{0.8} \\ Pr_x^{0.8} \end{Bmatrix}^{-1}\right) \right]^{-1} \quad (2.59)$$

Where, R_r is the temperature different ratio, δ represents the tube thickness (m), Pr_x is the shell type prandtl number, and V_i is tube side volume flowrate(m^3/s).

Moreover, the tube side pressure drop ΔP_t and the shell side pressure drop ΔP_x are determined by:

$$\Delta P_t = Np.\left[8.j_f.\left(\frac{1}{D_z - 2\delta}\right) + 2.5\right].\frac{\rho.V_t^2}{2} \quad (2.60)$$

$$log(j_f) = -1.329692 - 0.244832log(Re_t)$$

$$\Delta P_x = 8.j_f.\left(\frac{D_s}{D_z.C_{ef}}\right).\frac{\rho.V_t^2}{2} \quad (2.61)$$

$$log(j_f) = -0.578009 - 0.182013log(Re_x)$$

Where, j_f is tube (shell) side friction factor, ρ is steam density (kg/m^3), Re_t and Re_x are tube and shell side Reynold's number respectively.

In the HEN synthesis, a lot of effort has been done to develop mathematical models to optimize different objectives simultaneously in each iteration. Generally, a multi-objective nature approach of the HEN synthesis problem has been transformed into a single-objective problem. However, the true nature of the problem can be done by formulating several individual objective functions instead of only one phase. Then conflicting objectives function can be solved by using multi-objective optimization (Laukkanen *et al.*, 2010). Therefore, the method based on an interactive multi-objective optimization method, NIMBUS, was developed to find the best solution to satisfy the result without too much cognitive or computational load, which is a very important part in MINLP type problem. The NIMBUS method was based on the classification of objectives. Then, each iteration, it can tell how the objective values should change in order to get a more satisfactory solution. For example, some of the objective functions were allowed to be improved, unchanged, some to be impaired, and some to vary freely. Because it was necessary to allow some objective functions to be impaired and, hence, enhance others.

Typically the HEN problems are much immense with either large number of process streams or extended variables and can cause more computational load in the global optimum algorithms, especially, with the MINLP type problem. Therefore, bound contraction procedure for global optimization of bilinear MINLP problems was proposed (Faria *et al.*, 2011). Faria and Bagajewicz (2011) presented the relaxation methodology. The bound contraction procedure did not introduce any new integers or intervals for determining the global optimization solution. The reference values and the algorithm of this strategy were used to perform the bound contraction. As it shows below, variables are identified and updated in each interval at a time after a reference value has been calculated from a lower bound to run successive bound contraction steps. The procedure is repeated until the gap different value between the lower and upper bounds is satisfied and acceptable.

$$z_{ij} = y_j x_i \quad \forall i = 1, \ldots, n; \ \forall j = 1, \ldots, m \tag{2.62}$$

$$x_i^L \leq x_i \leq x_i^U \quad \forall i = 1, \ldots, n \tag{2.63}$$

$$y_j^L \leq y_j \leq y_j^U \quad \forall j = 1, \ldots, m \tag{2.64}$$

$$z_{ij} \geq y_j x_i^L \quad \forall i = 1, \ldots, n; \ \forall j = 1, \ldots, m \tag{2.65}$$

$$z_{ij} \geq y_j x_i^U \quad \forall i = 1, \ldots, n; \ \forall j = 1, \ldots, m \tag{2.66}$$

$$x_i^{ref} = f_x^{(w)}(z_{i1}, z_{i2}, \ldots, z_{im}; y_1, y_2, \ldots, y_m) \quad \forall i = 1, \ldots, n \tag{2.67}$$

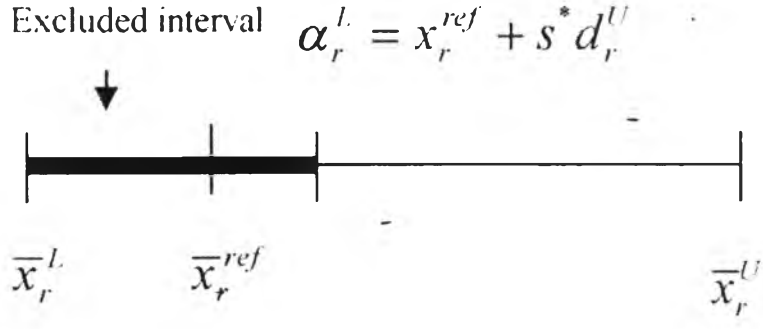


Figure 2.6 Interval exclusion for bound contraction (Faria *et al.*, 2011).

From the Eqs.2.62 to 2.67 and Figure.2.4 illustrated above, these briefly indicate the scenario of the main idea to find the global optimization in non-convex problem without the need to use an additional binary variable or partitioning the key variables into several intervals.