CHAPTER II
THEORETICAL BACKGROUND AND LITERATURE REVIEW

2.1 Crude Oil

Occurring naturally from the remains of plants and animals that died millions of years ago, crude oil is found in the pores of the rocks and earth's surface. Crude oil is in the form of raw material, which is unprocessed. Hence it needs to be extracted, processed and separated from its impurities. It is refined in a refinery and converted into useful petroleum products such as kerosene, diesel fuel, and Liquefied Petroleum Gas (LPG), gasoline and asphalt base. With the distillation method, the hydrocarbons can be separated at various boiling points in the oil refinery.

2.1.1 Crude Oil Composition

The chemical compositions of crude oils are surprisingly uniform even though their physical characteristics vary widely. The elementary composition of crude oil usually falls within the following ranges.

Table 2.1 Composition of crude oil

Element	Percent by weight
Carbon	84–87
Hydrogen	11–14
Sulfur	0–3
Nitrogen	0–0.6

The carbon and hydrogen present in crude oil are in compounds known as hydrocarbons. The three main types of hydrocarbon found in crude oil are paraffins (alkanes), naphthened (alicyclic alkanes) and aromatics. Other substances also present in crude oils in small quantities include oxygen and traces of metals, particularly vanadium and nickel. The presence of these substances may be significant in downstream refinery processes and may influence the refiners' choice of crudes, depending on the available process configuration. Inorganic substances such as salt are usually removed by electrostatic desalting prior to distillation: sand and other solid contaminants deposit in storage tanks or in process equipment, necessitating regular cleanout.

2.1.2 Crude Oil Assay and TBP Distillation Curves

When a refining company evaluates its own crude oils to determine the most desirable processing sequence to obtain the required products, its own laboratories will provide data concerning the distillation and processing of the oil and its fractions.

2.1.2.1 Crude Assay

The complete and definitive analysis of a crude oil is called crude assay. This is more detailed than a crude TBP curve. A complete crude assay contains some of the following data:

- Whole crude salt, gravity, viscosity, sulfur, light-end carbons, and the pour point.
- A TBP curve and a mid-volume plot of gravity, viscosity, sulfur, and the like.
- Light-end carbons analysis up to C8 or C9.
- Properties of fractions (naphthas, kerosenes, diesels, heavy diesels, vacuum gas oils, and resids). The properties required include yield as volume percent, gravity, sulfur, viscosity, octane number, diesel index, flash point, fire point, freeze point, smoke point, and pour point.
- Properties of the lube distillates if the crude is suitable for manufacture of lubes.
- Detailed studies of fractions for various properties and suitability for various end uses.

The results of crude oil assay testing provide extensive detailed hydrocarbon analysis data for refiners, oil traders and producers. Assay data help refineries determine if a crude oil feedstock is compatible for a particular petroleum refinery or if the crude oil could cause yield, quality, production, environmental and other problems. Furthermore information obtained from the petroleum assay is used for client marketing purposes. Feedstock assay data are an important tool in the refining process.

2.1.2.2 TBP Distillation Curves

The composition of any crude oil sample is approximated by a true boiling point (TBP) curve. The method used is basically a batch distillation operation, using a large number of stages, usually greater than 60, and high reflux to distillate ratio. The temperature at any point on the temperature-volumetric yield curve represents the true boiling point of the hydrocarbon material present at the given volume percent point distilled. TBP distillation curves are generally run only on the crude and not on petroleum products. Typical TBP curves of various crude oils are shown in Figures 2.1.

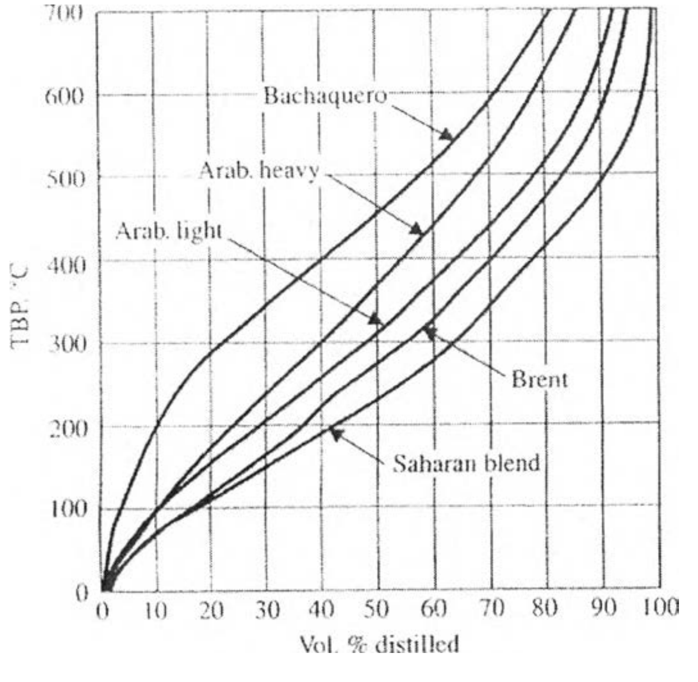

Figure 2.1 TBP distillation of crude oils. (Hori, "Crude Oil Processing. ",2000)

2.2 Crude Distillation Unit

Crude Distillation Unit (CDU), as shown in Figure 2.2, is the first process in the refining sequence and is vital to the profitability of refinery operations.

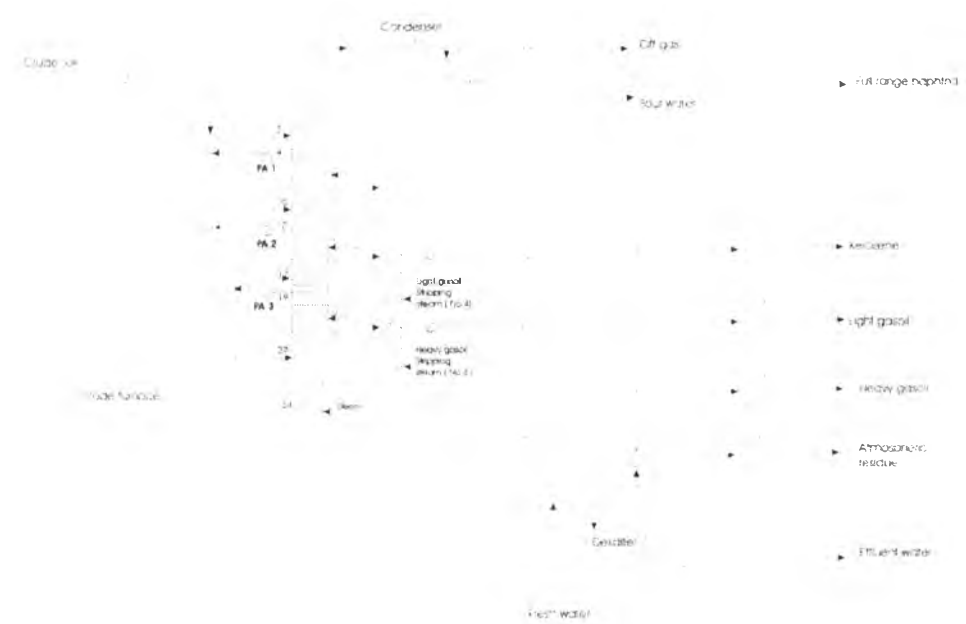

Figure 2.2 Crude Distillation Unit.

Crude oil distillation is one of the oldest continuous multi-component separations practiced. It is a pure physical process separating light and heavy fractions by making use of the different boiling points. Crude oil distillation contains a multiple of hydrocarbons and metal organics, in addition to sediments, water and waxes. The crude stills are the first major processing units in the refinery. They are used to separate the crude oils by distillation into fractions according to boiling point so that each of the processing units following will have feedstocks that meet their particular specifications. Higher efficiencies and lower costs are achieved if the crude oil separation is accomplished in two steps: first by fractionating the total crude oil at essentially atmospheric pressure; then by feeding the high-boiling bottoms fraction (topped or atmospheric reduced crude) from the atmospheric still to second fractionators operated at a high vacuum.

The vacuum still is employed to separate the heavier portion of the crude oil into fractions because the high temperatures necessary to vaporize the topped crude at atmospheric pressure cause thermal cracking to occur, with the resulting loss to dry gas, discoloration of the product, and equipment fouling due to coke formation. Typical fraction cut points and boiling ranges for atmospheric and vacuum still fractions are given in Tables 2.2 and 2.3.

Table 2.2 Boiling Ranges of Typical Crude Oil Fractions

	Boiling ranges, °F	
Fraction	ASM	TBP
Butanes and lighter		
Light straight-run naphtha (LSR)	90–220	90–190
Heavy straight-run naphtha (HSR)	180–400	190–380
Kerosine	330–540	380–520
Light gas oil (LGO)	420–640	520–610
Atmospheric gas oil (AGO)	550–830	610–800
Vacuum gas oil (VGO)	750–1050	800–1050
Vacuum reduced crude (VRC)	1050+	1050+

Table 2.3 TBP Cut Points for Various Crude Oil Fractions

Cut	IBP (°F)	EP (°F)	Processing use
LSR gasoline cut	90	180	Min. light gasoline
	90	190	Normal LSR cut
	80	220	Max. LSR cut
HSR gasoline (naphtha)	180	380	Max. reforming cut
	190	330	Max. jet fuel opr.
	220	330	Min. reforming cut
Kerosine	330	520	Max. kerosine cut
	330	480	Max. jet-50 cut
	380	520	Max. gasoline operation
Light gas oil	420	610[a]	Max. diesel fuel
	480	610[a]	Max. jet fuel
	520	610[a]	Max. kerosine
Heavy gas oil (HGO)	610	800	Catalytic cracker or hydrocracker feed
Vacuum gas oil	800	1050	Deasphalter or catalytic cracker feed
	800	950	Catalytic cracker or hydrocracker feed

[a] For maximum No. 2 diesel fuel production, end points as high as 650°F (343°C) can be used.
Note: In some specific locations, economics can dictate that all material between 330°F IBP and 800°F EP (166 to 427°C) be utilized as feed to a hydrocracker.

The energy efficiency of the distillation operation is also improved by using pump-around reflux. If sufficient reflux were produced in the overhead condenser to provide for all sidestream drawoffs as well as the required reflux, all of the heat energy would be exchanged at the bubble-point temperature of the overhead stream. By using pump-around reflux at lower points in the column, the heat transfer temperatures are higher and a higher fraction of the heat energy can be recovered by preheating the feed.

2.3 Heat Integration of Distillation

For many years, the standard heat integration are two main methods of research for heat exchanger network (HEN) retrofit. One is based on thermodynamic analysis including Pinch Analysis (Tjoe and Linnhoff *et al.*, 1986). Another is using Mathematical Programming (Yee and Grossmann,1991).

First, Pinch technology optimizes a HEN through the incorporation of thermodynamic properties of the process streams that set energy saving and cost targets prior to the design of HEN. Goal of pinch analysis is to maximize the process-to-process heat recovery and minimize the utility requirements of a system (T.Hallberg *et al.*,). The limitations of this technology, after the addition of the improvement methods, make it the less preferred method in an industrial setting.

On the other hand, A mixed Integer Linear Programming (MILP) proposed by Barboro and Bagajewicz (2005), It is capable in many real-world optimizing scenarios for HEN with non-isothermal mixing, incorporating various costs for exchanger area manipulation including adding new area to existing shell, adding area as a new shell, reducing area by plugging tubes and passing exchange. Retrofit MILP model by Yee and Grossmann (1987), this retrofit MILP model is based on transportation and transshipment models, which allow the model to quickly and effectively distribute heat between hot and cold streams. Moreover, they developed a two-step approach. First, they used their transshipment model to do retrofit network structure at different energy recovery levels. And the second, they optimized by using MINLP. Although the network structure is simplified, solving the MINLP model was still time consuming task and solution are still very often trapped at local optimum. Ciric and Floudas (1990), theycombined two–steps into a single step by using a MINP formulation to meanwhile optimize heat exchanger area, energy reassignment and other features of a HEN. Asante and Zhu proposed a step by step interactive approach for heat exchanger network retrofit by combining the features of Pinch and mathematical programming. They introduced a concept of network pinch that identifies the bottleneck of the network and the most effective change. An MILP model was formulated for this purpose. Once a topology change is accepted either the addition of a new exchanger or a new split, a relocation of an existing heat exchanger, the new topology will then be optimized as an NLP. The procedure is repeated until the designer could not find any more economical change and identifies a single topology change at a time in a sequential manner that may in theory yield a sub-optimal solution. Also, sensible user interaction is required for meaningful result.

Most recent results include the work of heat integration and heat exchanger network syntheses have been the subject of a significant research activity in process systems engineering.

Shenoy, Uday V. (1995) has been modified existing plants which have been achieved by various retrofitting techniques that may be classified into four board categories: computer search, mathematical programming, inspection and pinch technology. Jones *et al.,* (1986) studied about computer search technique that can be used to choose from a number of simulated MER networks and get a new network with the most favorable economics and minimal change. But this method may not prove efficient in many cases due to three reasons: the element of chance in hitting or missing the best network, the large amount of computational effort involved in simulating many networks, and the difficulty in retrofitting to identify a design having a structure reasonably close to the existing one and simultaneously transferring zero heat across the pinch. But Tjoe and Linhoff (1987) discussed about the method of retrofitting by inspection and computer search carry the potential risk of the network not being the optimum. While the use of mathematical programming makes strong computational demands. Retrofitting by pinch technology provides a promising alternative. This method has been successfully used in industry.

A retrofit example problem is first solved by inspection which has been tried as an intuitive method to achieve energy saving in a plant and then more systematically by pinch technology. Second is a retrofit-fixed heat transfer coefficient that is modification to provide targets and involves network modification to achieve the set targets. The targeting procedure is based on energy and area targets as well as on the concept of area efficiency. Tjoe and Linhoff (1986) plotted investment vs. savings is used to obtain a target for retrofit design.

Aguilera and Nasini (1996) and Papalexandri and Pistikopoulos(1994), who address flexibility and broader operability issues, respectively; Chang et al.(1994), who focus on structural HEN possibilities; Daichendt and Grossmann (1994), etc. While numerous HEN optimization issues have been addressed, industrial applicability of the proposed methods has been limited, as important features of industrial HENS cannot be efficiently accounted for. Mathematical programming-based approaches have been developed to address total cost minimization in HEN design and retrofit design problems (Floudas; 1995, Biegler et al., 1996). Turkay and Grossmann (1996), who applied disjunctive programming techniques to address the problem of discontinuous investment costs. Nielsen et al. (1997) have recently shown aspects of practical importance (mainly cost implications) in industrial HENS, that cannot be considered in current HEN design methods, as the latter have been presented in the literature. An attempt is made in this work to overcome the traditional limitations of mathematical programming based methods for HEN optimization and study systematically synthesis, design and operation issues in an industrial crude preheat system. A mass/heat exchange -based process representation framework, presented in earlier work (Papalexandri and Pistikopoulos, 1996) is used to model enhanced heat integration possibilities, where different streams, of temperature dependent heat capacities, can be mixed and lose their identity. Intermediate stream processing can be explicitly accounted for.

G.Athier *et al.,*(1998) has been derived from a grassroot design model is proposed. The master problem, related to structural optimization, is carried out by a simulated annealing (SA) procedure. For each generated network, the required additional area for existing exchangers and the size of the new exchangers are optimized by a Nonlinear Programming (NLP) algorithm. Papalexandri and Patsiatzis (1998) are considered in heat integration possibilities that involve different stream mixing and intermediate stream processing. Realistic heat exchange models are considered to calculate actual area requirements. Multiple objectives and trade-offs are investigated systematically. It is shown that the significant savings of a simultaneous optimization framework are realizable for industrial systems, without prohibitive computational requirements.

Briones and Kokossis (1999) studied only MILP models by using a two-step approach; screening and optimization. In the screening step, a MILP model was used for network modifications as well as the additional heat exchanger area. Range area targets were calculated and show the result into an investment–saving plot which identify the exact level of energy recovery and selected the existing matches that have high efficiency. The selected matches are accumulated retrofit network and the remaining matches will be considered for reassignment. After fixing the energy recover level in the second step. MILP model used to determine the remaining part of the network by utilizing unpracticed and new exchanger.

Vijaya Kumar Bulasara and Ramgopal Uppaluri (2009) studied about revamping of crude distillation unit (CDU) heat exchanger network (HEN) of a typical refinery based on pinch design method, two sub-cases of modify study have been considered namely (a) installation of new heat exchanger for the entire network and (b) reutilization of existing heat exchangers. The case for petroleum refineries is the most interesting in which one of the primary objectives of energy integration is to maximize the target temperature of crude oil stream before entering the furnace, which can drive reduction in furnace duties and maximization of energy recovery from the hot product streams from various distillation units.

Ebrahim Rezaei and Sirous Shafiei (2009) studied about the revamping of heat exchanger networks (HENs) using genetic algorithm (GA) coupled with nonlinear programming (NLP) and integer linear programming (ILP) methods. Structural modifications are carried out by the GA in which node representation is used for the addressing of exchanger locations. Continuous variables are handled using a modified NLP formulation for maximum energy recovery (MER). Simultaneous optimization of the NLP is replaced by a search loop to find the best minimum approach temperature and split ratios. In this way the NLP is converted to an LP procedure which is easier to solve. After each LP, an ILP problem is solved to determine the minimum investment cost of modifications. The ILP determines the elimination or reuse of current exchangers and/or introducing new ones to the network.

Robin Smith, Megan Jobson and Lu Chen (2010) studied about a methodology for heat exchanger network (HEN) retrofit, which is applicable to complex industrial revamps, considering existing networks and constraining the number of modifications. The network pinch approach has been modified and extended to apply to the HEN design in which the thermal properties of streams are temperature-dependent. The modified network pinch approach combines structural modifications and cost optimization in a single step to avoid missing cost-effective design solutions.

Most of all, majority of the works use mathematical programming according to two steps that are screening and optimization. Because solution of the HEN retrofit problem is necessary to consider about energy, heat transfer area and re-allocation of heat exchanger obviously that is very time consuming or the quality of solution cannot be guaranteed. The screening step is very important which determines or restricts the final topology of network. Screening step is good step when also simplifies the network structure that is solution time at the second step could be minimized. Most of the models used for the screening step had fixed energy consumption; therefore, approach–temperature at each enthalpy interval could be fixed. This assumption linearized the problem so that it could be solved as an MILP. The disadvantage of this model affects the quality of solution because the pre-selected energy consumption (or the network's minimum approach temperature). Moreover serious problem in fixing enthalpy intervals will generate a huge number of integer variables. So, it is often for assigning heat exchanger matches among those intervals. This significantly increases the solution time.

2.4 Area Targeting

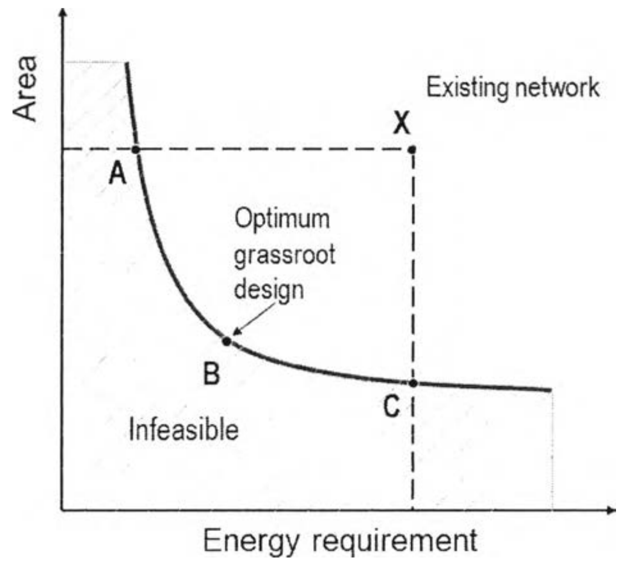

Figure 2.3 The relationship between area requirements and energy requirements for a current process relative to the grassroots design curve. (Texas A&M University. "Network Pinch Analysis." 122.)

It is necessary to understand the theory behind how pinch technology calculates the area for applying to determine the total network retrofit area for various ΔT_{min} values; Figure 2.3 illustrates the energy requirement versus area plot for a typical HEN retrofit process. The curve represents the optimum design curve for the HEN if it were developed for a grassroots situation. Which had our existing network been designed for a grassroots situation with the same energy requirements, Point X represents the current heat exchanger area for the total system as well as the energy requirements. Point C would correspond to the required area; likewise, if our existing network were a grassroots design and had the same amount of area, point A would correspond to the required energy. The optimum grassroots design would minimize the costs of both area and energy and thus have a location near point B.

The goal of the retrofit process is to increase energy savings and decrease total cost by moving X towards the target curve. As the ΔT_{min} is decreased, the energy requirements will decrease while the required area for the system will increase.

Going below the curve is not feasible because a retrofit cannot be better than the targeted grassroots design. If possible, the retrofitted design should reuse and try to improve on the use of existing area; however, if this is not feasible or not economic, area addition to the network will be considered to decrease the total energy requirements and find the optimum solution.

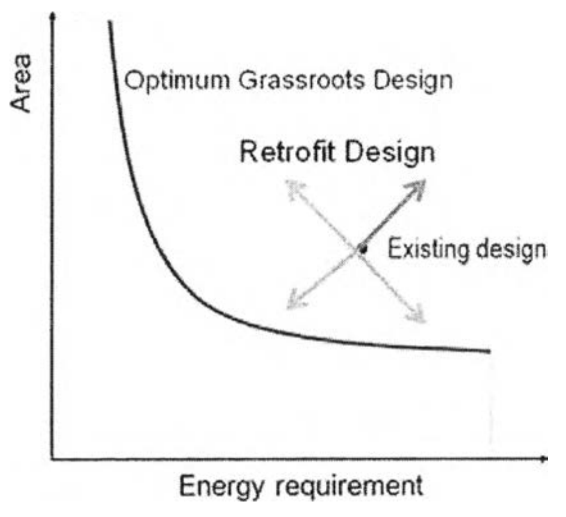

Figure 2.4 Relation between area and energy requirement, show the possible HEN changes that a current process could undergo for a retrofit to increase energy savings and decrease total cost.(Texas A&M University. "Network Pinch Analysis." 122.)

As a result, a retrofit design theoretically has four possible options to consider in Figure 2.4.

- **The up and to the right**, if the existing design moves in the direction of that, then the energy and area requirements will both increase; finding a more economical solution in this manner is highly unlikely.
- **The down and to the right**, if the existing design follows to that, then we will be decreasing area but increasing energy;

Theoretically, a more optimal design could be located here but the purpose of pinch technology is to reduce energy requirements and increase the use of area. Therefore, this region will be rejected. Thus, we have the two arrows pointing to the left to consider. Pinch technology recommends not ignoring area that has already been invested and so assumes that the down and to the left will not be economical. For now, we will follow this recommendation and assume pinch technology is correct. However, this is a limitation of pinch and we will try to improve upon it later. Therefore, we will assume that the up and to the left will be the direction we move to retrofit the HEN.

After improvement of pinch technology, these improvements will not ignore the area in down and to the left. The results for these improvements will fall somewhere in the figure that is to the left of the existing design. However, the specifics as to whether the optimum solution will lie above or below the existing design will be a result of the specifics of each retrofit case.

2.5 Retrofit Targeting Based on ΔT_{min} – Vertical Heat Transfer

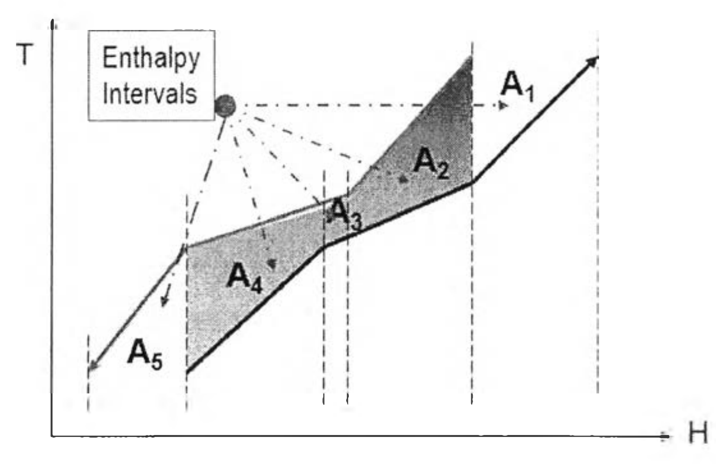

Figure 2.5 Vertical heat transfer. Using to calculate the network area for vertical enthalpy intervals. (Texas A&M University. "Network Pinch Analysis." 123)

We can determine A_{ideal} by calculating the area required for each separate enthalpy region and summing them as in Figure 2.5. The enthalpy regions where the hot and cold composite curves overlap represent process-to-process heat exchangers; conversely, the regions of no overlap correspond to utility exchangers. The areas for the utility exchangers will not be calculated at this stage of the retrofitting process because their duties are going to be reduced later when the overall network changes are made.

Moreover, because we do not know the specifics of the retrofitted design, we must assume that each exchanger in our network will have an equal area. This will allow us to determine our optimum ΔT_{min} by estimating the total cost.

Shenoy and Uday(1995), the idea area (A_{ideal}) for the process is calculated using Equation 2.1 where LMTD is the logarithmic mean temperature difference for the temperature interval. Qj is the enthalpy change of the j-th stream, hj is the heat transfer coefficient of the j-th stream, i is the i-th enthalpy interval, and j is the j-th stream. Equation 2.2 splits the summation over the streams existing in each enthalpy interval into two summations that were used in the calculations of A_{ideal} where h denotes a hot stream, and c denotes a cold stream. Equation 2.3 is the logarithmic mean temperature difference for each interval.

$$A = \sum_i \left(\frac{1}{LMTD}\right)_i \sum_j \left(\frac{Q_j}{h_j}\right)_i \tag{2.1}$$

$$\sum_i \left(\frac{Q_j}{h_j}\right) = (dT_h).\sum_{jh} \left(\frac{CP}{h}\right)_{jh} + (dT_h)_i \,.\sum_{jc} \left(\frac{CP}{h}\right)_{jc} \tag{2.2}$$

$$LMTD = \frac{(T_{h,i} - T_{c,i}) - (T_{h,i-1} - T_{c,i-1})}{\ln\left(\frac{T_{h,i} - T_{c,i}}{T_{h,i-1} - T_{c,i-1}}\right)} \tag{2.3}$$

2.6 Area Efficiency

Figure 2.6 shows an approach for retrofit targeting based on the concept of "Area efficiency". An area efficiency factor α can be determined for an existing network according to the following equation;

$$\alpha = \frac{(A_{ideal})_0}{(A_{existing})} = \text{Area Efficiency}$$

$$\Delta\alpha = \frac{A_{ideal_1} - A_{ideal_0}}{A_{retrofit} - A_{existing}} \qquad (2.4)$$

where; $A_{existing}$ = Existing surface area of the network

A_{ideal} = Target surface area for the new design at the existing energy consumption (Eex).

$A_{retrofit}$ = Retrofit surface area of the network

$\Delta\alpha \approx \alpha$ if $\alpha>0.9$ or $\Delta\alpha \approx 1$ if $\alpha<0.9$

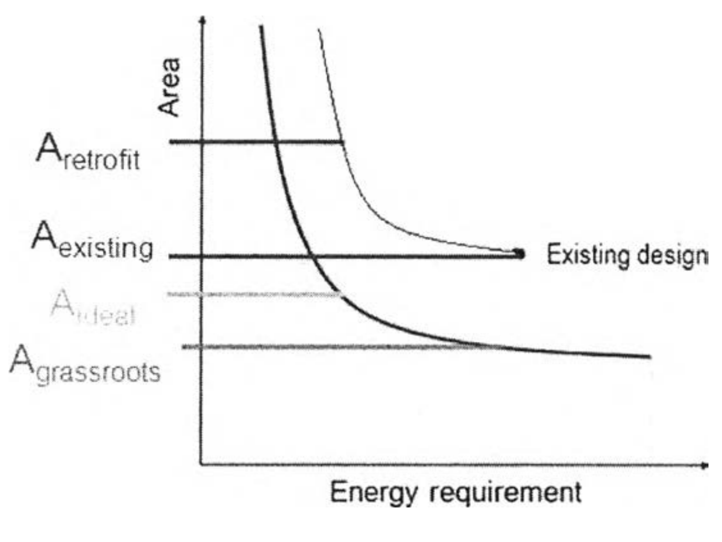

Figure 2.6 Area efficiency concepts (Texas A&M University. "Network Pinch Analysis." 123)

Area efficiency determines how close the existing network is to the new design area target. In order to set a retrofit target, one approach is to assume that the area efficiency of the new installed area is the same as the existing network as shown in Figure 2.6. Moreover the maximum retrofit area can be found by below Equation 2.5.

$$A_{retrofit} = \frac{(A_{ideal_1} - A_{ideal_0})}{\Delta\alpha} + A_{existing} \tag{2.5}$$

2.7 Cost Targeting

The next step in the retrofit process, we have to consider retrofit targeting based on ΔT_{min} that is after the composite curve have been created is to the optimum ΔT_{min} value based on which value provides the most economical design. To do this, the total network area and the utility requirements for the retrofit network calculated for each ΔT_{min} value. Then the costs of the area and energy requirements are calculated and the optimum value is determined. This section describes in detail supertargeting process (Hallberg Y. *et al.*,)

Shenoy and Uday (1995), the cost of a network basically comprises the operating cost and the capital cost. These cost contribute on are discussed below.

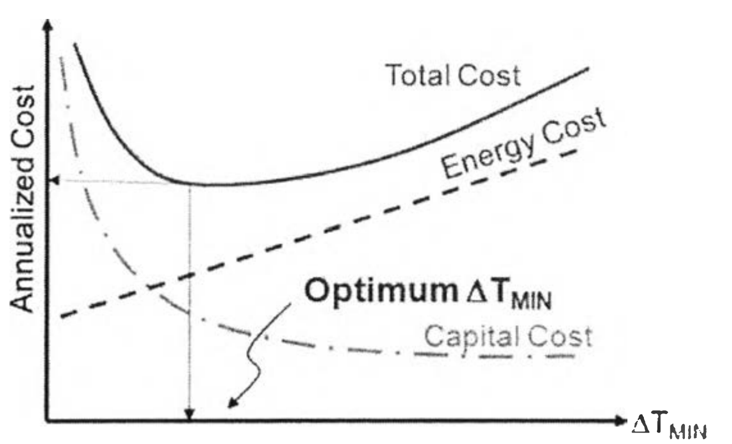

Figure 2.7 A typical Total Annualized Cost (TAC) vs. ΔTmin diagram. The minimum on the total cost curve corresponds to the optimum ΔT_{min} value.

We have to determine the optimum ΔT_{min} value prior to the design of the new process. To determine this value, we will use a Total Annualized Cost (TAC) vs. ΔT_{min} diagram for a constant α value of 1. Figure 2.7, show a typical TAC vs. ΔT_{min} diagram. The minimum on the TAC curve corresponds to the optimum value.

Total annualized cost (TAC) is a function of the operating cost (*OC*) and the capital cost (*CC*) according to Equation 2.6.

$$TAC = OC + CC \tag{2.6}$$

Because the operating costs and the capital costs are both a function of ΔT_{min}, a compromise must be made when a network design is to be retrofitted. As ΔT_{min} increases, the energy requirements will increase while the area requirements will decrease. Thus, the operating costs will increase. However, as ΔT_{min} decreases, the energy requirements will decrease while the area requirements increase. Thus, the capital costs will increase. As a result of how each cost curve behaves with ΔT_{min}, it is expected that the TAC curve when plotted with ΔT_{min} will have a minimum value. This value correlates to the optimum ΔT_{min}. The operating cost (OC) (in \$/year) is a function of the hot utility cost (CHU), the cold utility cost (CCU), and a discount factor according to Equations 2.7, 2.8, and 2.9, respectively. The utility cost factors in Equations 2.7 and 2.8 are the values for each examples which are studied. It has similar cost factors as displayed in amount and cost of each utility for the original HEN of each example. Operating costs are an expense that must be paid every year. The discount factor for the operating cost (in \$) is $1/(1.1)^{n-1}$ for year n.

$$C_{HU} = Q_{HU,min} \cdot \left(\frac{\frac{\$}{year}}{\frac{MJ}{hr}} \right) \cdot \left(\frac{3600\ s}{1\ hr} \right) \tag{2.7}$$

$$C_{CU} = Q_{CU,min} \cdot \left(\frac{\frac{\$}{year}}{\frac{MJ}{hr}} \right) \cdot \left(\frac{3600\ s}{1\ hr} \right) \tag{2.8}$$

$$OC = (C_{HU} + C_{CU}) . \left(\frac{1}{1.1^{n-1}} \right) \tag{2.9}$$

The capital cost (CC) is a function of the number of heat exchangers in a network and the area distribution for each exchanger as in Equation 2.8; furthermore, it is paid only once, not yearly like the operating costs. Because the optimum ΔT_{min}

value is still unknown at this point, the area distribution for each exchanger is not known. Therefore, it is still assumed here that each individual exchanger in the network has the same area.

In Equation 2.10, N_{min} is the minimum number of exchangers in the network, A retrofit is the retrofitted area for the new network, and a, b, and c are cost law coefficients that depend on the network itself. This equation assumes the retrofit network is constructed of only countercurrent heat exchangers and that each exchanger uses the same cost coefficients. N_{min} is calculated according to Equation 2.11. N_h is the number of hot streams, N_c is the number of cold streams, Nu is the number of utility streams, AP is above the pinch, and BP is below the pinch.

$$CC = N_{min}.\left[a + b.\left(\frac{A_{retrofit}}{N_{min}}\right)^c\right] \qquad (2.10)$$

$$N_{min} = [N_h + N_c + N_u - 1]_{AP} + [N_h + N_c + N_u - 1]_{BP} \qquad (2.11)$$

The TAC versus ΔT_{min} diagrams. Thus the optimum ΔT_{min} value is values represent an economic compromise between heat exchanger areas and utility requirements for the retrofitted networks.

2.8 Mathematical Programming Methods

Over last decade there have been considerable advances in mathematical programming techniques for the HEN retrofit problem. Yee and Grossmann (1987) proposed an MILP assignment transshipment formulation for retrofit HENs. It is an extension of the MILP transshipment model (Papoulias and Grossmann (1983)). Zhelev et *al*. (1987) developed an algorithm for retrofit HENs which a network is retrofitted through comparison of grassroots network design for the problem. Ciric and Floudus (1989) proposed a two-stage approach consisting of a match selection stage, and optimization stage. Central to this strategy is mathematical model for retrofit at level of matches. The match selections stage used a mixed integer linear programming (MILP) formulation that incorporates explicitly the cost associated with each potential match of streams and involves all possible options for modifications. The solution of this formulation provides information on which exchangers should be reassigned or newly installed, and whether there is a need to increase or decrease the area of the existing exchangers. The optimization stage takes advantage of this information, and a superstructure is postulated and formulated as a nonlinear programming (NLP) problem. The solution of the NLP provides the actual retrofitted network from optimizing the matching order and flow configuration. Unfortunately, the MILP model does not account for areas quite reliably and involves a large number of integer variables that make its application to industrial size problem difficult (Briones and Kokossis, 1999). These two-stage approaches were later combined into a single stage by Ciric and Floudas (1990), using a mixed integer nonlinear (MINLP) formulation to incorporate all possible stream matches, network configuration and existing exchanger reassignment in single mathematical formulation. Yee and Grossmann (1991) provided a systematic procedure which also had two-stage, in this procedure however a targeting or pre-screening stage and an optimization stage were used. In the pre-screening stage, the economic feasibility of the project is analyzed with lower bounds on cost for utility, additional area, and structural modifications. The bounds are used to construct a prescreening cost plot to estimate the maximum savings that can be achieved. However only the number of new units required to achieve the optimization investment determined was carried forward to the optimization stage. During the optimization stage, the heat recovery level was allowed to vary an MINLP formulation was used to simultaneously optimize the capital-energy trade off and all the network parameters. Because the MINLP model is very detailed, different types of binary variables are needed in their formulation. This issue may restrict the application of the model to small scale problems.

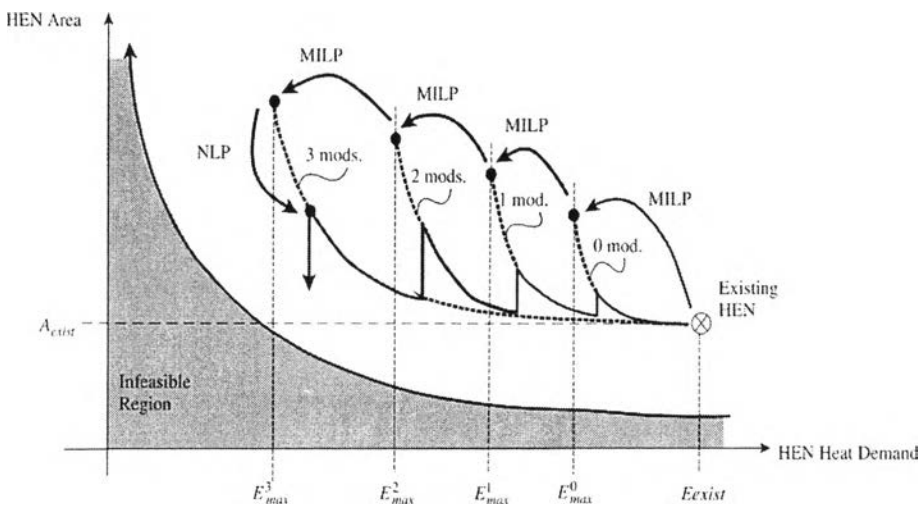

Figure 2.8 The retrofit can be proceed in a stepwise approach. (From Asante NDK and Zhu XX, 1997, Trans IChemE, 75A: 349, reproduced by permission of the Institution of Chemical Engineers)

2.8.1 MINLP Model for Grassroots Design

The MILP model is based on the stage-wise superstructure representation proposed by Yee and Grossmann (1990). The superstructure for the problem is show in Figure 2.9. Within each stage of the superstructure, potential exchangers between any pair of hot and cold streams can occur.

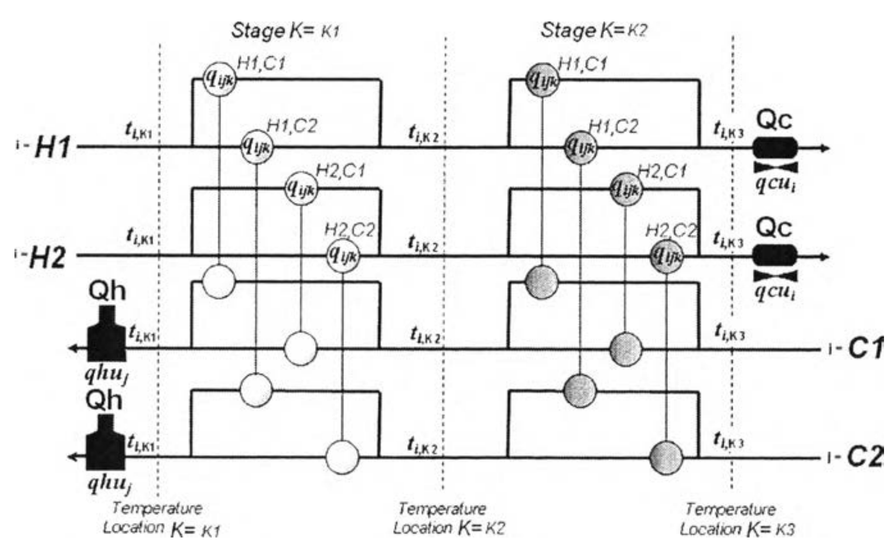

Figure 2.9 Two-stage superstructure.

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 steam. It is assumed that the outlets of the exchangers are isothermally mixed, which simplifies the calculation of the stream temperature for the next stage, since no information of flows is needed in the model. The outlet temperatures of each stage are treated as variables in the optimization. The number of stages should in general coincide with the number of temperature intervals to ensure maximum energy recovery. However, in most cases selecting the number of stages as the maximum of hot and cold streams suffices. A heater or cooler is placed at the outlet of the superstructure for each process stream. Optimization of the MINLP model identifies the least cost network embedded within the superstructure by identifying which exchangers are needed and the flow configuration of the streams. A major advantage of this model is its capability of easily handling constraints for forbidding stream splits. Process streams are divided into two sets, set HP for hot streams, represented by index i, and set CP for cold streams, represented by index j. Index k is used to denote the superstructure stage given by the sets ST. Indices HU and CU correspond to the heating and cooling utilities respectively. Also, the following parameters and variables are used in the formulation:

<u>Parameters</u>

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

β = exponent for area cost

NOK = total number of stages

Ω = upper bound for heat exchanger

Γ = upper bound for temperature difference

Variables

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

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

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

q_{ijk} = 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 stream 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_{ijk} = 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

With above definitions, the formulation can now be presented.

2.8.1.1 Overall Heat Balance for each Stream

$$(TOUT_j - TIN_j)F_j = \sum_{k \in ST}\sum_{i \in HP} q_{ijk} + qhu_j \qquad j \in CP$$

$$(TIN_i - TOUT_i)F_i = \sum_{k \in ST}\sum_{j \in CP} q_{ijk} + qcu_i \qquad i \in HP \qquad (1)$$

2.8.1.2 Heat Balance of each Stream at each Stage

$$(t_{j,k} - t_{j,k+1})F_j = \sum_{i \in HP} q_{ijk} \qquad j \in CP,\ k \in ST$$

$$(t_{i,k} - t_{i,k+1})F_i = \sum_{j \in CP} q_{ijk} \qquad i \in HP,\ k \in ST \qquad (2)$$

2.8.1.3 Assignment of Superstructure Inlet Temperature

$$TIN_j = t_{j,N+1} \qquad j \in CP$$

$$TIN_i = t_{i,1} \qquad i \in HP \qquad (3)$$

2.8.1.4 Feasibility of Temperature

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

$$TOUT_j \geq t_{j,1} \qquad j \in CP$$

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

$$TOUT_i \leq t_{i,N+1} \qquad i \in HP \qquad (4)$$

2.8.1.5 Hot and Cold Utility Load

$$(TOUT_j - t_{j,1})F_j = qhu_j \qquad j \in CP$$

$$(t_{i,N} - TOUT)F_i = qcu_i \qquad i \in HP \qquad (5)$$

2.8.1.6 Logical Constraints

$$q_{ijk} - \Omega z_{ijk} \leq 0 \qquad i \in HP,\ j \in CP,\ k \in ST$$

$$qhu_j - \Omega zhu_j \leq 0 \qquad j \in CP$$

$$qcu_i - \Omega zcu_i \leq 0 \qquad i \in HP \qquad (6)$$

z_{ijk}, zcu_i, $zhu_{j = 0,1}$

2.8.1.7 Calculation of Approach Temperatures

$$dt_{ijk} \leq t_{i,k} - t_{j,k} + \Gamma(1 - z_{ijk}) \qquad i \in HP,\ j \in CP,\ k \in ST$$

$$dt_{ijk} \leq t_{i,k+1} - t_{j,k+1} + \Gamma(1 - z_{ijk}) \qquad i \in HP,\ j \in CP,\ k \in ST$$

$$dthu_j \leq TOUT_{HU} - t_{j,1} + \Gamma(1 - zhu_j) \qquad j \in CP$$

$$dtcu_i \leq t_{i,NOK+1} - TOUT_{CU} + \Gamma(1 - zcu_i) \quad i \in HP \qquad (7)$$

2.8.1.8 Objective Function

$$LMTD \approx \left[(dt1 \times dt2) \times (dt1 + dt2)/2\right]^{1/3} \tag{8}$$

min

$$\sum_{i \in HP} CCUqcu_i + \sum_{j \in CP} CHUqhu_j + \sum_{i \in HP}\sum_{j \in CP}\sum_{k \in ST} CF_{ij} z_{ijk} + \sum_{i \in HP} CF_{i,CU} zcu_i + \sum_{j \in CP} CF_{j,HU} zhu_j$$

$$+ \sum_{i \in HP}\sum_{j \in CP}\sum_{k \in ST} C_{ij}\left[\frac{q_{ijk}}{U_{ij}\left[(dt_{ijk}\, dt_{ijk+1})(dt_{ijk} + dt_{ijk+1})\right]^{1/3}}\right]^{\beta_{ij}}$$

$$+ \sum_{i \in HP} C_{i,CU}\left[\frac{qcu_i}{\left(U_{i,CU}\left[(dtcu_i)(TOUT_i - TIN_{CU})\{dtcu_i + (TOUT_i - TIN_{CU})\}/2\right]^{1/3}\right)}\right]^{\beta_{i,CU}}$$

$$+ \sum_{j \in CP} C_{HU,j}\left[\frac{qhu_j}{\left(U_{HU,j}\left[(dthu_j)(TIN_{HU} - TOUT_j)\{dthu_j + (TIN_{HU} - TOUT_j)\}/2\right]^{1/3}\right)}\right]^{\beta_{j,HU}} \tag{9}$$

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

The continuous variables (t, q, qhu, qcu, dt, dtcu, dthu) are non-negative and the discrete variables z, zcu, zhu are 0-1. The nonlinearities in the objective function may lead to more than one local optimal solution due to their nonconvex nature.

Papalexandri and Pisikopoulos (1993) addressed the problem of redesigning a HEN in order to improve its flexibility. The multiperiod MINLP approach of Floudas and Grossmann (1987) is utilized in the generation of a multiperiod hyperstructure network representation used in the simultaneous optimization of the operation costs and retrofit investment costs of the retrofit HENS problem. The desired flexibility target is achieved through an iterative procedure between the flexibility analysis and the MINLP retrofit HENS problem. Papalexandri and Pisikopoulos (1993) presented the retrofit of HEN with variable operating conditions. With the assumption of no dual streams, a multiperiod network representation is used in an MINLP formulation of the retrofit HENS problem. The

MINLP model couples synthesis techniques for HEN multiperiod operation and retrofit strategies. An iterative scheme may be used to integrate this problem with flexibility analysis. Konukman et *al.* (1995) presented a controllable design of heat exchanger networks as constrained nonlinear optimization problem. The objective of this method is to find the individual exchanger areas and bypass fractions which minimize the total annualized cost (or the total area) of the given heat exchanger network structure and, at the same time, to satisfy all the target temperature constraints (hard or soft) for a set of disturbances predefined in all possible directions. This is achieved by solving only one constrained optimization problem which considers the exchanger model equations (heat transfer and mixing) and constraints (resiliency index, heat load and the minimum approach temperature) simultaneously for all possible predefined disturbance directions. Nielsen et *al.* (1996) presented an object-oriented modeling which is used to create a HENs problem representation and simulated annealing to solve this problem in order to extend HENs to include concurrent exchangers as well as heat capacity flow rates that are not constant. The computer software HEN Explorer is developed in this approach to HENs. Nielsen et *al.* (1997) used an industrial retrofit HENs problem as an example for presenting a realistic HENs problem. Zhelev et *al.* (1998) developed an operability analysis approach for existing HENs in which networks working in conditions of process stream parameter variation. Athier et *al.* (1998) proposed a two-level strategy for retrofit design. A simulated annealing algorithm is used to solve the master problem of generating and iteratively modifying a HEN topology. The slave problem involves NLP optimization of the operating parameters of the network. Ma, Hui, and Yee (2000) proposed an MILP model for HEN retrofit. A two-step solution procedure is proposed to overcome the problems associated with the nonconvexities of the MINLP model. First the constant approach temperature MILP model is solved to determine the fixed network structure, and then the MINLP model is solved for determining match reassignments. Silva and Zemp (2000) presented a new approach considering the distribution of heat transfer area and pressure drop in retrofit. The problem is described as a non-linear model, and the additional area required for the new network condition and available pressure drop are estimated based on economical optimization (or process requirements). Zhang and Zhu (2000) proposed a systematic method for HEN retrofit which modification to the network topology is considered simultaneously with changes to the process parameters such as stream flow rates and temperatures.

2.8.2 MILP Retrofit Design Model (Barbaro et *al.*)

The retrofit model is developed from the grass-root model, that is, the basic structure of the grass-root model is conserved and additional sets of constraints are included to consider the network modifications. The model relies on a transshipment concept, more specifically, the temperature span of each stream in the problem is divided into several smaller temperature intervals and then each temperature interval of a hot stream is considered to exchange heat with temperature intervals of cold streams observing the rules of heat balance and heat exchange feasibility, etc. Binary variables are used to indicate the existence of heat exchanger between a hot stream "*i*" and a cold stream "*j*" in an interval "*m*". The model employs a one-step strategy to simultaneously optimize both the network structure and the heat exchanger areas. The objective is to minimize the total cost, which includes the utilities cost (i.e. operating cost) and the investment cost of the heat exchanger network.

In retrofit cases there are several exchangers that already present in the network and one wants to determine changes to this network that will allow a net reduction in the total annual cost. To achieve this objective, there are several options, namely:

- Addition of new heat exchangers units
- Area expansion/reduction of existing exchangers
- Relocation of existing units.

These options are aimed at enhancing the heat integration among process streams and reducing the use of utilities and therefore the operation cost. In essence, the retrofit problem is to optimally add new exchangers, add area to existing exchangers and/or relocate them (if necessary) such that a certain economic objective is met. Among others, one can

i) Maximize the cost saving on utilities minus the annualized capital cost.

ii) Maximize the net present value of the retrofit.

iii) Maximize the return of the investment.

iv) Maximize the utility cost savings subject to a certain capital investment limit.

Indeed, the MILP is more practical optimizing scenarios, such as non-isothermal mixing, exchanger relocation, repiping costs, and incorporating various costs for exchanger area manipulation. The MILP also maintains the complex of the retrofit problem by not making any of the simplifying assumptions. Moreover the ability of the MILP is to easily change the objective function. This allows the user to optimize a variety of cost and profit variables to generate an optimal solution for various design constraints.

2.9 Combining Pinch and Mathematical Programming Methods

Asante and Zhu (1996, 1997, 1999) combined mathematical optimization techniques with a better understanding of the retrofit problem, based on thermodynamic analysis and practical engineering, to produce a systematic procedure capable of efficiently solving industrial-size retrofit problems. The network pinch concept provides new insight to the HEN retrofit problem and plays an important role in selecting promising modifications, forming the foundation of the new method. This concept, when applied to mathematical formulation, significantly simplified the mathematical models while maintaining good quality of solutions. This approach allows the design tasks to be automated with user interactions. In addition, this procedure also employs a two-stage approach for retrofit HEN design. The first stage is the diagnosis stage which is made up two steps. In the first step the HEN bottleneck is identified and in the second step a mixed integer linear programming (MILP) formulation is used to select a single modification which will best overcome the identified bottleneck. These two steps are repeated in a loop to yield the required set of promising topology modification. In the second stage, the optimization stage, the HEN obtained after implementation of the modifications is optimized using non-linear optimization techniques to minimize the cost of additional surface area employed. However, the success of this approach is sensible to the order of MILPs and suboptimal networks may be obtained by different users for the same problem. Kovabvc and Glavibvc (1995) proposed the combined thermodynamic and computational methods for retrofit HENs. The grand composite and extended grand composite curves are used to eliminate unattractive structures. MINLP is used for optimizing the network using a superstructure. Briones and Kokossis (1996) presented a rigorous and systematic optimization method for the retrofit design of heat exchanger networks. The approach addresses the problem as a multi-task effort and applies a decomposition scheme which makes use of both mathematical programming and pinch analysis methods. The different tasks include targets for structural modifications and heat transfer area changes, the development and optimization of the retrofitted network and the analysis of its complexity against economic penalties and trade-offs. The decomposition stages embed targeting information which supports screening and facilitates an effective optimization search. As such, the decomposition not only bypasses the limitations of past decomposition techniques but exploits its features toward the development of an interactive design tool. Marechal and Kvalitventzeff (1996) combined pinch analysis and mathematical techniques. The analyze step uses the pinch method to propose a set of utilities that may satisfy the minimum energy requirement. The generate step uses a mixed integer linear programming (MILP) optimization to select the utilities to be used and calculates their optimal flow rates. Bruno, Fernandez, Castells and Grossmann (1998) presented an MINLP model for performing structural and parameter optimization of utility plants. The combined methods combine advantages of the thermodynamic, heuristic and mathematical methods by using many boundaries. Briones and Kokossis (1999) also combined the use of thermodynamics and mathematical programming techniques, two-step methodology similar to the grassroots designs, the methodology includes a targeting and an optimization stage. In the first step, two MILP models (HEAT and TAME model) are solved for auditing of existing network and screening of the most promising modifications. These MILPs are employed by targeting procedure and determine the tradeoff among energy, number of units, structural modification and heat transfer area. A superstructure is constructed at the optimization step to account for all possible configurations within a network. This methodology reports improvement up to 40% against the established techniques. Varbanov et al. (2000) proposed two-stage procedure for a correct solution of the optimization problem. Using pinch analysis techniques, the suggested methodology combines the heuristic and mathematical programming approaches in their best aspects. The first stage, an appropriate HEN retrofit superstructure is to be built by using pinch analysis and heuristic path construction, while at the second one the optimal set of retrofit modifications is obtained using mathematical programming. These two integrated components result in simple and efficient retrofit procedure. Kovac-Kralj et *al.* (2000) presented the using rigorous models for simultaneous parameter and structural optimization of an existing complex and energy intensive continuous. The method that was recently developed to sequentially optimize retrofits has been extended to a stepwise simultaneous superstructural approach, using available process simulators and optimization software capabilities. An extended procedure has been employed for retrofits using a three-step approach: (i) generation of a process superstructure by pinch analysis; (ii) formulation of a mixed integer nonlinear programming (MINLP) model and its simplification into a relaxed nonlinear programming (NLP) model; (iii) simultaneous optimization, first by a process simulator and then by the NLP algorithm. Zhu et *al.* (2000) developed a targeting strategy for allowing heat transfer enhancement to be an option for HEN retrofit.

From the above listed technologies, it is necessary for a design method to allow for both automated and interactive generation of retrofit design. The automation of a design process can save time significantly, while interaction allows users to assess modifications on a much wider basis including qualitative aspects.