STRATEGIES FOR OPTIMIZATION IN HEAT EXCHANGER NETWORK DESIGN

A THESIS SUBMITTED IN FULFILMENT
OF THE REQUIREMENT FOR THE DEGREE OF

DOCTOR OF PHILOSOPHY

by

(Frank) Xin X. Zhu
B.E. (Mechanical Engineering)
M.S. (Energy Engineering)
Shanghai Maritime University of China

January 1994

Department of Chemical Engineering
The University of Adelaide
Australia

Awarded 1994

CERTIFICATE OF ORIGINALITY

I hereby declare that this submission is my own work and that, to the best of my knowledge and belief, it contains no material previously published or written by another person nor material which to a substantial extent has been accepted for the award of any other degree or diploma of a university or other institute of higher learning, except where due knowledge is made in the text.

I give consent to this copy of my thesis, when deposited in the University Library, being available for photocopying and loan.

SIGNATURE: .... DATE: 7/3/94

This Ph.D. Dissertation is dedicated to

my wife, Ms. J. Y. Shao,

and my daughter, Kathy M. J. Zhu

for their support and understanding

Acknowledgements

A thesis as this could not have come about without help and encouragement from some very special people. I offer my heartful thanks with a handshake or hug (as appropriate) to the following people:

* To Dr. John R. Roach who is responsible for first introducing my interest in this project and has provided continual guidance during the two and half years of my Ph.D study.

* To Dr. Brian K.O'Neill for his invaluable assistance and helpful suggestions. I owe a strong debt to him, for his advice which contributed to the production of this thesis.

* To Dr. Robert R. Wood, who has provided numerous, invaluable comments and encouragement over the period of my Ph.D study. Particularly, I like to express my thanks for his careful review of this thesis.

* To Professor J. B. Agnew, as the head of the department, for the encouragement to spend these years at the University of Adelaide.

* To Australian Research Council Grant No. A89031580.

* To Mr. T.S. Tran, the computing engineer in this department, for his assistance in the development of necessary software required for this study.

* To clerical staff, Mrs M.H. Barrow, Mrs E.M. Minerds and Mrs J.M. Holman for their willingness to help.

* To my parents and parents-in-law for their faith, love, understanding and encouragement. Words can not express ...

* And most of all, as always, to my wife, Jean, who has shown her love, understanding, support, encouragement and inspiration. She was as happy as I was when I said to her, "I finally finished my Ph.D. Study."

SUMMARY

Though the established Pinch Design Method (PDM) – a thermodynamic and heuristic approach, has produced the most extensive list of good projects in industry for improved heat integration, two major limitations exist in the PDM, i.e. the use of *single* ΔT_{min} and the *strict pinch decomposition*. On the other hand, purely mathematical programming approaches do not always meet with success when applied to realistic industrial–scale problems. There has been a very *little connection* between these two major approaches. It is suggested that the PDM approach would benefit by adoption of some of the mathematical programming methods in terms of *optimization* whilst the latter approaches would benefit from the *physical insights* which can be obtained by the application of the thermodynamic methods.

Therefore, the development of ideas to break the limitations in the PDM and to combine the advantages of both thermodynamic and mathematical programming approaches become two strong motivations of this study.

The principle objective of this research is to develop a new method for the conceptual design of HEN's. The general approach is essentially that which has been successfully used in the overall project to date, viz. to examine the physical structure of the problem with a view to reducing its complexity by identifying the dominant constraints and then applying thermodynamic principles and finding heuristics to produce sound initial designs. These initial designs can then be optimized using conventional non-linear optimization techniques in the subset of the problem's initial dimensionality. A 'block method' has been devised for this purpose which has proved to be successful in producing effective designs. The 'block' concept is means

of simplifying the overall design problem structure by reducing the number of effective temperature-enthalpy intervals in the composite curves.

The 'block method' has been extended to handle problems with significantly different film coefficients and a new targeting procedure to cope with different film coefficients is presented. The interesting phenomenon discovered in this work is that by changing the individual ΔT-contributions, different stream structures can be screened and selected prior to design.

Mathematical programming models based on 'block decomposition' and a 'block-based superstructure' are proposed. Although the block concept leads to a similar superstructure approach to that of the stage method (Yee et al, 1990), the block concept provides the additional physical insights for efficient mathematical models and a large number of inferior alternatives are eliminated from consideration in the NLP optimization. More importantly, the optimization starts in a good region which is broadly located using the general targeting procedure (Linnhoff and Ahmad, 1986a & b) and thus the possibility of finding the global optimum is enhanced. In a sense, the block method provides a bridge between the heuristic (PDM) methodology and mathematical programming techniques which have hitherto been quite distinct.

Work associated with traditional energy relaxation is also presented. An interesting outcome of this work is that the parameters, i.e. temperatures and heat loads in a heat exchanger network can be represented as an analogy based on Kirchhoff's Law. This presentation greatly simplifies the task for loop-breaking and makes it much more deterministic.

Ideas for future work following the development of the block method are suggested. Those include the application to the retrofit problems.

TABLE OF CONTENTS

LIST OF FIGURES

LIST OF TABLES

CHAPTER 1

INTRODUCTION

The study of the synthesis of heat exchanger networks (HENS) has become a classical example of addressing the issue of complexity in process design and synthesis problems. Considerable study and progress in this area has been made in the past two decades. The basic principles for the detailed understanding of the problem are well established, however, there are no methods available so far, which can guarantee optimal solutions for general situations. Thus, practical engineering calls for the improvement of the current methods or the development of new methods which can provide designs satisfying the requirements of cost effectiveness, operability and controllability.

1.1 The HENS Problem

Many chemical process plants produce hot streams as heat sources to be cooled and cold process streams as heat sinks to be heated. There are also hot utility streams as supplementary heat sources to heat process streams and cold utility streams as supplementary heat sinks to cool process streams. Heat exchangers, heaters and coolers are exploited for process-process, process-hot utility, and process-cold utility heat transfer, respectively. The whole system of heat exchangers including associated utilities is referred to as a heat exchanger network.

The industrial heat exchanger network synthesis (HENS) problem is very complex and involves combinatorial problems in the "matching" between hot and cold streams to enhance heat recovery, temperature dependent physical and transport properties, the choice of flow configuration and materials of construction for the heat exchangers, the combination of "hard" and "soft" problem data (some target temperatures must be met, while others may be varied within limits if this is of advantage for the total process economy), various kinds of constraints (forbidden and compulsory matches) and different types of streams (liquid, vapor and mixed phase) (Gundersen and Naess, 1988). Pressure drop limitation and cost of piping are also important.

Practically, the heat exchanger network must be developed to meet design objectives, which include a quantitative part (cost of exchangers, piping and instrumentation, heaters and coolers), and a largely qualitative part (safety, operability, flexibility and controllability). Because of the nature of the qualitative part of the objectives, some of the qualitative aspects cannot easily be formulated. Thus, it makes it difficult to establish a single objective function to evaluate the design. To cope with realistic problems, some logical and practical assumptions must be applied to simplify the ideal model. As a consequence, the production of quantitative cost effective designs has become the main objective.

However, satisfying the economic objectives does not guarantee that the solution will be practical. A network should not only save money but also be simple, operable and controllable. Usually, problems associated with the operability, controllability etc. are closely related to the complexity of a network. A complicated network may create difficulties in achieving smooth operation of the whole plant and may introduce strong interaction and dependence between exchangers. Therefore, to achieve a low cost and simple network structure is the main objective of this study.

1.2 The Motivations of this Research

Though the Pinch Design Method (PDM) has produced a most extensive list of good projects in industry for improved heat integration, two major limitations exist in the PDM, i.e. the use of *single* ΔT_{min} and the *strict pinch decomposition*. This situation calls for the further improvement of the current methods.

It has also been discovered that there has been a very *little connection and linkage* between the two major approaches, i.e. thermodynamic and heuristic methods and mathematical programming methods. However, the former approaches should adopt the advantages of mathematical programming methods in terms of *optimization* whilst the latter approaches would benefit from the necessary *physical insights* which can usually be obtainable from the application of the thermodynamic methods. Obviously, the combination of the advantages of both approaches is of great importance for finding optimal solutions to HEN synthesis problems. Any work aiming for this combination would make a great contribution.

Therefore, how to break the limitations in the PDM and how to combine the advantages of both thermodynamic and mathematical programming approaches become two strong motivations for this study.

1.3 The Objective and General Methodology

The objective of this research is to develop a novel method for the conceptual design of HEN, which should account for the two facts mentioned above. The general methodology to be followed is essentially that which has been successfully used in the overall project to date, viz. to examine the physical structure of the problem with a view to reducing its complexity by identifying the dominant constraints and then applying thermodynamic principles and finding heuristics to produce sound initial designs. These initial designs can then be optimized using conventional non-linear optimization techniques in the subset of the problem's initial dimensionality. The 'block method' has been devised for this purpose and has so far proved to be a very promising method for industrial application.

1.4 Organization of this Thesis

Chapter 2 is a review of the various methods for HENS. This review focuses on the analysis of these methods and their inherent advantages and disadvantages. This analysis should help to discover the new avenues for improving the current methods. Chapter 3 presents the 'block' concept and the detailed 'block method' which combines the thermodynamic principles and heuristic rules with mathematical optimization approaches. In this Chapter, the mixed integer linear programming (MILP) for match selection associated with the block method is also presented. The sequential approach for match selection used widely in the current methods is compared with the simultaneous approach applied in the block method. As well, the issues about stream splitting problems are also addressed.

Chapter 4 extends the block method for problems with significantly different film coefficients. The new targeting procedure to cope with different film coefficients is presented. The interesting phenomenon discovered in this work is that by changing the individual ΔT-contributions, different stream structures can be screened prior to design. Thus, the promising stream structures can be selected for design.

Chapter 5 introduces the pure mathematical programming models which are built based on the block decomposition and the block-based superstructure. It is shown that the block concept provides necessary physical insights of HEN synthesis for mathematical models, which eliminates a large number of inferior alternatives from consideration in optimization and thus improve the efficiency of solving an NLP problem. More importantly as the optimization starts at a good region which is located using the targeting procedure (Linnhoff and Ahmad, 1986a & b, Zhu et al, 1993a, 1994), the possibility of finding the global optimum is enhanced.

Chapter 6 describes the work associated with the energy relaxation. The interesting discovery of this work is that the parameters, i.e. temperatures and heat loads in a heat exchanger network can be represented by Kirchhoff' Law. This presentation greatly simplifies the task for loop-breaking and makes it much more deterministic for the detailed calculation of the potential energy penalty associated with the removal of an exchanger from a network.

Chapter 7 suggests the possible future works to be done following the development of the block method. From the practical application point of view, the retrofit study is of great interest. As well, the extensions of this method to consider exchanger pressure drop, different material constructions, detailed exchanger design etc are also very important.

CHAPTER 2

LITERATURE REVIEW

SUMMARY

Process synthesis has generated considerable interest in the past two decades. Heat exchanger network synthesis (HENS), a major problem in process synthesis, is arguably the most studied example and the basic principles for a detailed understanding of the problem are well established. Considerable progress has been made along three lines of research. These are referred as thermodynamic and evolutionary methods, mathematical programming strategies and knowledge based systems. Excellent reviews have been presented by Nishida et al (1981), Stephanopoulos (1982), Hohmann (1984) and Gundersen and Naess (1988). In particular, the final review of Gundersen and Naess provides a comprehensive view of the state of art in HEN synthesis prior to 1988. The current review is going to identify the three phases of HENS research, outlined the various methods and critically analyzed these methods to find appropriate avenues for further improvement.

Although the Pinch Design Method (PDM) dominates in industrial applications for improved heat integration, the major limitations in the PDM arise from the use of a single ΔT_{min} and the strict pinch decomposition. Overcoming these limitations is a key focus of recent research in HENS.

A more significant issue also arises. There has been little progress on linking the research in the thermodynamic or heuristic methodology with the research in mathematical programming strategies. Both these approaches have distinct strengths. Clearly, establishing such a linkage would provide a significant contribution to the field of process integration or conceptual design.

2.1 Introduction

As well as being important from the point of view of general process synthesis, the study of HENS from the view point of energy conservation is of considerable importance. The problem represents a real-life situation and basic insights gleaned by such analysis have lead to 30-50% energy savings in many process industries (Linnhoff and Vredeveld, 1984).

The 'modern' HENS problem was first formulated by Masso and Rudd (1969) and many researches have since proposed a variety of different design algorithms for HEN synthesis (Hohmann, 1971; Nishida et al, 1977; Linnhoff and Flower, 1978a & b; Boland and Linnhoff, 1979; Su, 1979; Linnhoff and Hindmarsh, 1983; Papoulias and Grossmann, 1983; Floudas et al, 1986; Trivedi et al, 1989; Linnhoff and Ahmad, 1990; Ahmad et al, 1990; Yee et al , 1990; Yee and Grossmann, 1990; Ciric and Floudas, 1991; Rev and Fonyo, 1991; Wood et al, 1991; Suaysompol et al, 1991a & b; Zhu et al, 1994, 1993a & b).

The design objective of a heat exchanger network (HEN) includes quantitative considerations(cost of exchanger equipment and external utilities), coupled with qualitative elements (safety, operability, flexibility and controllability). This makes it difficult to establish a single objective function to evaluate a HEN design (Gundersen and Naess, 1988). Ease of operability is a highly desirable goal for any process design but slightly different topologies posses vastly different operability characteristics (Grossmann and Morari, 1984). Given the current state of knowledge, it is extremely difficult to consider the operability of a network in the initial stage of design (Halemane and Grossmann, 1983; Beautyman and Cornish, 1984; Saboo and Morari, 1984; Townsend and Morari, 1984; Calandranis and Stephanopoulos, 1985; Grossmann and Floudas, 1985; Swaney and Grossmann, 1985; Terrill, 1985; Trivedi et al, 1989). Therefore, the objective in HEN synthesis is to generate feasible networks with low total costs and simple network structures. These networks can then be further analyzed on the basis of their operability.

The key reviews in the area of heat exchanger network (HEN) synthesis are the excellent studies of Nishida et al (1981), Stephanopoulos (1982), Hohmann (1984) and Gundersen and Naess (1988). In particular, the most recent review surveys in detail most of work done prior to 1988 and provides a detailed state of art in HEN synthesis. The present review focuses on the analysis of previous and current methods to reveal their associated advantages and disadvantages. This analysis may help to discover the new avenues for further improvement of HEN methods.

2.2 Problem Definition and Statement

Problem Definition

Masso and Rudd (1969) provided the classical definition for the HEN synthesis as follows:

Heat exchanger network design is undertaken to cope with a situation where a variety of process streams are to undergo simultaneous state changes achievable by the addition and/or removal of heat. Economic advantages concurrent with the efficient use of the process streams, as heating or cooling media, serve as the incentive for carefully administering the specification of auxiliary equipment and facilities such as water coolers and steam or fired heaters. Under the usual circumstances, however, it is not clear beforehand how to go about matching heat demands and supplies in such a manner as to optimize the performance of the required system. This problem differs from that where the operation of an existing network is being optimized by proper selection of its internal temperatures, flow rates, heat exchanger areas, etc. For the *situation at hand, there is no previous information on what the network looks like: there is no available structure.*

Problem Statement

In HEN synthesis, some of the qualitative constraints can be expressed explicitly. Thus, with these constraints defined, Yee and Grossmann (1990) stated the heat exchanger network synthesis problem as follows:

Given are a set of hot process streams to be cooled and a set of cold streams to be heated. Specified are also each hot and cold stream's heat capacity flow rates and the initial and target temperatures stated as either exact values or inequalities. Given also are a set of hot utilities and a set of cold utilities and their corresponding temperatures. The objective then is to determine the heat exchanger network which exhibits the least annual cost. The solution defines the network by providing the following:

1. Utilities required.
2. Stream matches and the number of units.
3. Heat loads and operating temperatures of each exchanger.
4. Network configuration and flows for all branches.
5. Area for each exchanger.

The objective of least annual cost includes the optimal trade-off of multiple targets, i.e. minimum heat transfer area, minimum units or shells and minimum utility consumption. These trade-offs are summarized by Figure 2.1.

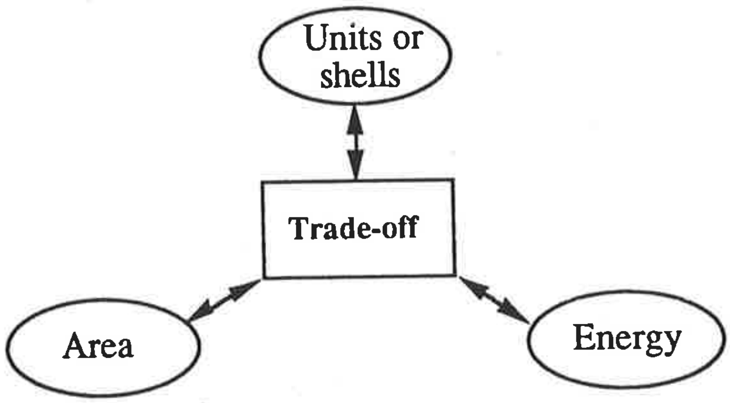


Figure 2.1: Trade-off in the HEN synthesis

2.3 History of HEN Synthesis

Three Design Phases

Three distinct phases can be identified in the development of HEN synthesis. Early methods (phase 1) normally emphasized the investment cost and employed minimum area as the design criterion and guide for selecting matches. The trade-off between energy, area and units was not considered. The methods developed during this period included those by Nishida et al. (1971), Hohmann (1971), Nishida et al.(1977) and Umeda et al. (1978). If the driving forces are appropriately applied, the "fast" heuristic method proposed by Ponton and Donaldson (1974) normally provides near-minimal area solution (Gundersen and Naess, 1988).

After the steep rise in petroleum price in 1973 (the so–called "energy crisis"), the energy cost became dominant in chemical processes and it was found that any improvements in reducing capital investment yielded only modest returns as discussed by Rather (1982). Thus, reducing the energy consumption was the objective of research and various methods were developed for either new heat exchanger networks or retrofit problems. This resulted in the discovery of important and fundamental concepts such as the heat recovery pinch as a bottleneck for reducing energy consumption (Umeda et al, 1978; Linnhoff et al, 1979). The fundamental understanding of the heat recovery pinch, including the decomposition effect was presented (Linnhoff et al 1979; Linnhoff and Turner, 1981; Linnhoff et al; 1982; Linnhoff and Hindmarsh, 1983; Linnhoff and Vredeveld, 1984). Since then, Linnhoff and his coworkers, first within ICI and later at UMIST have developed and refined the Pinch Technology.

The philosophy applied to most phase 2 methods was stated by Gundersen and Grossmann (1990):

"Designs that achieve maximum energy recovery (MER) in the fewest number of units (U_{min}) are near-optimal in total annual costs".

However, because of the strict pinch decomposition and the use of one global variable (ΔT_{min}) in the Pinch Design Method (PDM), the initial network produced is usually quite complicated and the evolution of the initial network can be a complex task (Su, 1979; Linnhoff et al, 1982; Trivedi et al, 1990). Rev and Fonyo (1986) invented the pseudo-pinch concept, and Challand et al (1981) and Colbert (1982) produced the concept of Dual-Temperature Approaches (DTA), to overcome the weakness from the strict pinch decomposition. Trivedi et al (1989) and Wood et al (1991) applied these two concepts to HEN synthesis problems and developed a new method , so–called Pseudo-Pinch Design Method (PPDM). Suaysompol and Wood (1991a) improved on the PPDM and developed the Flexible Pinch Design Method (FPDM). The PPDM and FPDM focus on the network simplification while achieving maximum energy recovery. Consequently, the flexibility for design at pinch is increased and the need for network evolution is reduced. Ciric and Floudas (1990) applied the concepts of the pseudo-pinch and dual-temperature approaches to their optimization model and found simpler networks can be obtained by the relaxation of the assumption of no heat flow across the pinch point.

Since it is very difficult to find the global optimum for a design problem directly (because of non–linearities and high dimensionality), the general philosophy of various methods used was to design an initial network by focusing on a simple target (the energy target) and then evolve this network towards the other targets (area and units). This strategy proved to be quite successful and has been applied to HEN synthesis for a long period. However, since the inherent nature of HEN synthesis is a combinatorial problem coupled with multiple targets, a network should be optimized *simultaneously* based on the trade-off between capital and energy costs. It is not surprising to find that in some cases, the methods relying on the evolutionary design philosophy may fail to provide near global optimal solutions. Therefore, the focus of current research has shifted to simultaneous optimization.

Current methods (designated phase 3) emphasize considerations of the total cost (capital and energy). Phase 3 methods were first introduced by Ahmad and Linnhoff (1984) and Townsend and Linnhoff (1984). Research into the development of thermodynamic and evolutionary methods accounts for both the energy-area or energy-capital trade-off systematically. Improved versions of the Pinch Design Method (PDM) (Linnhoff and Ahmad, 1990) yield better solutions by utilizing the 'Driving Force Plot' (DFP) and the 'Remaining Problem Analysis' (RPA). With these procedures, designs evolve by a *sequential* choice of matches and the designer provides significant input into the choice of matches and hence the solution process. The design outcome is a network which is close to the area target while achieving the optimal energy consumption. Subsequently, the number of units in a network is reduced by using the evolution strategy (Linnhoff and Hindmarsh, 1983).

Using the Phase 3 research philosophy, recent applications of mathematical programming (Ciric and Floudas, 1991; Yee and Grossmann, 1990; Yee et al, 1990) seek to arrive at such minimal-cost solutions. The work of Grossmann and his coworkers appears to be particularly promising, as a superstructure is used, which restricts the solution to reasonably practicable topologies. Yee and Grossmann (1990) formulated the synthesis problem as a mixed integer non-linear (MINLP) problem. Annual cost, comprising of utility cost, area cost as well as fixed charges for exchanger units are optimized simultaneously. As well, this MINLP model can account for design constraints such as forbidden, required or restricted matches. However, convergence to local optimal is still a potential difficulty with such methods (Quesada and Grossmann, 1993), but these workers are making progress in developing and improving a branch and bound approach, which has a convex under-estimator.

Three Design Methodologies

In terms of methodology, research has been progressing along three different lines. These are the use of thermodynamic concepts, mathematical programming technologies and the application of knowledge based systems for process design. Despite a number of inherent shortcomings, industrial application of the methods has been dominated by the Pinch Design Method (PDM).

As stated, the two major design algorithms are the thermodynamic and mathematical programming approaches. The former methodology mainly relies on physical insights into HEN synthesis. The latter approach involves a rigorous formulation of the problem and provides a superior search technique for optimization.

The early work in the field of mathematical programming was carried out mainly in the early 80's (Kobayashi et al, 1971; Cerda et al, 1983; Cerda and Westerberg, 1983; Papoulias and Grossmann, 1983; Floudas et al, 1985; Floudas et al, 1986; Saboo et al, 1986). Major progress in this area occurred in recent years (Floudas and Ciric, 1989; Gundersen and Grossmann 1990; Colberg and Morari, 1990; Yee et al 1990; Yee and Grossmann, 1990; Ciric and Floudas, 1991). The key problem which plagues mathematical programming is how to discover the global optimum among possibly many local optima resulting from the non-convex nature of the problem. Attempts aimed at providing a general algorithm for finding the global optimum have been conducted by a number of workers (Floudas et al, 1989, Floudas and Visweswaran, 1990, Visweswaran and Floudas, 1990, Viswanathan and Grossmann, 1990, Quesada and Grossmann, 1993).

The third approach has not been received as much attention. Despite a very rapid growth in the application of knowledge-based systems or expert systems in many other areas, the techniques have had little impact on the activity related to HEN synthesis (Gundersen and Naess, 1988). The basic methodology used in expert systems for HEN synthesis is that a problem is reduced to several simpler subproblems and solved based on proposed theorems (e.g., the search techniques in artificial intelligence). Strictly speaking, these theorems are not rigorous physical insights of HEN synthesis, but are used in connection with the chosen inference mechanism (e.g., the forward chaining inference method). Two major problems, i.e. the low computational efficiency and the difficulties in the representation of the knowledge in HEN synthesis, impede the application. However, research has been carried out to try to overcome these problems. The expert systems developed recently include those by Grimes et al. (1982), Niida et al. (1986), Calandranis and Stephanopoulos (1985), Viswanathan and Evans (1986, 1987), Chen et al (1989) and

Suaysompol and Wood (1991b). The apparent advantage of using knowledge-based techniques is the flexibility in applying, or combining, several methods for subproblems within a HEN. It is easy to modify or improve the capabilities of the system by expanding the contents of the knowledge base.

2.4 State of Art in HEN Synthesis

The three key stages in HEN synthesis are targeting, synthesis and optimization. Targets involve estimates of the best (limiting) theoretical performance of a heat exchanger network. The synthesis stage is concerned with matching of hot and cold streams and sequencing of the resulting exchangers. Optimization involves both topological and parameter improvements that reduce the total annual cost. These three stages also constitute a complete process of optimal HEN synthesis and design.

2.4.1 Targets

Targets are established prior to design. These provide lower bounds for the design problems. Possible targets include the targets for energy, heat transfer area, number of units or shells and total annual cost.

The Energy Target

The correct energy target has been established for the unconstrained case by several researchers. Hohmann (1971) used the feasibility table, Linnhoff and Flower (1978a) developed the problem table analysis (PTA) and Umeda et al (1978) employed the temperature-heat content (T-Q) diagram to get the utility targets. The PTA is the best known method and has been widely used for energy targeting.

For the situation with constrained matches (forbidden, imposed matches), an LP transportation model was developed by Cerda and Westerberg (1983) to predict the energy target and later an LP transshipment model was proposed by Papoulias and Grossmann (1983) to reduce the size of the transportation model.

The Area Target

When considering heat transfer area, one should distinguish between minimum area design procedures which include strategies for the network development that minimize total area, and targeting algorithms for calculating an area target ahead of design (Gundersen and Naess, 1988). The area target is calculated for specified utility loads.

The concept of an area target was introduced independently by Hohmann (1971) and Nishida et al (1971). Hohmann proposed a method for the calculation of total surface area. By assuming an average overall heat transfer coefficient (U) and dividing the composite curves into simple counter-current sections based on 'kink points', the area for each section is calculated by the following equation:

$$A_j = \frac{Q_j}{U \Delta T_{LMj}} \tag{2.1}$$

where the subscript j refers to a counter-current section on the composite curves. The sum of the section areas A_j is the total minimum area which can be expressed as:

$$A_{min} = \frac{1}{U} \sum_j \frac{Q_j}{\Delta T_{LMj}} \tag{2.2}$$

Nishida et al (1971) addressed the calculation for the minimum area target in the heat content diagram by matching streams in the order of decreasing temperatures. Nishida et al (1977) refined this approach by taking the utility into account. Utilities are not necessarily placed at the extremes, but located 'optimally' with respect to their temperatures. When all film coefficients are equal and vertical counter-current heat transfer is assumed, the expression for the area target is identical to that of Hohmann .

Townsend and Linnhoff (1984) extended these methods to account for different film coefficients. Since the assumption of an average overall heat transfer coefficient is an extreme simplification, they suggested the following formula (the so–called Bath formula):

$$A_{min} = \sum_k \frac{1}{\Delta T_{LMk}} \sum_j \left(\frac{q_j}{h_j}\right)_k \tag{2.3}$$

where subscript k refers to an enthalpy interval defined by 'kinks' on the composite curves.

This formula was first presented without proof or explanation and a detailed proof was later provided by Linnhoff and Ahmad (1990). This area target like Hohmann's (Eq. (2.2)) is exact only if all film coefficients are equal and that the heat exchange is strictly vertical. Provided that film coefficients only differ slightly, the Bath formula yields a satisfactory approximation. Ahmad (1985) and Townsend (1989) showed that providing film coefficients differ by less than one order of magnitude, this simple area calculation usually predicts an area not larger than 10% of the true area target which is determined by mathematical programming methods. Although the simple area target gives a good estimate of the area requirement for many problems, the area target may be poorly estimated in cases of significantly different film coefficients.

To handle problems with significantly different film coefficients, Nishimura (1975, 1980) first proposed a general approach but only for problems with a single hot (cold) versus multiple cold (hot) streams. Ahmad (1985) extrapolated Nishimura's results to a general case, i.e. the individual contribution ΔT_i for stream i was related to its film coefficient through the equation:

$$\Delta T_i = \frac{C}{\sqrt{h_i}} \tag{2.4}$$

where C is a constant that is adjusted until the heat recovery level obtained by using the individual ΔT–contributions is the same as when using a single global ΔT_{min} (HRAT). This resulted in a more complex procedure and a new area target. It provided the first systematic approach to exploit differences in film coefficients. In dealing with individual stream vertical shifts in each enthalpy interval, Ahmad (1985) proposed a modified area targeting formula (the so–called pseudo-BATH formula).

Another important contribution to individual approach temperature difference was made by Fraser (1989a) who proposed the minimum heat flux for the design of HEN's which led to an individual minimum approach temperature for each stream using the relation

$$(\Delta T_{min})_i = \frac{2Q''_{min}}{h_i} \tag{2.5}$$

where Q''_{min} is the minimum heat flux and $\frac{1}{2}(\Delta T_{min})_i$ is equivalent to the temperature difference between the stream and the wall. This idea was derived from industrial practice (Fraser, 1989b).

Rev and Fonyo (1991) noted that the determination of ΔT–contributions using the approach suggested by Ahmad (1985) may be ambiguous. Hence, they introduced the diverse pinch approach to remedy the inherent drawbacks in the method of Ahmad (1985). The difference between these two approaches is that Rev and Fonyo applied individual shifting at the very beginning and not in a later phase of the design that was done by Ahmad. Ahmad applied individual shifts while maintaining the original (uniform) pinch and the corresponding vertical intervals (Rev and Fonyo, 1993). The use of the diverse pinch concept for stream shifting has a clear effect on the distribution of the heat flux. Similar to Fraser's (1989a) proposal, Rev and Fonyo (1991) suggested an approximately uniform heat flux $Q'' = Q/A$ by setting ΔT_i contributions proportional to $1/h_i$. In their work, a shifted set of composite curves is obtained. The area calculation based on the modified composite curves has a similar form to the Bath formula, and was named the diverse Bath formula by Rev and Fonyo.

The previous algorithms for the prediction of the area target are based on the assumed film coefficients. However, exchangers are normally not designed on the basis of an assumed film coefficient, or to achieve a particular coefficient, but rather on the basis of allowable pressure drops. The coefficient assumed during the targeting phase may be inconsistent with that finally achieved during detailed exchanger design. This inconsistency can result in poor targeting.(Polley et al, 1990). Hence, Polley et al suggested that the network area prediction should be done based on stream pressure drops rather than on assumed film coefficients to reflect the reality of practical design. They identified two major advantages for this approach. First, it removes the subjectivity in the selection of the coefficients used in targeting. Second, it makes the targeting procedure more consistent with exchanger design procedures. In their approach for targeting area, the pressure drop is related to the heat transfer area and thus the Bath formula is extended to include pressure drop considerations. Polley et al (1990, 1991) proved that this approach can provide a more realistic area prediction which is consistent with the subsequent detailed exchanger design.

A rigorous area target, even for the situation with a large variation in film coefficients, can be discovered using a linear programming (LP) transportation model

(Saboo et al, 1986). The approach suggested by Saboo et al. commences using the temperature intervals (TI's) based on the 'kink points' in the composite curves. The TI's are then made successively smaller and new LP's are solved until either the area calculated converges within a specified tolerance or until the problem becomes prohibitively large.

Using the calculus of variations, Nishimura (1980) developed a rigorous area target for the special case of one hot stream versus multiple cold streams or vice versa. Nishimura showed that this area target can be achieved by a complex network structure in which the approach temperatures are inversely proportional to the square root of the corresponding film coefficients.

Colberg and Morari (1990) developed a pair of NLP models for the area target and the capital cost target. These two models can handle problems involving unequal film coefficients and constrained matches. The NLP formulation is based on the temperature intervals defined by 'kinks' and the initial solution for the NLP models is provided by using the heat cascade corresponding to the composite curves. The area or capital cost target is calculated for an associated network. By contrast, the area calculated by the Bath formula or the LP model by Saboo et al (1986) is associated with a very complicated network structure. As well, the NLP model can give a more precise estimate for the area target.

By means of a simple superstructure, Yee et al (1990) presented a pair of NLP models, one for simultaneous energy and area targeting, and the other for area targeting with a fixed utility requirement. The models are devised based on stages rather than TI's. Thus, the number of variables involved in the NLP models are greatly reduced compared to the previous methods. The models can provide a good prediction of the area target associated with a feasible network. In the models, the non-linear constraints are avoided and the non-linear terms only appear in the objective function: this treatment produces high robustness and good solution efficiency.

The Unit Target

Hohmann (1971) proposed the (N-l) rule for the unit target where N is the total number of streams including utility streams. Boland and Linnhoff (1979) extended this rule by Euler's theorem and gave a more general unit target as:

$$U_{min} = N - S + L \tag{2.6}$$

where S is the number of disconnected subnetworks and L the number of loops. Linnhoff and Turner (1981) introduced the unit target by applying (N-l) rule above and below pinch. For the case with constrained matches and multiple utilities, the minimum number of units while achieving MER can be predicted by a MILP transportation model (Cerda and Westerberg, 1983) or a MILP transshipment model (Papoulias and Grossmann, 1983).

It is believed that (N-l) networks cannot always be found (Linnhoff et al. 1979, Grossmann, 1985). For many practical problems, stream splitting as a technique is often required to reduce the number of units. Wood et al (1985) raised an interesting issue by demonstrating that by using a novel arrangement of stream splitting, mixing and by-passes, some problems may be designed to conform to the U_{min} target.

The Shell Target

Colbert (1982) and Hohmann (1984) pointed out that when non-counter current exchangers are used, the number of shells is often of greater importance than the number of units. In practice, industrial heat exchanger units are composed of multipass shell-and-tube units. The number of shells required by the network plays a significant part in the cost of the final design.

All the shell targeting approaches are based on the composite curves. Shiroko and Umeda (1983) proposed a stepwise approach to estimate the number of shells from the composite curves by a graphical procedure. Ahmad (1985) presented a coherent targeting and design strategy for minimum number of shells and near-minimum area in networks of 1-2 exchangers. This is based on analysis of the minimum number of shells required for the temperature distribution of the composite curves.

Trivedi et al (1987) presented a different method for targeting the number of shells. This 'stepping-off' approach which is analogous to the McCabe–Thiele construction, is based on the composite curves. The number of steps over the temperature range of a stream presents the number of shells it requires. The total number of shells is thus calculated for all hot and cold streams separately. Whichever number of shells is larger, whether for hot streams or cold, determines the shell target. Shell targeting by this method is very straightforward; however, this method can sometimes lead to an under-estimate of the required number of shells and is not consistently reliable (Ahmad and Smith, 1989).

Johns (1987) targeted the number of shells based on the enthalpy intervals defined by 'kinks' on the composite curves. Ahmad and Smith (1989) exploited both the enthalpy intervals and stream contribution concepts to target the number of shells. The latter approach to shell targeting was based on the more practical X_p model (Ahmad et al, 1988). In this model, the determination of the number of shells can ensure the correction factor F_n is larger than a specified value (e.g. 0.75 or 0.80) for 1-2 exchangers. The X_p model also avoids steep slope regions where there exists a very high sensitivity to changes in process conditions. As well, the X_p model allows temperature crosses in the exchanger shells and thus can assure a more realistic design.

Suaysompol (1991) modified the method suggested by Ahmad and Smith (1989) to account for streams, area and units. The modified model gives the achievable instead of the theoretical minimum number of shells. Such a number of shells may be achieved by the Flexible Pinch Design Method (FPDM) (Suaysompol and Wood 1991a).

Total Annual Cost Target (Capital and Energy)

Targets for energy, heat transfer area and the number of units or shells, enable the capital cost target and total annual cost to be predicted. By calculating the total annual cost for various ΔT_{min} (HRAT), the optimal ΔT_{min} (HRAT) corresponding to the least total annual cost can be located. This provides a good initial point for synthesis. This idea is fundamental to the supertargeting approach (Ahmad and Linnhoff,1984 & 1989; Ahmad 1985; Linnhoff and Ahmad,1986a & b).

Prior to the supertargeting method, the minimum approach temperature ΔT_{min} (HRAT) was determined by experience. However, even with experience, the chosen ΔT_{min} (HRAT) may not be optimal. A poorly estimated ΔT_{min} (HRAT) may lead to a network which can never be evolved to the optimal solution. This phenomenon was referred to as the topology trap related to ΔT_{min} (HRAT) by Linnhoff and Ahmad (1986a & b, 1990). Thus, prediction of the optimal ΔT_{min} (HRAT) using total annual cost targeting represented a significant advance.

However, two assumptions are necessary for the supertargeting approach. First, the simple area target is calculated using the Bath formula and second the total heat transfer area is evenly allocated between the minimum number of units. As discussed, the area target based on the Bath formula is not rigorous and associated with a 'spaghetti structure'. An obvious question that arises is "should the rigorous target by Colberg and Morari (1990) or Yee et al. (1990) be employed?". The assumption of an equal allocation of heat transfer area over the minimum number of units also affects the capital cost calculation when the exponent of exchanger cost models is not unity. Ahmad et al (1990) argued as follows: "suppose the capital cost predicted by applying the Bath formula is not close to the true target, it does not matter as long as the slope of the cost curve follows the true cost target curve. In this case, the correct optimal ΔT_{min} (HRAT) could still be obtained." This suggests that though the cost curve from the supertargeting is not exact, the key importance is not for precision, but simply to avoid a complete miss of an estimated 'optimal' starting point. A complete miss may result in an inferior design.

Rev and Fonyo (1991) proposed a similar supertargeting approach. The sole difference is in that unequal film coefficients are considered by using individual ΔT-contributions and total heat transfer area is calculated by the so–called diverse Bath formula.

The more reliable targeting method is that developed by Yee et al (1990). In their work, a simple yet general superstructure for heat integration was presented. This superstructure used a stage-wise representation. Within each stage, heat transfer is possible between each hot and cold stream. A NLP model was introduced to simultaneously target for area and energy cost while properly accounting for constrained matches.

2.4.2 Synthesis

In this section, the most significant methods for HEN synthesis in each of the three phases are critically discussed with a view of discovering the important problems in HEN synthesis for which better solutions might be sought.

Phase 1 Methods – design for minimum area

Most early methods used minimum area as the design criterion and the guide for selecting matches. The outstanding method in this phase was the thermodynamic evolutionary synthesis method proposed by Nishida et al (1971, 1977). This method appeared to be suitable for the solution of realistic problems. It employed the following procedure: first ensure maximum energy recovery, then minimize heat transfer area and finally evolve an initial network to minimize the total cost by following a number of heuristic rules. The prime tool guiding match determination was the heat content diagram adopted by Siirola (1974). This represents the streams according to their temperatures and heat capacities.

The cold utility is calculated as follows: if any temperatures of the coldest section of a hot stream minus ΔT_{min} are less than the lowest supply temperature of any cold stream, this section should be served by cold utility. The sum of heat loads of such sections gives the minimum cold utility requirement. The hot utility is calculated in a similar manner. With utility requirement calculated as above, hot and cold streams, including utilities, are matched in decreasing order of their temperatures. Thus, the basic strategy is thermodynamically and systematically orientated. This strategy was totally different from the strategy employed by some other early methods where matches were selected by favouring large driving-force matches which would cause other matches subsequently placed to have smaller driving forces. The disadvantage is that the net result may be an increased area requirement for the HEN and a large utility consumption. Essentially, this kind of strategy is based on the unit design rather than the network synthesis.

The inherent drawbacks in the method suggested by Nishida et al are related to the calculation of the minimum utility requirement and match selection. The method cannot correctly predict the minimum utilities requirement (Linnhoff and Flower, 1978b). With the utility consumption fixed according to the calculation suggested, the design at pinch region may have driving forces less than the minimum approach temperature (ΔT_{min}). In order to retain ΔT_{min} for matches at the pinch or avoid thermodynamic infeasibility, a lot of stream splitting at the pinch may be unavoidable. In addition, when introducing matches according to the heuristic rules suggested by Nishida et al., excessive stream splitting may occur at an early stage of synthesis.

Another well known method in this phase is the fast algorithm proposed by Ponton and Donaldson(1974). This method uses heuristics that allow fast synthesis of a single heat exchanger network with a low area requirement, rather than producing alternative networks and then selecting the best from among them. Two heuristics are used to select matches:

Heuristic 1: Match the hottest hot stream with the cold stream with highest target temperature.

Heuristic 2: The two streams should exchange as much energy as possible without allowing their driving forces to be less then ΔT_{min}.

The first heuristic identifies the two streams to be matched whilst the second heuristic determines how much heat should exchange between these two streams. The heuristic approach quickly and efficiently yields good solutions though not necessarily the best.

However, the network generated by the Ponton and Donaldson method usually severely violates the minimum energy consumption and if fixed utilities are a requirement in the synthesis, the assigned network structure becomes over-complicated (Stephanopoulos, 1982; Rev and Fonyo, 1986). The fundamental reason underlying these two problems is that a systematic safeguard against individual matches which prejudice an overall optimum for the whole network is not provided (Linnhoff and Flower 1978b).

In summary, since the methods in phase 1 lack sufficient physical insight to the HEN synthesis, the heuristic rules produced are neither general nor rigorous. Hence, the networks synthesized are not necessarily optimal (Stephanopoulos, 1982).

Phase 2 Methods – design for MER and U_{min}

The steep rise of energy cost provided the motivation for developing synthesis methods to reduce operating cost. The discovery of the heat recovery pinch (Umeda et al., 1978, Linnhoff et al., 1979) as a bottleneck for energy savings resulted in increased efforts in academia and industry in developing systematic methods for both retrofit and new designs. The pinch concept forms the basis of the best known method, i.e. the Pinch Design Method (PDM). Good introductions to this method are provided by Linnhoff et al (1979), Linnhoff et al (1982) and Linnhoff and Hindmarsh (1983). The greatest contribution of the PDM to this area of chemical engineering is the insight it supplied to the application of fundamental thermodynamic principles to efficient heat recovery and process integration.

In this review, the PDM developed in the early 80's is referred as the old version of the PDM which is classified in the phase 2 category. The old version of the PDM aims for MER design. Since then, the PDM has been improved at UMIST. The new version of the PDM can achieve MER and near-minimum area simultaneously. Thus, it is referred to as a phase 3 method.

In the PDM, three basic rules have to be strictly adhered to in order to achieve maximum energy recovery. These are

- *Do not transfer energy across the pinch*
- *Do not use cold utilities above the pinch*
- *Do not use hot utilities below the pinch*

According to the first rule, the system is divided into two subsystems at the pinch. Design starts at the most constrained region (the pinch) and matches are selected by employing CP matching rules (Linnhoff and Hindmarsh, 1983). To reduce the number of units, each exchanger is made as large as possible. This heuristic is referred to as the 'tick-off' rule (Linnhoff and Hindmarsh, 1983). Subsequently, the two separately synthesized subnetworks (above and below the pinch) are merged together to achieve MER design. The network generated in this way usually has more units than the unit target. It then is evolved to reduce the number of units using an energy relaxation approach (Linnhoff and Hindmarsh, 1983).

However, the major limitations of the Pinch Design Method are the use of a single ΔT_{min} (HRAT) for all heat exchangers in synthesis and the strict pinch decomposition (Rev and Fonyo, 1986; Trivedi et al,1989; Gundersen and Grossmann ,1990; Colberg and Morari ,1990; Ciric and Floudas,1990; Rev and Fonyo, 1991; Wood et al,1991; Jezowski, 1991). They all observed that these two constraints are too rigid for optimal heat exchanger network synthesis. Gundersen and Grossmann (1990) showed another topology trap caused by a single ΔT_{min} (HRAT). Therefore, substantial research has been conducted to remedy these two deficiencies.

Wood et al (1985) showed that by avoiding the strict pinch decomposition and allowing exchangers to cross the pinch, using stream splitting and bypassing, it is often possible to obtain a U_{min} design while achieving MER.

Similar work (Jones and Rippin (1985) and Jezowski (1990)) split those streams passing through the pinch in such a way so that the hot and cold stream branches matched in an exchanger have identical heat capacity flowrates. Two exchangers on both sides of the pinch may be merged into one. In this manner, there is no heat flow across the pinch despite exchangers operating across the pinch. As a result, the network is simplified but without energy penalty. However, it was demonstrated by Jezowski (1990) that such matches often incur a severe area penalty as a result of the narrow temperature profiles occurring in these exchangers. As well, Rev and Fonyo (1986) pointed out that blind insistence on the pinch rules can produce overly complicated networks. Thus, they proposed an approach where strict pinch decomposition is relaxed and a small amount of heat leakage across the pinch is allowed.

Another important work along this line is the introduction of the concept of Dual Temperature Approaches (DTA), i.e. the Heat Recovery Approach temperature (HRAT) and the Exchanger Minimum Approach Temperature (EMAT). The dual temperature approach (DTA) was first suggested by Challand et al. (1981) and Colbert (1982) and then further developed by Trivedi et al (1989) and Wood et al (1991). In the first dual temperature approach (DTA) proposed by Challand et al (1981) and

Colbert (1982), the initial design is generated based on the temperature interval (TI) method developed by Linnhoff and Flower(1978a). Then the design is simplified by applying the evolutionary strategy of Linnhoff and Flower (1978b) or loop breaking techniques by Su and Motard (1984). The DTA approach has been implemented in HEXTRAN which is a software package for HEN synthesis. Because of the large number of temperature intervals, the initial network generated by this method usually possesses a complicated structure. During network evolution, utility consumption is fixed at the utility target, thus significant effort is required to simplify the network. Nevertheless, the dual temperature concept is powerful in that the flexibility is provided by this concept and the limitation from a single ΔT_{min} is partially removed.

Mainly following this concept, Trivedi et al. (1989) proposed a new method, namely Pseudo Pinch Design Method (PPDM). In the PPDM, the system is decomposed into two subsystems at the pseudo pinch. The design strategy is similar to the PDM but it retains the flexibility from dual temperature concept. In PPDM, HRAT and EMAT were optimization variables. Gundersen and Grossmann (1988) proved, however, that in their vertical MILP model EMAT is not an optimization variable. Similarly, Colberg and Morari (1990) allow EMAT to vary in the range (δ-HRAT) where δ is a small number.

Recently, more progress along the research of providing simple designs has been achieved by the work done by Suaysompol and Wood (1991a & b). The methodology of this method is similar to the that of the Pseudo Pinch Design Method (PPDM). The difference is the PPDM starts a design at EMAT and fixes utility consumption at HRAT(ΔT_{min}). Thus, it allows net energy across the pinch with the amount of the difference of utility consumptions between EMAT and HRAT. To give larger driving forces for exchangers at the first place, FPDM starts a design at HRAT and permits heat flow across the pinch with same amount, thus no extra utilities are required as energy criss-crossing the pinch is balanced. For match selection, FPDM uses simple and effective heuristic rules, i.e. preferring subequality matches for one side of the pseudo pinch and searching for mirror image matches in the other side rather than the CP matching rules in the PPDM. The subequality match is defined as the match constructed by a pair of streams having same amount of heat which can be adjusted by shifting these two streams across the pinch. The mirror image match is the one having same pair of streams as the match on the other side of the pinch. These two kind of matches are formed to aim for network simplification. Examples proved that the networks produced by the FPDM are usually simpler than that obtained by the PDM. However, since the FPDM merely focuses on network simplification, it is not surprising to find that in some instances, a simple network may require a large capital investment. The other limitation of the FPDM is that the stream splitting has not been considered.

The mathematical programming studies carried out in phase 2 stage should also be mentioned. As stated, the heuristic rule espoused in the phase 2 stage is maximum energy recovery (MER) plus minimum number of units (U_{min}). Following this rule, Cerda and Westerberg (1983) formulated the HEN synthesis problem into a transportation model (MILP) which could handle restricted matches. Papoulias and Grossmann (1983) formulated the transshipment model for MER and U_{min} design. Based on the solution from the transportation model, the optimal network configuration is determined by a NLP model presented by Floudas et al. (1986). This approach has been implemented into the software known as MAGNETS (Floudas et al., 1986).

The common drawback inherent in all phase 2 methods is that attention is focused on the achievement of maximum energy recovery. Considerations of capital cost are ignored. However, should a number of designs all achieve MER and U_{min} targets, they are considered equally good based on this heuristic. However, significant differences may be in capital costs. This phenomenon has been demonstrated by Gundersen and Grossmann (1990) using a five stream problem. They presented four designs produced using MAGNETS. All four designs achieved MER and U_{min} targets. Obviously, these four designs are superior to designs that fail to meet the energy target by a significant amount. However, comparing the four designs, one was 63% larger in area incurring 36% penalty in capital cost compared with the best solution. Obviously, this design cannot be accepted as near optimal. With the widespread use of Pinch Technology in industry, most companies are able to produce MER designs. The question is how to distinguish between designs achieving MER and U_{min} in terms of total annual cost.

In addition, should a design only consider the maximum energy recovery and the minimum number of units, the possibility exists when reducing the number of units, that removal of one unit may incur small energy penalty but require a large additional heat transfer area. A significant total cost penalty may result. Thus, the disadvantage of the approach applied in phase 2 was that the trade-offs between energy, units and capital cost cannot be considered simultaneously and this approach can often lead to suboptimal networks. This drawback has motivated research to develop new methods which can solve the above problems. Such methods are referred to as phase 3 methods.

Phase 3 Methods – design for minimum total annual cost

As stated, the original PDM leads to networks with maximum energy recovery (MER). The philosophy of the improved PDM (Linnhoff and Ahmad, 1990) is to achieve minimum area designs while achieving MER. The new version of PDM yields improved solutions by utilizing the new CP-rules, 'Driving Force Plot' (DFP) and the 'Remaining Problem Analysis' (PRA). A match is selected initially by the new CP-rules together with the 'tick-off' rule. Then, the DFP or RPA is employed to check if this tick-off is appropriate. The new version of the Pinch Design Method (PDM) has achieved a significant improvement over the old version of the PDM.

The two major contributions from the improved PDM are the new methods for match selection, i.e. new CP-rules, the DFP and the RPA, and the determination of the 'optimal' ΔT_{min} (HRAT) which is used as a starting point of synthesis. The new methods for match selection provide more deterministic guidelines for selecting matches featuring the minimum-area requirement. The location of the optimal ΔT_{min} (HRAT) gives a designer the confidence that the current synthesis is been carried out at an 'optimal' condition and towards a near optimal design. To start a design at this optimal point is of utmost importance to avoid the topology trap (Linnhoff and Ahmad, 1986a & b, 1990).

Ahmad et al (1990) extended the PDM to handle situations with different film coefficients. A set of linear equations are constructed for shifting streams along the pinch point according to their film coefficients. As a consequence, the streams with small film coefficients are assigned large ΔT-contributions at the pinch and vice versa. The ΔT-contributions determined as such maintain the enthalpy balance at pinch, hence no extra utility is required. Ahmad (1985) has shown that this approach does lead to an improved minimum area design. The individual ΔT-contributions are usually considered at pinch or regions with narrow-spaced composite curves.

Besides the Pinch Design Method, Jezowski (1991) suggested an approach which combines the dual temperature approaches to allow energy criss-crossing the pinch with the fast algorithm by Ponton and Donaldson (1974) for match selection. In this approach, the effect of the area required for each match on the remaining problem is analyzed by the RPA (Linnhoff and Ahmad, 1990). The reason for the application of the Ponton-Donaldson method is that this algorithm is in broad agreement with principles of area targeting. Since it requires significant computation to discover a match with the combined application of the Ponton–Donaldson fast algorithm and the RPA (Linnhoff and Ahmad, 1990), this approach is restricted to small-scale problems. This severely limits its application.

Dolan et al. (1987, 1989) proposed the method to account for all types of costs simultaneously and applied the simulated annealing algorithm as a synthesis technique. Although this iterative type gave good results for some problems, a very large number of trials is required and the computational effort is very expensive.

A parallel development using phase 3 principles is a substantial body of work in the area of mathematical programming. Yee and Grossmann (1988) formulated an extensive MINLP model for retrofit problems where the piping layout is also considered. In this approach, operating cost and capital cost are considered simultaneously in the search for a least cost network. Recently, Ciric and Floudas (1991) proposed an approach for optimizing the different costs simultaneously. This approach embeds both strict pinch transshipment and pseudo pinch transshipment models. Both models are based on the hyperstructure model of Floudas and Ciric (1989) to select the optimal HEN configuration, and a modified version of the transshipment model of Papoulias and Grossmann (1983) to select optimal heat loads.

In order to reduce the size of a NLP model and to provide networks of moderate complexity, Yee et al (1990) presented a stage-wise superstructure which is simpler than the superstructure (Floudas et al., 1986) and hyperstructure (Floudas and Ciric, 1989). In the same work, based on the simplifying assumption for isothermal mixing of streams, Yee and Grossmann (1990) formulated the HEN synthesis problem as a MINLP model in which all constraints are linear. The solution scheme determines the least annual cost network by optimizing simultaneously the utility requirement (HRAT), the minimum approach temperature (EMAT), the number of units and the heat transfer area.

2.4.3 Optimization

Optimization of the network involves both topology and parameter changes to the initially synthesized design in order to minimize the total annual cost. Two approaches are used for optimizations, namely evolutionary and NLP optimization. Several methods presented in 70's have been named evolutionary but qualify as optimization methods (Linnhoff and Flower, 1978b; McGallard and Westerberg, 1972; Nishida et al, 1977; Shah and Westerberg, 1975; Umeda et al, 1978).

Linnhoff and Hindmarsh (1983) presented the evolutionary method, so-called "energy relaxation", to evolve MER networks towards non-MER designs with increased energy consumption, but a reduced number of exchangers. This is achieved by sequentially breaking loops and restoring the global ΔT_{min} through a 'path' in the network. Evolution was also used by Grimes et al (1982). The interesting feature of their evolutionary approach is that dummy exchangers with zero initial loads may be added and then loads are shifted to search through different topologies.

Su and Motard (1984) presented a loop breaking procedure for evolving MER designs. They defined the loop levels and suggested the heuristic of breaking loops according to their levels, i.e. start from the loop of first level and then second level loops and so on. Basically, this is an automated approach with a similar goal to the PDM. Trivedi et al (1990) also used this heuristic and presented the systematic energy relaxation approach which is based on the best-first searching technique. This approach identifies constrained exchangers in each loop together with those exchangers which are candidates for removal.

Recently, a more deterministic method to guide this evolution is presented by Zhu et al (1993c). It is based on the application of Kirchhoff's Law to the network. The potential energy penalties associated with breaking loops by removing units can be calculated. Thus the minimum energy penalty can be discovered and the unit to be removed to constitute an optimal solution can be identified. The minimum energy penalty path may be followed until a final network is discovered. In such a way, the designer can undertake the loop-breaking phase of network design with confidence.

Essentially, the previous evolutionary approaches are energy-oriented. In other words, the goal is to minimize the total energy penalty through network evolution by reducing the number of units rather than the total cost. Therefore, when applying the evolutionary approach, it is clear that the solutions are not necessarily optimal in terms of total cost and the evolution of a network is a highly complex task.

A straightforward idea is to adopt the advantages of mathematical optimization techniques in searching for optimal solutions. This strategy differs from the pure mathematical programming models which merely rely on the optimization techniques without the aid of the thermodynamic or heuristic methods provided by physical insights. The initial network obtained from the thermodynamic approaches provides a starting point for optimization. Ptacnik and Klemes (1988) proposed a method where the optimization proceeds along loops, paths and stream-splits since these situations offer the degrees of freedom for manipulating the network cost. Recently, a more general optimization approach is proposed by Zhu et al (1993a). This method views the whole initial network as a single optimization problem and formulates a NLP model for cost optimization. In this method, dummy heaters and coolers with zero initial heat loads can be added for streams without such units. This enlarges the variable search space and provides the possibility of replacing process-process exchangers with utility exchangers.

2.5 Critical Analysis of Synthesis Methods

The synthesis of optimal heat exchanger network is a large combinatorial problem. The designer searches among the alternative networks for the one with the least annual cost and a simple network structure. Previously, the various methods developed for finding the optimal solutions have been outlined. In this section, the major advantages and disadvantages related to the current methods will be discussed. Since the Pinch Design Method (PDM) is the best known method for both academic and industrial applications, it will be the main focus for critical analysis to establish potentially new avenues for improvement.

Pinch Design Method (PDM) *(Linnhoff and Hindmarsh, 1983; Linnhoff and Ahmad, 1990)*

To date, Pinch Technology dominates the industrial applications aimed at improving heat integration. This is undoubtedly a consequence of its outstanding advantages over other methods, particularly with regard to physical insights. Adopting the more rigorous guidelines in the improved PDM, one usually can obtain good solutions for HEN problems. However, a number of shortcomings still exist in the PDM.

First, the driving force plot (DFP) considers only temperatures, neglecting the effects of heat transfer duty and film coefficient on the heat transfer area and the consequent cost. As a result, if several possible matches exist with temperature profiles that reasonably fit the DFP, the match with minimum area penalty cannot be identified. In addition, the DFP may mislead the designer about the matches, the heat loads of matches and stream split ratios, when streams possess very different film coefficients (many processes have more than one order of magnitude of difference in these conditions). In this case, it is no longer appropriate to use DFP as the guideline for selecting matches. This is because streams with large film coefficients should be assigned small driving forces and streams with low film coefficients should be assigned large driving forces to achieve minimum-area designs. Driving forces assigned in such a manner no longer follow the DFP.

Second, the PDM uses the *sequential* approach for match selection. The nature of the *sequential* approach is virtually the same as the best first search. The sequential approach (best first) selects one match at a time. Though this approach can usually select a best option at any stage, it may not be necessarily to find a best solution for the whole problem.

This can be explained more clearly by using two (above the pinch) networks , the one in Figure 2.2 produced by the DFP and the other one (Figure 2.3) by applying the RPA (Linnhoff and Ahmad, 1990). The match 1 in Figure 2.2 has a smaller area penalty (0.1%) than that of the match 1 (6.1%) in Figure 2.3. By applying the sequential match choice (best first search), obviously, the match 1 in Figure 2.2 should be selected. Then the design continues using the sequential match choice until the network in Figure 2.2 is produced. By contrast, the match 1 in Figure 2.3 is selected though it has a relatively large area penalty but it creates good conditions for later matches. As a result, the better design (Figure 2.3) is obtained.

For the sequential match approach, whenever it is found at any stage that a design incurs a large area penalty, the design process needs to back track to the stage where the problem is caused. Consider Figure 2.2 again for illustration. After the match 1 is determined, the design continues until it is found that the match 4 incurs a large area penalty of 11.1%. From the analysis, it is discovered that the match 1 caused the problem and then the design must be restarted from the very beginning.

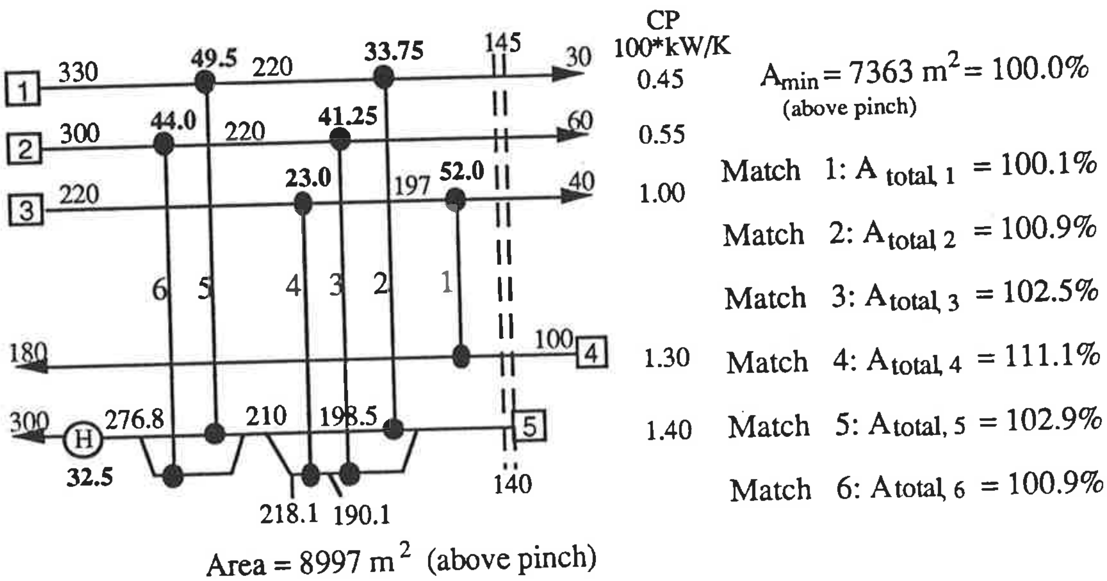


Figure 2.2: The Pinch design (above pinch) using the DFP method

(Linnhoff and Ahmad, 1990)

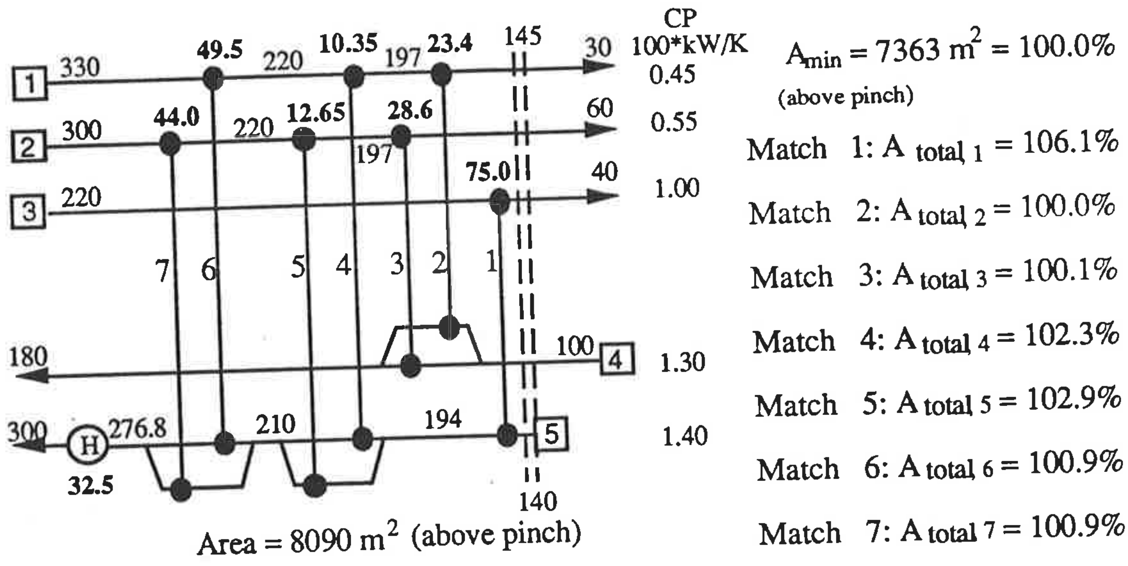


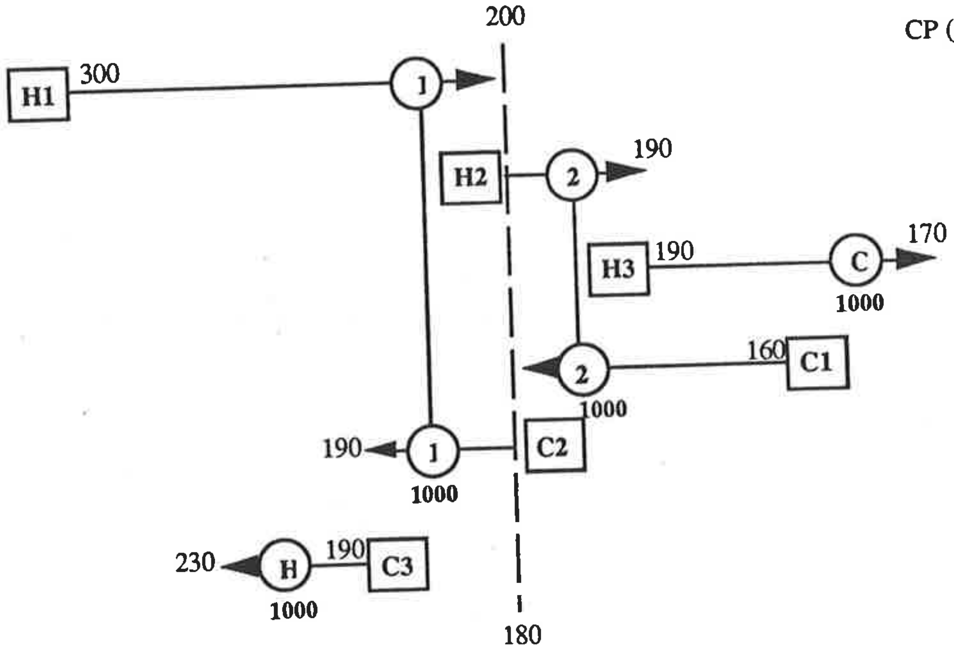
Figure 2.3: The Pinch design (above pinch) employing the RPA method

(Linnhoff and Ahmad, 1990)

From the above discussion, it may be seen that though the match selected by the sequential match choice (best first) has least area penalty at one stage, the design may not achieve the overall minimum-area requirement. Even if all matches selected have tolerable area penalties, whether or not these matches give the best solution to a problem in terms of area, is still uncertain. In a worst case, if some match is discovered incurring a large area penalty, a design has to be back tracked. Further, it is not usually an easy task to identify which match(es) has caused a problem. These observations show that the sequential approach may not always be able to produce optimal solutions.

The third problem arises from the strict pinch decomposition (Rev and Fonyo, 1986; Trivedi et al,1989; Gundersen and Grossmann ,1990; Ciric and Floudas,1990; Wood et al,1991; Jezowski, 1991). The strict pinch decomposition results in two subproblems, one above the pinch and the other below the pinch. These two subproblems are in "enthalpy balance". Clearly, two effects automatically result for each of these two subproblems, i.e. no energy leakage through the pinch and fixed utility consumptions. Hence, there exists little freedom for manipulation of matches. As a result, a large number of matches may be necessary for each subproblem. Merging of two subnetworks may result in an over-complicated network. However, by permitting a small energy leakage through the pinch and a small relaxation for utility consumption, the freedom and flexibility for design can be greatly increased. The small penalty of a slightly higher utility consumption can be compensated by a much simplified network coupled with a low area and total cost requirement.

Finally and perhaps most significantly, the major limitation with the PDM from an industrial point of view is the use of a single ΔT_{min} (HRAT) (Ciric and Floudas, 1990; Gundersen and Grossmann, 1990; Colberg and Morari, 1990; Rev and Fonyo, 1991; Jezowski, 1991). By a simple example, Gundersen and Grossmann (1990) have demonstrated that forcing a single ΔT_{min} for all exchangers in a network may put the designer into another kind of topology trap. This effect was demonstrated using a six-stream problem by Gundersen and Grossmann. Figure 2.4 is the design produced using the PDM and Figure 2.5 represents the design generated by systematically criss-crossing at pinch (Gundersen and Grossmann, 1990). The pinch design (Figure 2.4) has 27.5% excess area and 20% excess cost compared to the design (Figure 2.5) violating the pinch rules. Because of the use of single ΔT_{min} coupled with strict pinch decomposition, the PDM can never achieve the design in Figure 2.5. More importantly, the strict pinch decomposition and the use of a single ΔT_{min} may generate networks containing more than minimum number of units, potentially leading to higher cost exchanger networks (Ciric and Floudas, 1990).



CP ($kW\ K^{-1}$)	h ($W\ m^{-2}K^{-1}$)
10	100
100	1000
50	1000
50	100
100	1000
25	1000

Figure 2.4: Pinch design with HRAT = 20°C
(Gundersen and Grossmann, 1990)

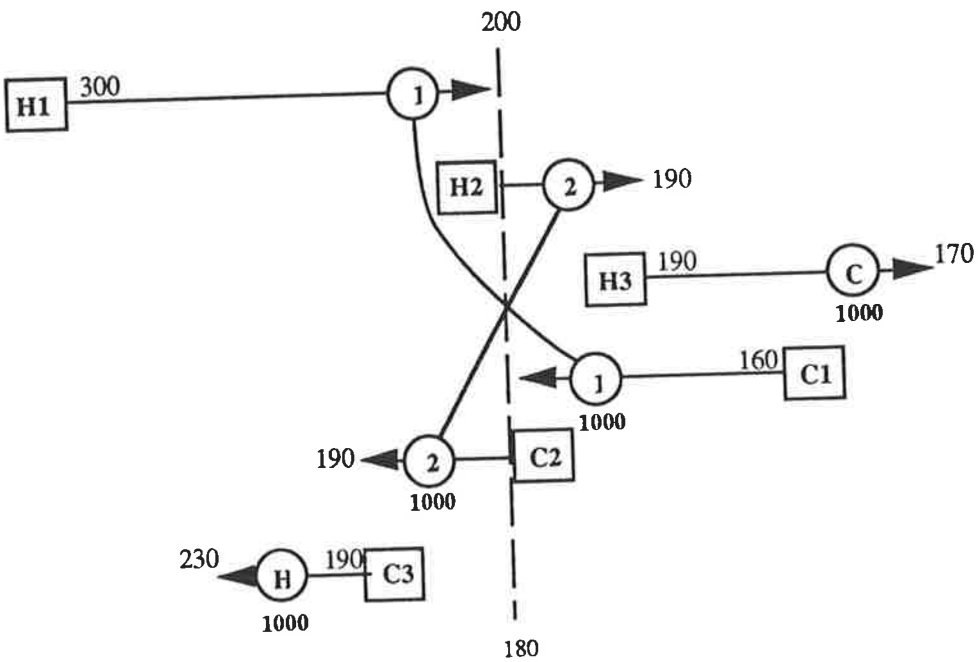


Figure 2.5: Criss-cross design with HRAT = 20°C
(Gundersen and Grossmann, 1990)

Pseudo Pinch Design Method (PPDM) (Trivedi et al, 1989)

In the PPDM, the two approach temperatures, HRAT and EMAT, are used respectively to target the minimum energy requirement and size heat exchangers. Thus, it provides a more flexible synthesis environment. The design strategy is similar to that of the PDM except the PPDM employs different CP matching rules for selecting matches. During the evolutionary stage, a specified loop breaking strategy (Trivedi et al, 1990) applies. Because of the application of EMAT for sizing heat exchangers, stream splitting at the pinch is reduced. Hence, simpler networks compared to those from the PDM may be achieved. However, there are two drawbacks associated with this method. First, the CP matching rules do not consider the area factor and thus some matches at the pinch may incur a significant capital penalty. The evolution strategy only considers the minimum energy penalty rather than the trade-off of operating cost and capital cost. Furthermore, the minimum energy penalty is not guaranteed when using the evolution approach suggested by Trivedi et al (1990).

The latter version of the PPDM (Wood et al, 1991) employs a number of features in the FPDM which is described below.

Flexible Pinch Design Method (FPDM) (Suaysompol and Wood, 1991a,b)

The FPDM is an extension of the PPDM. It aims for network simplification. The FPDM allows energy criss-crossing at the pinch while retaining the energy target. Match selection is achieved by following simple heuristic rules, which simplify the synthesis task. Evolution is easy, often, there is no need for loop breaking. By means of criss-crossing through the pinch and the heuristic rules for match selection, particularly in cases with a parallel profile of the composite curves, a simple network with low total cost can be designed. However, this method only addresses network simplification and fails to consider the trade-off between units and area. Consequently, it is occasionally possible to suggest a simple network possessing a large area and capital cost. Furthermore, the splitting problem is not addressed in the FPDM. However, splitting is often required in industrial applications.

Given these limitations, the computer program FLEXNET uses the A^* search strategy to find the design based on the FPDM heuristics which is of lowest total cost (Suaysompol and Wood, 1991b).

The Method Proposed by Jezowski (1991)

This method seeks to achieve simple networks with low capital cost by combining the dual temperature concept (Challand and Colbert, 1981) and the Ponton-Donaldson fast algorithm (1974). It has been demonstrated by Jezowski (1991) that for many small problems, the method produces low cost networks. However, since the heuristics in the Ponton-Donaldson method are not rigorous, it requires a lot of trial-and-error to find a good match when using the remaining problem analysis (RPA) (Linnhoff and Ahmad, 1990) to asses matches. Thus, this method is impractical for the solutions of large-scale problems.

Mathematical Programming Approaches

Recently, research concerning the application of mathematical programming has made significant progresses for both targeting and synthesis of heat exchanger networks. The key concept is the use of simple and reliable superstructures (Floudas and Ciric, 1989; Ciric and Floudas, 1990 & 1991; Yee et al., 1990; Yee and Grossmann, 1990). Such methods look attractive for further development. At present, the practical application of the methods is impeded by some notable deficiencies.

First, the nature of MINLP problem is non-convex and several local optima may exist. These complicate the search for the global optimum. Clearly, if possible, production of a rigorous and robust algorithm for finding the global or near global optimum in HEN synthesis is necessary. Second, most current mathematical algorithms involve a large number of variables. This renders them impractical when dealing with large-scale problems. The third problem is that no method exists for reliably generating a good initial solution for the problem. Conventional NLP techniques heavily rely on a very good initial solution to ensure the solution quality. If a poor initial guess is provided, the problem may fail to converge or converge to an inferior solution.

The final problem is that the mathematical programming approach is somewhat cumbersome if more networks than one optimal solution are required. In practice, the designer would prefer to select among alternative networks to find that network which is economical, operable and controllable. As well, a designer cannot influence the decision process and has little interaction with the design process.

2.6 Practical Engineering Considerations

Satisfying the economic objectives used as criteria during synthesis does not guarantee that the solution will be practical. A network should not only save money but also be simple, operable and controllable. These factors demand serious consideration, as an optimal 'economic' network may render the total process unstable or inoperable (Stephanopoulos, 1982).

The following effects from the MER designs have been found by Stephanopoulos (1982). In order to obtain a MER design, one tends to recover heat from process streams as much as possible by producing many process-process exchangers. The creation of such heat exchanger networks will increase the integration in a chemical plant. This also complicates its operation and control. The increased interaction among the process units in a network will create difficulties in smooth operation of the whole chemical plant (propagation of disturbances, instabilities). A second effect is that in a highly connected network, fewer independent variables are available for free manipulation. The third effect is the process response will be slower. Recycle loops usually lengthen response time. Fewer independent manipulative variables and slower process response cause additional problems for effective control of the whole process. The existence of these problems calls for the exploitation of networks containing several disconnected subnetworks or featuring a low degree of interaction among the processing units.

Therefore, from both the economic and practical points of view, a designer should investigate a number of alternative designs and examine the process very carefully to ensure the network selected is economical, operable and controllable.

2.7 Discussion and Conclusions

So far, pinch technology has produced the most extensive list of good projects in industry for improved heat integration. The major task for improving the PDM is to break the limitations from the use of single ΔT_{min} and the strict pinch decomposition. It is also important to produce more rigorous and reliable criteria for directly measuring area or capital cost requirement in selecting matches to reduce the match uncertainty.

Both the thermodynamic and mathematical programming methodologies have distinct individual advantages. The former methodology mainly relies on the physical insight into HEN synthesis whilst the latter approach is superior in searching technique. Previous work has paid little attention to the linkage between research in the thermodynamic and mathematical approaches. The work aiming for this linkage will make a great contribution to the field of process integration or conceptual design.

In order to overcome the drawbacks in the PDM and to provide a research bridge between the thermodynamic and mathematical approaches, the 'block' method has been developed (Zhu et, 1993a & b, 1994). The 'block' concept is proposed based on physical insights from the composite curves. The HEN synthesis problem is decomposed into a number of 'blocks'. The blocks are determined so that streams in each block have similar requirements for driving forces; but streams in different blocks have different approach temperature requirements. The connection between blocks is achieved by employing a heuristic import/export rule (Zhu et al, 1993a). The near-minimum area and near-MER design with a relatively simple network structure is achieved by applying a number of newly formulated heuristic rules (Zhu et al, 1993a). Hence, the pinch decomposition is not a necessary requirement when the block concept is used. As well, the maximum energy recovery (MER) constraint is relaxed and the use of different minimum temperature approaches is permitted. These relaxations provide more opportunities and greater flexibility in searching for optimal designs.

The NLP optimization techniques are also applied in this method. The application of the NLP optimization techniques in this case is different from the pure mathematical programming which merely relies on the optimization methods without the aid of thermodynamic methods. In the 'block method', an important improvement in the searching of the global optimum is to find the proper initial network (near-minimum area, near-MER and near-minimum units), that is already relatively close to the global optimum. This kind of initial design is provided as the starting point for optimization. This strategy enhances the advantages of both thermodynamic and mathematical programming approaches.

Regarding the pure mathematical programming, another benefit from the application of the 'block' concept is that it provides a physical basis for the superstructure. This superstructure is similar to that from the stage method (Yee et al, 1990) although the stage was derived without physical basis. A good starting point of optimization can be provided by employing the supertargeting approaches (Linnhoff and Ahmad, 1986a & 1986b; Zhu et al, 1993a, 1994) and the initialization procedures associated with block-based superstructure (Zhu et al, 1993b). By starting optimization at a good initial solution, the possibility of finding the global optimum is increased and the topology traps are avoided.

It is expected that the synthesis of heat exchanger networks will enter a new phase at the end of which practical designs can be evolved for problems encountered in chemical engineering practice, with the typical resources, e.g. a desktop computer or work station with appropriate software modules (U.S. National Research Council, 1988). Experience has shown that the application of heuristic methods or mathematical programming alone to the solution of engineering problems each have their own advantages and shortcomings. It becomes obvious that sophisticated software packages should take advantage of the blend of methods presented in this review. Mathematical programming has the advantage in targeting either for unconstrained or restricted cases. Good initial solutions may be provided using heuristic methods. MINLP optimization of these initial designs may provide a number of promising alternative designs. The best design among them would then be determined after qualitative analysis of safety, operability, flexibility and controllability by applying expert system methodology.

CHAPTER 3

THE 'BLOCK' METHOD — AREA TARGETING PRINCIPLES

SUMMARY

An alternative new heuristic method is proposed to combine the advantages of design methodology based on heuristics and mathematical programming techniques. This method does not rely on pinch decomposition although it does not preclude it. The composite curves are decomposed into a number of 'blocks' (which may exceed the two blocks formed by pinch decomposition). Within each block, a good set of design matches can then be simultaneously selected with any matching constraints taken into account by parallel examination of the **whole set** of possible matches. Usually an initial design closely approaches the area and energy targets with a small number of units. This initial design is optimized further in total cost terms by applying non–linear optimization techniques.

3.1 Introduction

The goal of current methods is to carry out the energy–area or the energy–capital trade–off systematically and achieve initial networks reasonably close to the global–minimum total cost. Current versions of the Pinch Design Method (PDM) (Linnhoff and Ahmad, 1990) yield improved solutions by utilizing the 'Driving Force Plot' (DFP) and the 'Remaining Problem Analysis' (RPA). With these procedures, designs evolve by a **sequential** choice of matches and the designer provides significant input into the choice of matches and hence the solution process. However, it is not always clear which of a number of candidate matches should be chosen, although some will be critical in the determination of the eventual cost of the completed network.

The new method proposed here incorporates the concept of total cost (energy and capital) targets and hence determines an optimal HRAT (network approach temperature) prior to initial design. This work is similar to the supertargeting approach of Linnhoff and Ahmad (1986a,b). However, whilst being guided by HRAT and MER, the block method then proceeds by using *area–targeting* concepts. The philosophy of this method is to seek a minimum or near–minimum area design coupled with near–minimum units while approaching the utility target at the optimal HRAT. This objective is similar to that of Linnhoff and Ahmad (1990) but it is achieved by a different approach. The basic methodology is to decompose the composite curves into a minimum number of blocks each of which includes one or more of the enthalpy intervals defined by the 'kink points' in the composite curves. For each block, a straight line segment approximates each composite curve giving a 'quasi–composite' (Figure 3.1) for both hot and cold streams and provides a good approximation to the true composite curves. The concept of pinch decomposition is ***not*** a requirement; however, the pinch may still be used as a block boundary if appropriate. The area for any match in a block is readily calculated and the results of the complete set of such computations may be stored in a 'matching matrix'. Examination of this complete set of area requirements enables a good *set* of matches to be obtained for each block *simultaneously* whilst also accounting for any constraints on matches. This selection process is implemented with a set of 'within–block' matching rules which permit the import/export of energy from/to adjacent blocks.

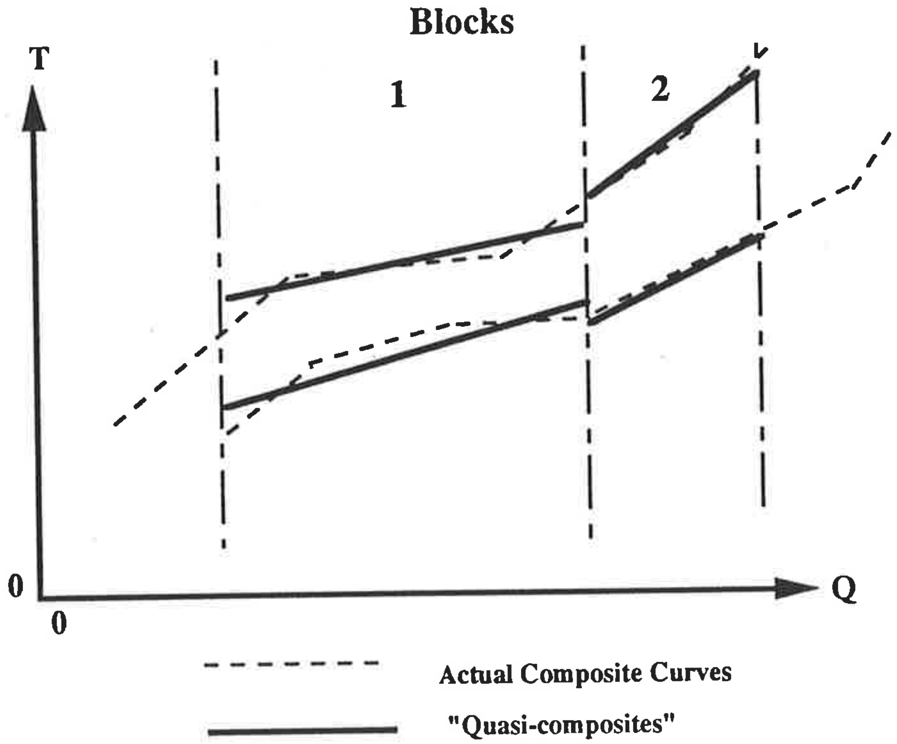


Figure 3.1: Quasi–composite curves and blocks

The final outcome is an **initial** design for subsequent NLP optimization which has few splits and a close approach to all targets (i.e. energy, area, units and cost targets).

A variety of methods have been used to decompose the overall network synthesis problem into sub-problems, which facilitate the matching process. Thus division into temperature intervals was used by Linnhoff and Flower (1978) and this procedure was greatly simplified when the pinch decomposition was discovered by Linnhoff and Hindmarsh (1983). Mathematical programming methods also have used similar approaches, with temperature intervals being used by Colberg and Morari (1990) and smaller number of stages by Yee et al (1990). Although the stage concept proposed by Yee et al was derived without the physical basis of Figure 3.1, both the block and stage-based methods lead to similar superstructure approaches. These methods will be discussed and compared in Chapter 5 in which it is also demonstrated that the block decomposition provides a sound basis for mathematical programming approach to the optimization of heat exchanger networks.

3.2 Brief Review of The Improved Pinch Design Method

The original Pinch Design Method (PDM) (Linnhoff and Hindmarsh, 1983) led to networks with maximum energy recovery. However, the improved PDM (Linnhoff and Ahmad, 1990, Ahmad et al, 1990) aims for maximum energy recovery and minimum area designs. This is achieved by implementing a hierarchy of methods. They are ranked in increasing order of sophistication.

3.2.1 New CP–Rules in the PDM

The original CP–rules (Linnhoff and Hindmarsh, 1983) merely ensure that the temperature profiles of matches at the pinch diverge away from the pinch. They fail to guarantee a good fit to the composite curves. A modified CP–rule (Linnhoff and Ahmad, 1990)

$$\left.\frac{CP_H}{CP_C}\right|_{pinch\ match} = \left.\frac{CP_{hot\ composite}}{CP_{cold\ composit}}\right|_{pinch} \tag{3.1}$$

yields an improved fit of the temperature profiles of matches situated at the pinch. However, when the tick–off heuristic (Linnhoff and Hindmarsh, 1983) is applied, though the temperature profile of a match selected using the above rule can follow the composite curves at pinch region well, it may deviate significantly from the composite curves in regions away from the pinch. Clearly, the larger the duty the worse the situation. Thus, the requirement of near minimum area is still not guaranteed. Thus, the driving force plot and remaining problem analysis are used to check whether a tick–off match selected by the above heuristic is appropriate.

3.2.2 Driving Force Plot (DFP)

The DFP was introduced by Linnhoff and Vredeveld (1984) and extended by Ahmad (1985) to supplement the CP–rule (equation (3.1)). When a match is selected by using the CP–rule plus the tick–off rule (Linnhoff and Hindmarsh, 1983), the DFP is used to check whether a tick–off is appropriate. It provides a guideline for selection of matches whose driving forces closely approach the corresponding driving force plot. Unfortunately, the DFP considers only temperatures, neglecting the effect of heat transfer duty and film coefficients on heat transfer area for the network. As a result, if several possible matches exist with temperature profiles that reasonably fit the DFP, the minimum area matches are not identified. In addition, the DFP may be misleading if the film heat transfer coefficients are not equal for all streams.

3.2.3 Remaining Problem Analysis (RPA)

The RPA was developed to quantitatively assess matches in area terms compared to the qualitative analysis of matches by the DFP. Thus, the RPA improves on the DFP. Two definitions of the RPA exist (Linnhoff and Ahmad, 1990). The first is based on individual matches and remaining problem consists of full stream data excluding only the hot and cold streams currently being analyzed. Assume the minimum overall area is A_{min}, area requirement for the match m being analyzed is a_m and the minimum overall area for the remaining problem excluding this match is $A_{r,m}$. Thus, the minimum overall area requirement is defined as

$$A_{total,m} = a_m + A_{r,m} \tag{3.2}$$
$$area\ penalty = A_{total,m} - A_{min} \tag{3.3}$$

This definition isolates each match and consequently can not consider the effect of interactions of matches on network area.

The second RPA is defined on a cumulative basis. It considers the total area of all placed matches and defines the remaining problem to be only the stream elements awaiting matches. It is expressed as

$$A'_{total,m} = \sum_{i=1}^{m} a_i + A'_{r,m} \tag{3.4}$$

and the area penalty is defined as

$$area\ penalty = A'_{total,m} - A_{min} \tag{3.5}$$

where $A'_{total,m}$ and $A'_{r,m}$ are similar to $A_{total,m}$ and $A_{r,m}$ except that the prime denotes the alternative definition of the remaining problem. This cumulative based RPA has the advantage of reporting the progress of all the matches together in the design up to that point. Its disadvantage is that the area penalty associated with a match depends on its sequence. It is a function of previously allocated matches. Linnhoff and Ahmad (1990) suggested that if the area penalty obtained on the cumulative match basis remains within 10% of the area target then the influence of sequencing on individual match penalties is small and can be ignored. In the rare case, where a design with a larger penalty is to be completed, then the individual match area penalties should also be evaluated for subsequent matches to isolate the error due to the chosen sequence.

In application, the DFP is first used to determine a number of promising matches whose driving forces of reasonably fit the driving force plot. These are then assessed quantitatively using the RPA. As a result , the best match in the current stage is selected. This kind of match choice is referred to the ***sequential*** match selection. It will be discussed in detail in section 3.9.

3.3 The Concept of A 'BLOCK'

The principle idea in the improved pinch methods is to ensure temperature profiles of matches to closely approach the composite curves in order to achieve minimum area design. A whole system is partitioned into two independent sub–systems at pinch and then the CP–rules, the DFP and the RPA are applied to these two sub–systems, respectively. In this study, a new alternative way to achieve the goal of closely approaching all targets (energy, area, total cost based on either unit or shells) is proposed. First, the composite curves may be partitioned into a number of blocks each of which spans several composite segments with similar profiles. With a proper match selection, the temperature profiles of matches in a block reasonably approach the corresponding composite curves. Thus, the design problem is greatly simplified by decomposition into several sub–systems. The search for minimum area design for these sub–systems is an easy task. These sub–systems are not independent but are connected by applying an import/export rule (Section 3.4.2). In this new method, the qualitative analysis of driving forces is completed in the determination of blocks and the quantitative assessment of matches is carried out by detailed area calculation.

3.3.1 Physical Insights and Examples of Design Outcomes

The actual composite curves may be used to determine the 'ideal' exchanger profiles in a HEN with approximately equal heat transfer coefficients. The minimum area target (Bath formula) based on enthalpy intervals defined by the 'kink' points has been presented by Townsend and Linnhoff (1984) as follows:

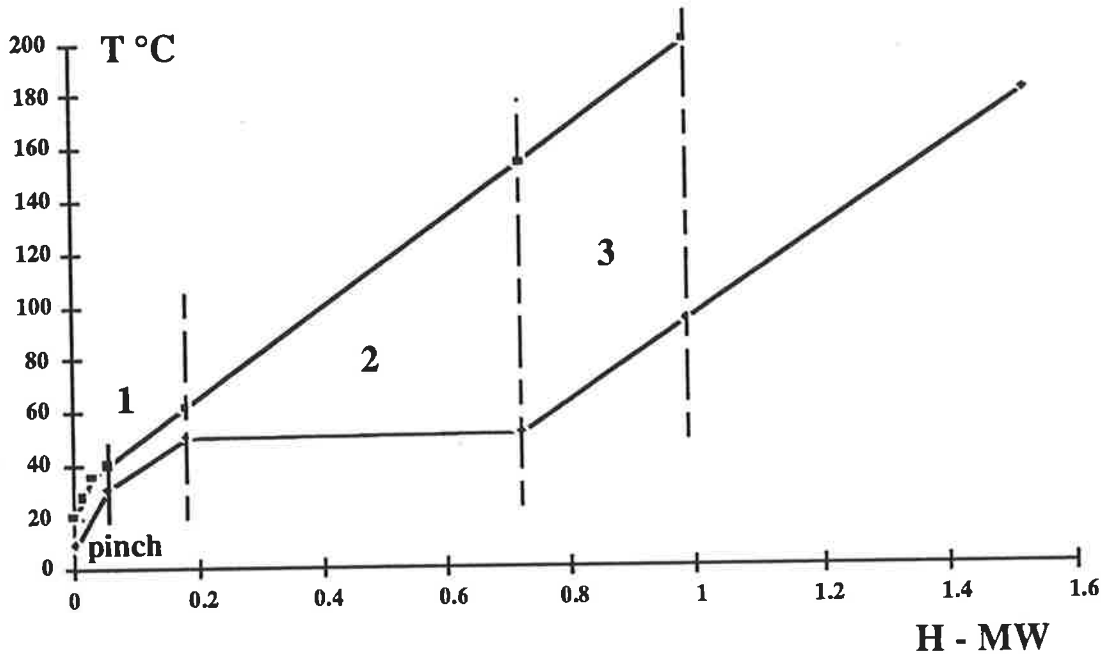
$$A_{min} = \sum_{i}^{intervals} \frac{1}{\Delta T_{lm_i}} \sum_{j}^{streams} \left[\frac{q_j}{h_j}\right]_i \tag{3.6}$$

This formula, although not exact, is based on vertical heat transfer. If a HEN is synthesized using the enthalpy intervals defined by the 'kinks' and the temperature profiles of the matches exactly follow the composite curves, then the resulting HEN will achieve both the area and utility targets. However, such networks possess an excessive number of units. They are known as a 'spaghetti structure' (Colberg & Morari, 1990).

To approach both the area and utility targets with near minimum units, the concept of a block as outlined previously is used. The composite curves are first partitioned into a number of such blocks. (Typically, each block spans a number of 'kink point' enthalpy intervals and the hot (cold) composite segments between 'kink points' within a block have similar temperature profiles). Next for each block, a 'within–block' sub–network is then synthesized. Obviously, the number of enthalpy intervals used to synthesize a HEN is greatly reduced compared to the 'spaghetti structure' and the combined use of a stream 'tick–off' rule and an import/export rule (Section 3.4.2), minimizes the number of units in each block. It is believed that a reasonably simple network facilitates the search for the optimal solution. The application of the tick–off rule and the import/export rule leads to network simplification by allowing criss–crossing. A network may not achieve the area and energy targets exactly as a result of 'criss–crossing'. However, significant network simplification may result. As a consequence, a network designed using this philosophy features near–minimum area and near–maximum energy recovery coupled with a simple structure.

Three examples are presented to introduce the block concept and to illustrate the benefits derived from it. It produces simple and effective designs easily, the detailed procedures for which are presented in Section 3.4.

The first example (Figures 3.2a–c) was presented by Linnhoff and Ahmad (1990). The relevant composite curves are presented in Figure 3.2a. From the composite curves, three regions may be readily identified. Region 1 is characterized by closely–spaced curves and includes the pinch. Region 2 contains a close temperature approach at one end, whilst in region 3, the composite curves are widely–spaced. To avoid incurring large area penalties, these characteristics should be carefully considered.



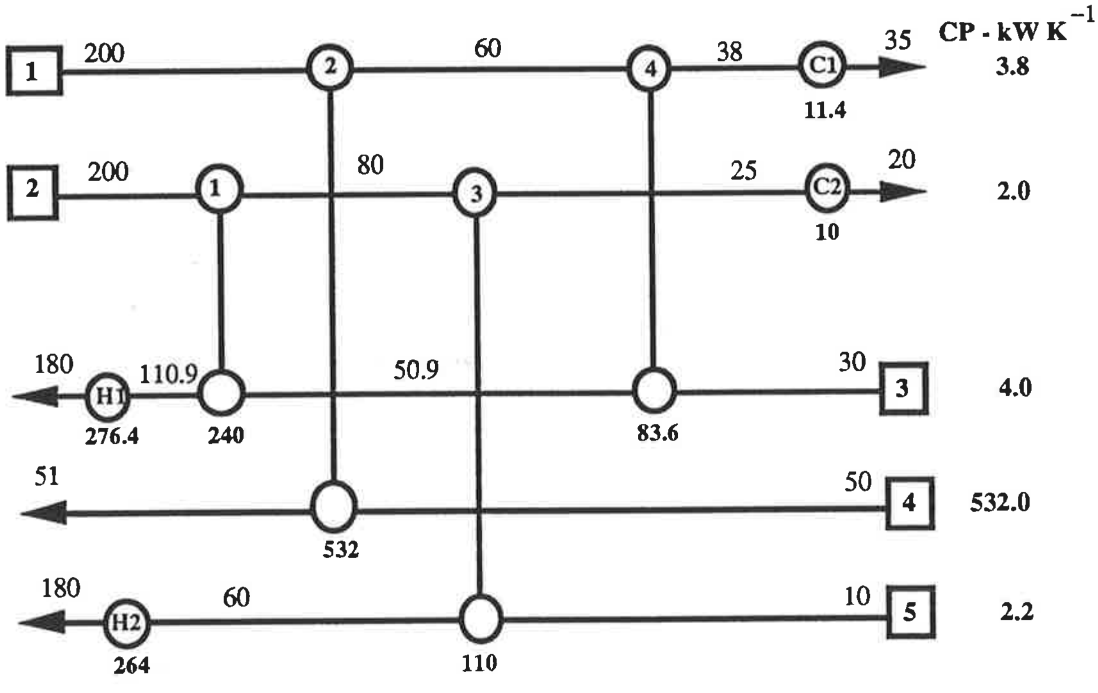
Targets (HRAT = 10 K): Q_H = 534 kW; Q_C = 15 kW; Area = 382 m^2

U = 100 W $m^{-2}K^{-1}$ for all matches

Utilities: Hot oil: 230 °C – 200 °C; Chilled water: 1 °C – 15 °C

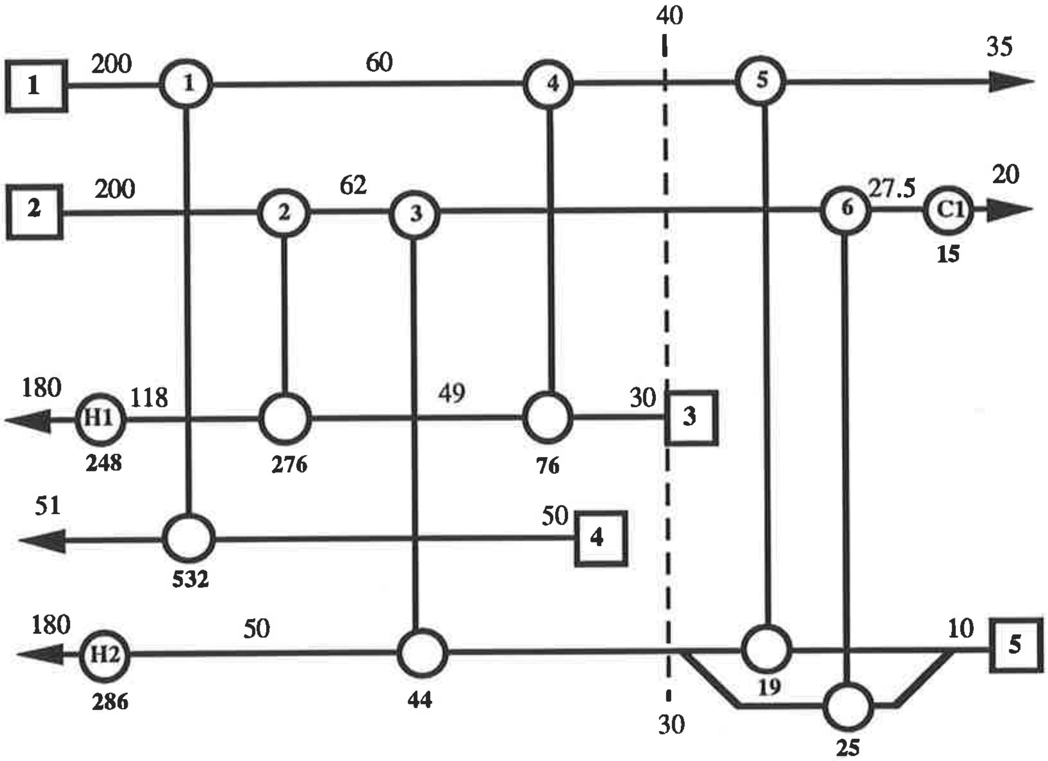
Figure 3.2a: Composite curves for example 1

If we define three blocks corresponding to the regions, then an initial network design may be easily deduced (Figure 3.2b). This network contains eight units with an area requirement of 392 m^2, hot utility consumption of 540.4 kW and a cold utility requirement of 21.4 kW (utility targets are not always exactly achieved because of the import/export rule). Interestingly, the pinch does not constitute a block boundary as the composite curves below it are short and possess a similar profile to the curves in the narrow region above the pinch. These portions are combined into a single block. The design produced compares well with the network (Figure 3.2c) devised by Linnhoff and Ahmad (1990) using the 'Driving Force Plot'. Their network achieves the energy target with an area of 438 m^2 and nine units. Linnhoff and Ahmad only provided the 'above pinch' design. The complete design is straightforward and is provided by the author.



Q_H = 540.4 kW; Q_C = 21.4 kW; Area = 392 m^2

Figure 3.2b: Initial design applying the block concept for example 1



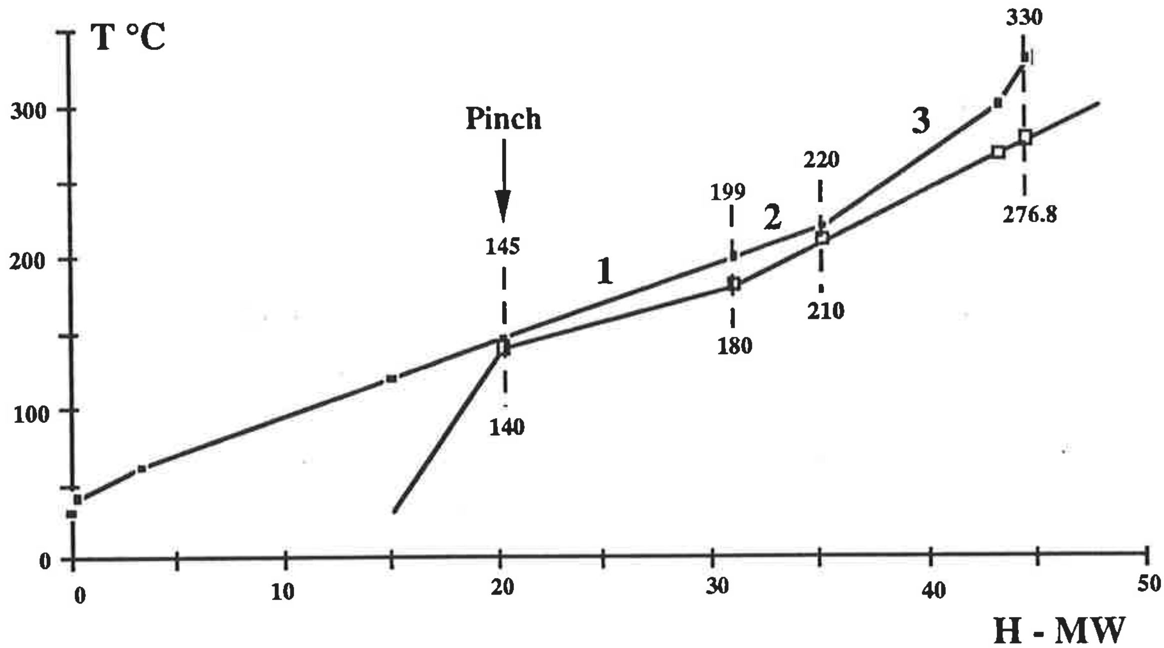
Q_H = 534 kW; Q_C = 15 kW; Area = 438 m^2

Figure 3.2c: Initial design applying the DFP for example 1

(Linnhoff & Ahmad,1990)

The second problem (Figures 3.3) is also taken from Linnhoff and Ahmad (1990). If we focus only on the above–pinch design, the pinch will form the boundary for region 1 (Figure 3.3a).

Three regions are indicated on the figure. All are characterized by close temperature approaches and region 2 is similar in profile to both regions 1 and 3. Clearly, region 2 may be combined with either region. As region 1 has a particularly narrow profile, to avoid a high level of 'criss–crossing' regions 2 and 3 are combined to define a two block geometry.



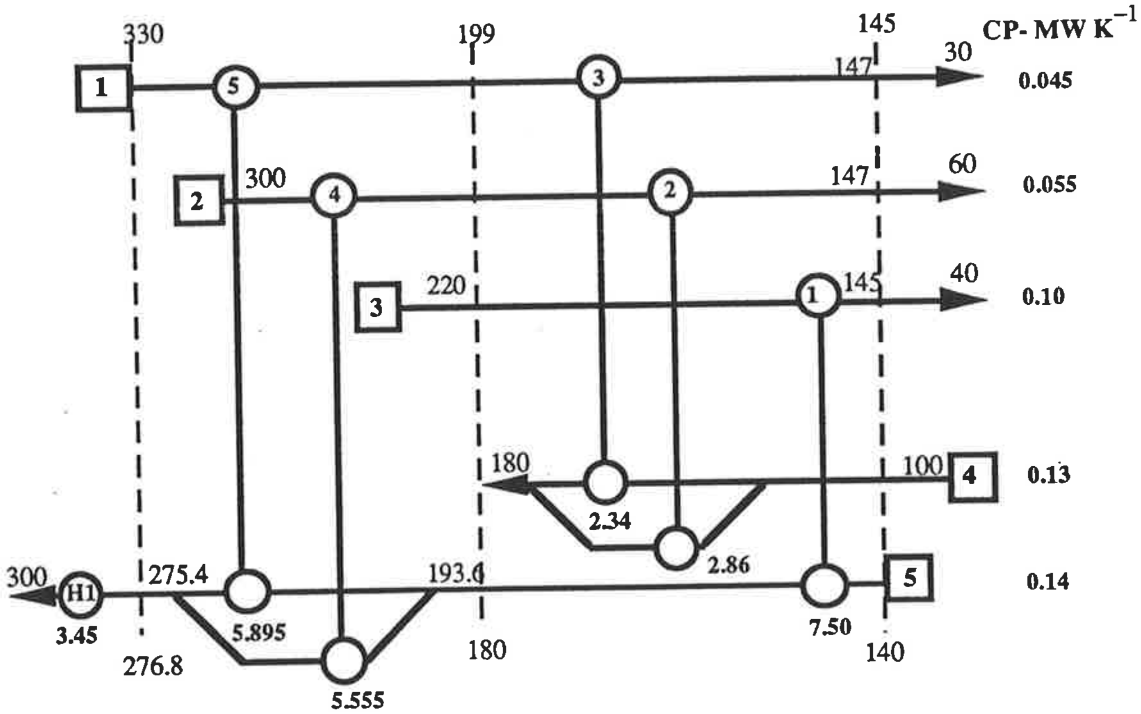
Targets (above pinch; HRAT = 5K): Q_H = 3.25 MW; Area = 7363 m^2

U = 250 W m^{-2} K^{-1} for all matches

Utilities: Hot oil: 350 °C – 330 °C; Cooling water: 10 °C – 30 °C

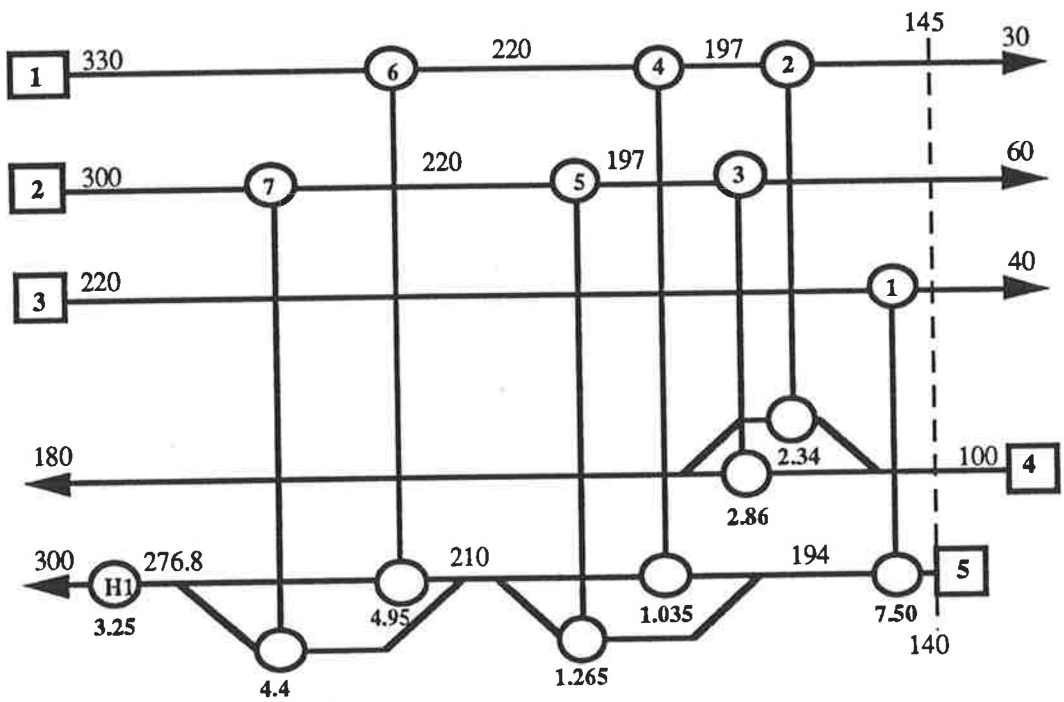
Figure 3.3a: Composite curves for example 2

The resulting network is illustrated in Figure 3.3b. The hot utility requirement is 3.45 MW (0.2 MW greater than the target) and the total area required is 7310 m^2 (53 m^2 below the area target). Again this design compares favorably with Figure 3.3c obtained from RPA (the DFP design had excessive area) which achieves the energy target but requires 8090 m^2 of exchanger area (9.9% greater than the target). In addition , the network of Linnhoff and Ahmad (Figure 3.3c) is more complex than the block design and requires two additional units. It is possible to reduce this complexity by combining matches 4 with 6 and 5 with 7 respectively. Unfortunately, this incurs an area penalty of 196 m^2. Clearly, the new network (Figure 3.3b) allows a small amount of 'criss–crossing' of the pinch on matches 2 and 3. This results in a small energy penalty but provides a substantial area benefit.



$Q_H = 3.45$ MW; Area = 7310 m^2

Figure 3.3b: Initial design applying the block concept for example 2 (above pinch)

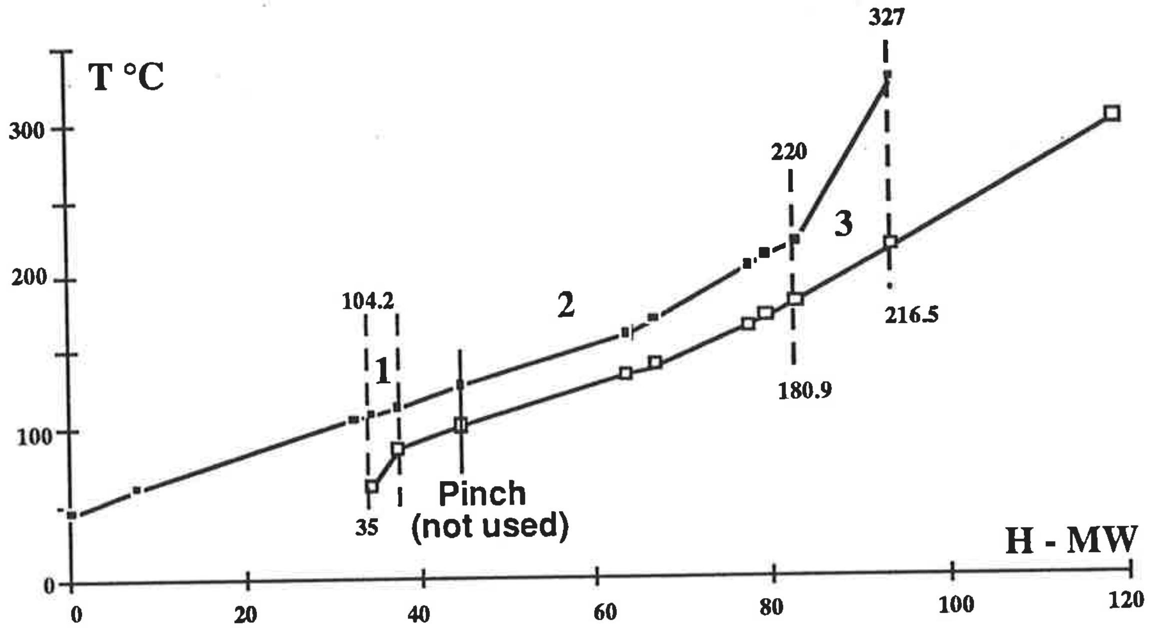


$Q_H = 3.25$ MW; Area = 8090 m^2

Figure 3.3c: Initial design applying the RPA for example 2 (above pinch)

(Linnhoff & Ahmad, 1990)

The final example is the well–known aromatics problem discussed by Linnhoff and Ahmad (1990). Three distinctive regions may be identified on the composite curves (Figure 3.4a).



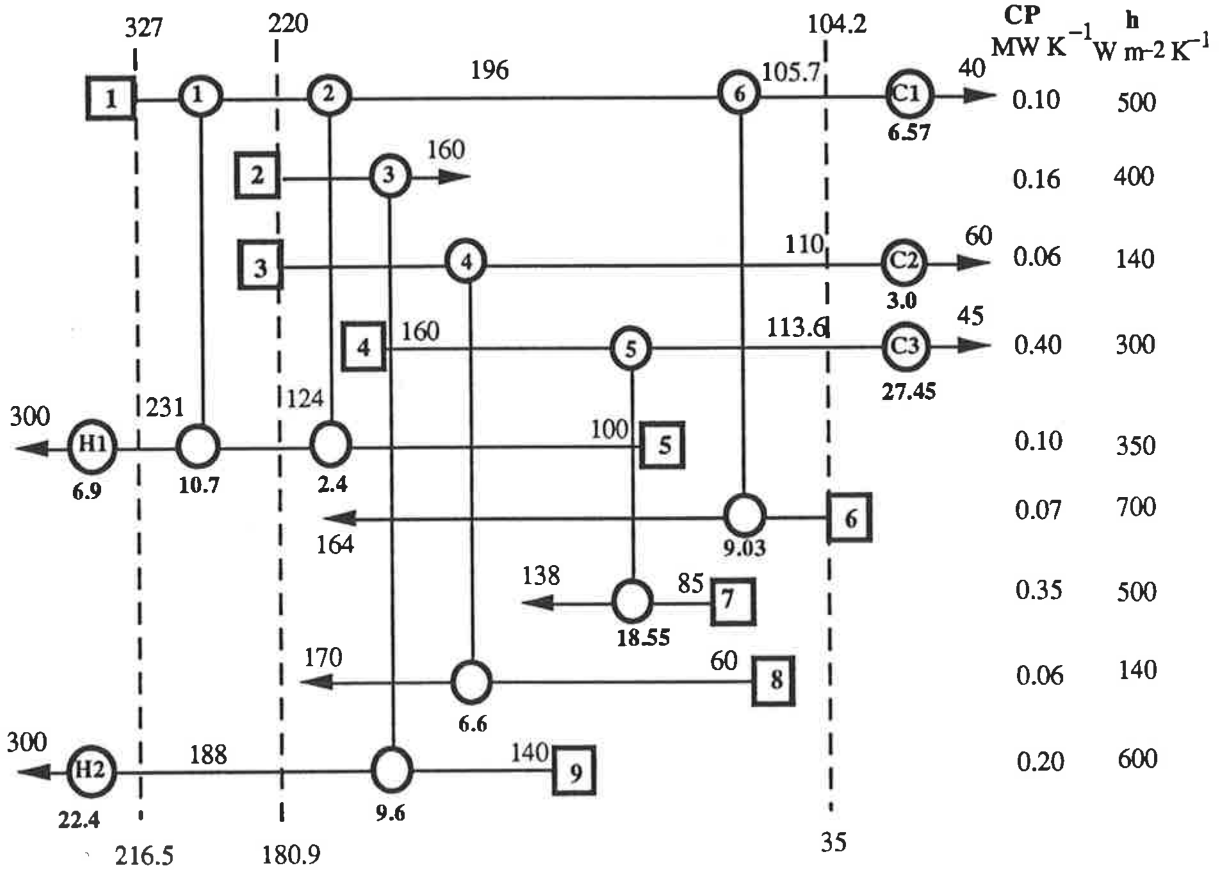
Targets (HRAT = 26 K): Q_H = 25.04 MW; Q_C = 32.76 MW; Area = 16984 m^2

Utilities: Hot utility: 330 °C – 250 °C; h = 500 W $m^{-2}K^{-1}$

Cooling water: 15 °C – 30 °C, h = 500 W $m^{-2}K^{-1}$

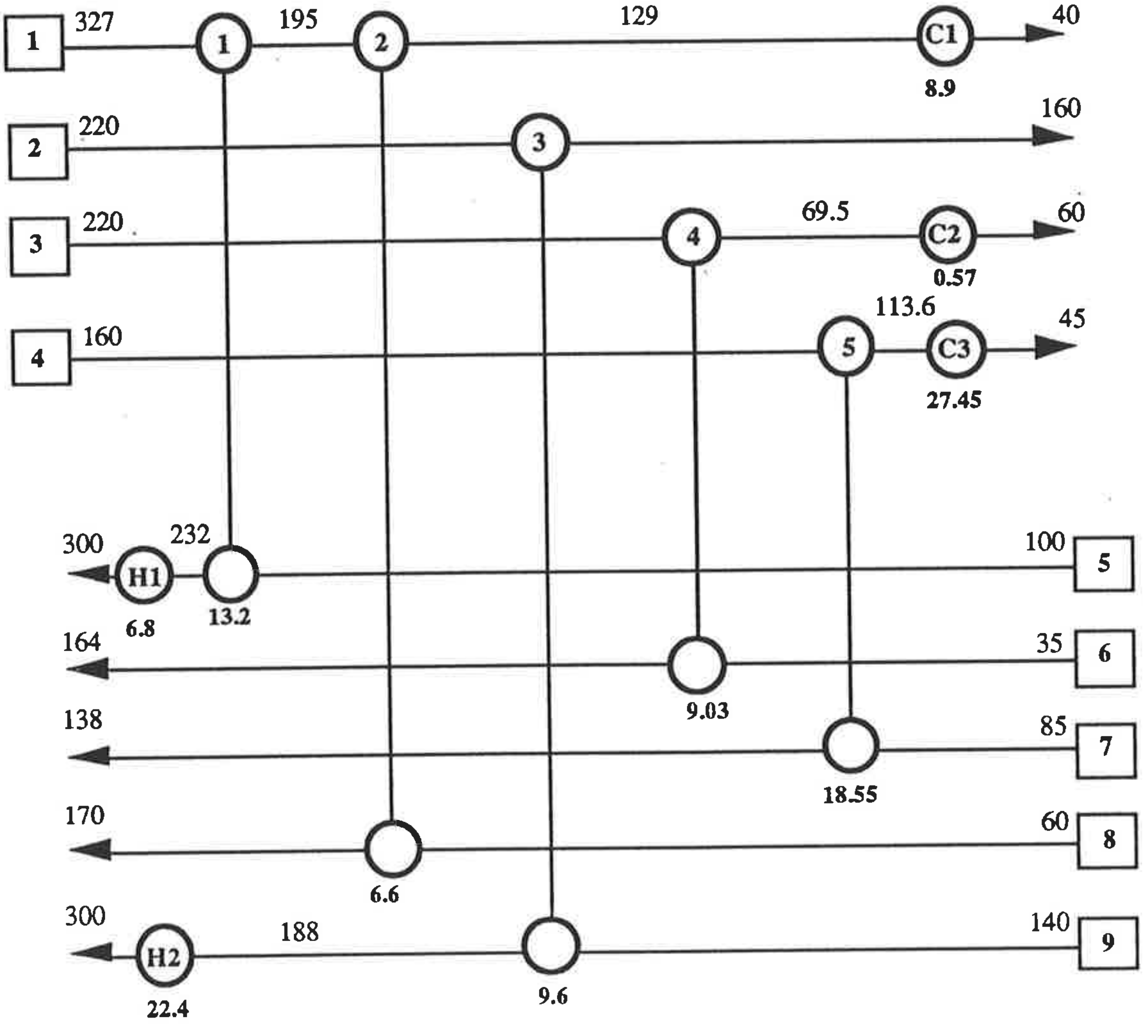
Figure 3.4a: Composite curves for example 3 (Aromatics plant)

Region 1 is small relative to both 2 and 3 and it is logically combined with region 2. Again, this produces a two–block system and block 1 spans the pinch point. The initial design resulting from this decomposition is illustrated in Figure 3.4b. It requires 29.3 MW of hot utility and 37.02 MW of cold utility coupled with an area requirement of 15,762 m^2. This initial design has 11 units (one greater than the unit target). The other alternative design by applying the block concept is shown in Figure 3.4c, which needs 16166 m^2 of overall heat transfer area with 29.2 MW of hot utility and 36.9 MW of cold utility. By contrast, the initial design (Figure 3.4d) provided by the improved pinch algorithm (Linnhoff and Ahmad, 1990) achieves the energy target and has 17,716 m^2 of area# and 17 units (an excess of 7 over the unit target). The block designs (Figures 3.4b-c) may require more utility consumption than the pinch design (Figure 3.4d). However, the trade-off between energy and capital will be carried out in the subsequent cost optimization. The focus of a block initial design is to find a good initial solution with a low area requirement (approaching the area target) and a simple network structure (approaching the unit target) with utility consumption reasonably close to the corresponding energy target. It is believed that such an initial design will provide advantages for the cost optimization.



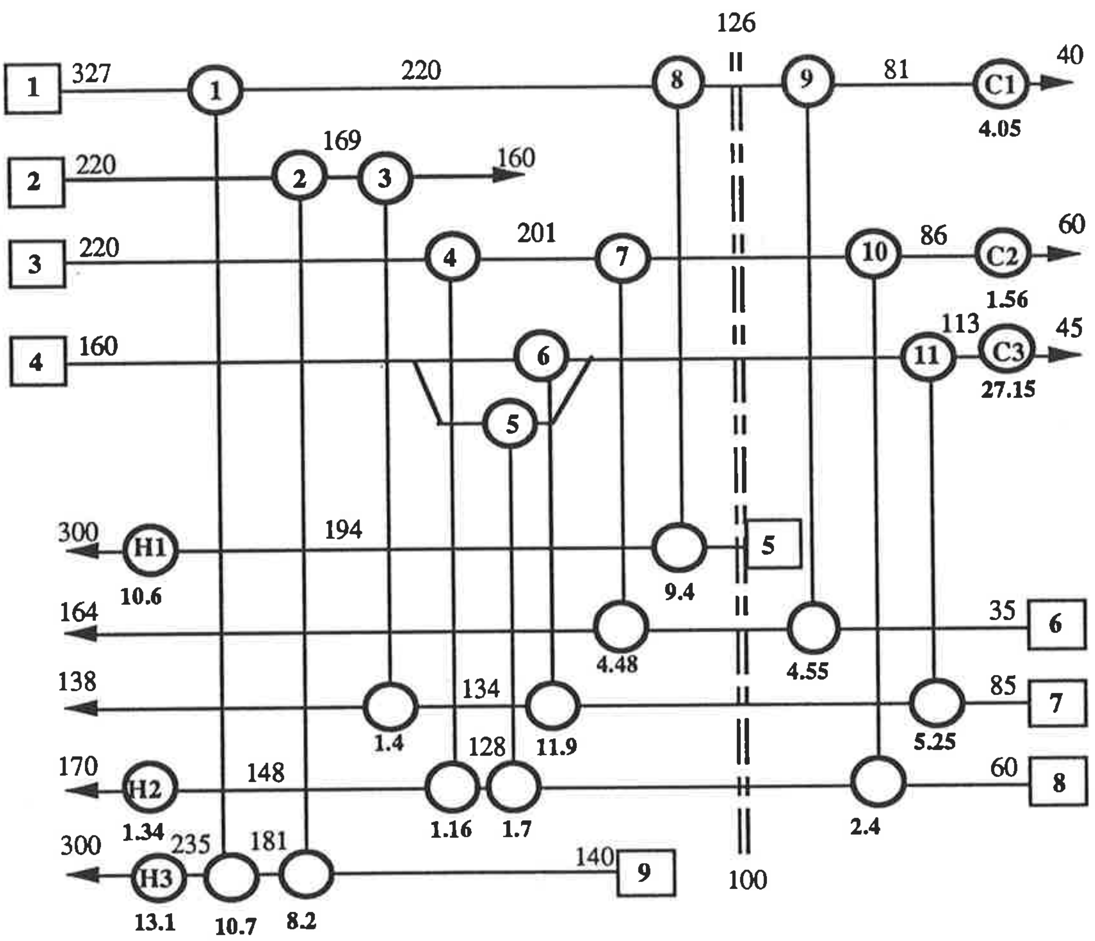
Q_H = 29.3 MW; Q_C= 37.02 MW; Area = 15762 m^2

Figure 3.4b: Initial design applying the block concept for example 3



Q_H = 29.2 MW; Q_C= 36.9 MW; Area = 16166 m^2

Figure 3.4c: Alternative initial design applying the block concept for example 3



Q_H = 25.04 MW; Q_C= 32.76 MW; Area = 17716# m^2

Figure 3.4d: Initial design applying the PDM for example 3

(Linnhoff & Ahmad, 1990)

Linnhoff & Ahmad (1990) did not publish the area calculation for their initial design (Figure 3.4d).

This figure was provided by a reviewer for the paper of Zhu et al (1993a).

3.3.2 Discussion of the 'Block' Concept

The three previous examples confirm that simple, efficient designs may be readily obtained by application of the block concept. A block can span a large number of enthalpy intervals and provides extended possibilities for matching to reduce the area requirement. The block method differs significantly from the pinch method and its variants. First, decomposition is in terms of blocks rather than strictly imposed by the pinch. The pinch may be neglected when it is contained within a block. Second, the design is not constrained by the energy target. Relaxation of this energy constraint can be beneficial, if associated with network simplification or reduced area, as the optimal HRAT merely provides an initial estimate of the true optimal conditions. The designer should not be constrained in the initial stages of a design to rigidly adhere to targets as this may result in an overly complex design. Normally, relaxation provides the designer with some flexibility and results in simpler initial designs as illustrated in the previous examples. Finally, in the block method, a match is evaluated on the basis of area. Such a calculation accounts for the effects of terminal temperatures, heat loads and the heat transfer coefficients. By contrast, the Driving Force Plot is based solely on temperatures. A final benefit is that match selection is undertaken in a more *simultaneous* manner rather than *sequentially* as in the pinch methodology (see Section 3.9).

3.4 Details of the 'Block' Method

A central driving force behind the block method is the combination of the advantages of thermodynamic or heuristic and mathematical programming methodologies. This is achieved in a two–step process. In the first step of design, the designer can provide a significant input based on his/her experience and knowledge, and thereby guide the decision process. The key aim of this stage is to seek initial designs close to all targets at the estimated optimal condition. As mentioned above, such designs provide good initial solutions for the subsequent cost optimization. If a superior initial solution can be provided for the NLP optimization, the likelihood of finding the global optimum is increased. The next step is to optimize and evolve this initial network to produce a final design. The evolution of a network by employing energy relaxation is believed the most difficult task in HEN synthesis (Linnhoff et al, 1982). In the block method this task is fulfilled using non–linear optimization techniques and computers.

To provide initial solutions, two approaches are considered viz. an automated solution utilizing computer techniques or a simplified method employing hand computation. The computer solution follows a prescribed algorithm whereas hand calculation requires more input from designers. Consequently, it is more flexible and provides more opportunity to exploit a designer's detailed knowledge and experience.

3.4.1 Determination of the 'Blocks'

For the situation with approximately equal film coefficients, the minimum area based on *quasi–composite curves* (Figure 3.1) can be expressed as:

$$A_{min} = \sum_{i}^{blocks} \frac{1}{\Delta T_{lm_i}} \sum_{j}^{streams} \left[\frac{q_j}{h_j}\right]_i \tag{3.7}$$

where h_j is the heat transfer coefficient of the jth stream, q_j is the heat load of the stream in the ith block and ΔT_{lm_i} is the logarithmic mean temperature difference of this block on the quasi–composites. The quasi–composites are determined by least–squares fitting. If the number of blocks is fixed, the appropriate minimum area can be calculated using equation (3.7). This may then be compared to the minimum area target using the *actual* composite curves using equation (3.6). If a constraint is placed on the permissible deviation from this area target, the optimal number of blocks may be defined as the smallest number of blocks achieving the given deviation (e.g. typically 5–10%).

This method of block determination is appropriate for automated synthesis by computer. However, for hand calculation, a simpler strategy is applied. The blocks can be determined by careful consideration of the composite curves. Enthalpy intervals with similar profiles may be combined into a single block. The block determination is based on the qualitative analysis of the composite curves and qualitative trade–off between area and the number of units. Generally speaking, fewer blocks tend to produce an initial design with fewer units but it may require more overall area. The principle for determining the number of blocks is that a small sacrifice in area is tolerated to improve network simplification. In some instances, a problem requires only two blocks and even a single block for nearly parallel composite curves.

In some cases, a number of different block decompositions may be possible. Alternative designs based on the differing block definitions should be produced and compared to select the best designs. This is not a difficult task.

Given a suitable set of blocks, the synthesis of a HEN proceeds block by block. Network synthesis commences at the most constrained block, i.e.the narrowest spaced block (either at a pinch point or within the block containing the pinch point). The matches are quantitatively assessed by doing area calculations and selected by a simultaneous choice approach rather than the sequential choice approach used in the PDM.

3.4.2 Selection Rules

Matches in each block are selected according to the following rules.

3.4.2.1 Rule 1: Tick–off Rule

Each match must 'tick–off' (i.e. completely match) at least one stream section within the block. Although similar to the 'tick–off' heuristic of Linnhoff and Hindmarsh (1983), there are differences as will be discussed later.

3.4.2.2 Rule 2: Import or Export of Energy

This rule is used for preferred matches which have different available enthalpy changes within a block or which need some small adjustment to achieve a favorable 'tick–off' situation. Energy may be imported from or exported to a neighboring block(s) to balance the enthalpy changes for matches between the section of hot stream i and the section of cold stream j within a block and so simplify the network. The rules governing such transactions are as follows:

For a block with $CP_{hot\ quasi\text{–}composite} < CP_{cold\ quasi\text{–}composite}$

If $CP_{Hi} \leq CP_{Cj}$, then energy may be imported to supplement the stream undergoing the smaller enthalpy change. If $CP_{Hi} > CP_{Cj}$, energy may be exported from the stream undergoing the larger enthalpy change.

For a block with $CP_{hot\ quasi\text{–}composite} > CP_{cold\ quasi\text{–}composite}$

If $CP_{Hi} \geq CP_{Cj}$, then energy may be imported to supplement the stream undergoing the smaller enthalpy change. If $CP_{Hi} < CP_{Cj}$, energy may be exported from the stream undergoing the larger enthalpy change.

For a block with $CP_{hot\ quasi\text{–}composite} \cong CP_{cold\ quasi\text{–}composite}$

If $CP_{Hi} \cong CP_{Cj}$, then energy may be imported to supplement the stream undergoing the smaller enthalpy change. If CP_{Hi} is significantly different to CP_{Cj}, then energy may be exported from the stream undergoing the larger enthalpy change.

The general rule is to allow the import or export of small amounts of energy for blocks with narrow profiles and to allow the import or export of relatively large amounts of energy for block with a wide spacing. This rule is based on simple thermodynamics. Large import or export of energy to a region where the composite curves closely approach one another will incur a significant area penalty. By contrast, widely spaced regions on the curves can tolerate relatively large import or export of energy. As a guide–line, energy import or export for a stream should be limited to a relatively small amount (about 5–10% of the amount of energy that the stream has in a corresponding block) in the narrow regions of the composite curves and to roughly 20–25% in the wider regions unless special circumstances pertain.

For hand calculation, if the quasi–composite curves are not used as the basis for synthesis, then the above general rule should guide the design.

Special circumstances may pertain where variations of these rules are desirable. For example, a stream may contain a small amount of energy relative to other streams within a block. The energy associated with this stream may be exported to an adjacent block to avoid introduction of a small exchanger. An instance of this occurs in Case Study 2. Normally, energy is imported for only one stream section. Occasionally, energy import can occur for both stream sections.

Consider the kth block in Figure 3.5. In this block, hot stream H_i possesses 250 kW of energy and cold stream C_j requires 240 kW of heating. Matching these streams means that H_i has a residual 10 kW of energy within the block which would require an additional small unit. Suppose that stream C_j requires 200 kW of heating and that H_i has a cooling demand of 15 kW in the adjacent (k+1) block. Returning to the potential match between these streams in the kth block. If we import 10 kW of energy to heat C_j, then two stream sections can be ticked off but the section of H_i in the (k+1)th block requiring 15 kW of cooling still remains. This section will necessitate the installation of a small exchanger. Alternatively, if we import for both streams (i.e. 15 kW for H_i and 25 kW for C_j from the (k+1)th block, then not only are the two streams in the kth block ticked off, as well, the small section of H_i in the (k+1)th block is also ticked off. This eliminates the need for one of the small exchangers.

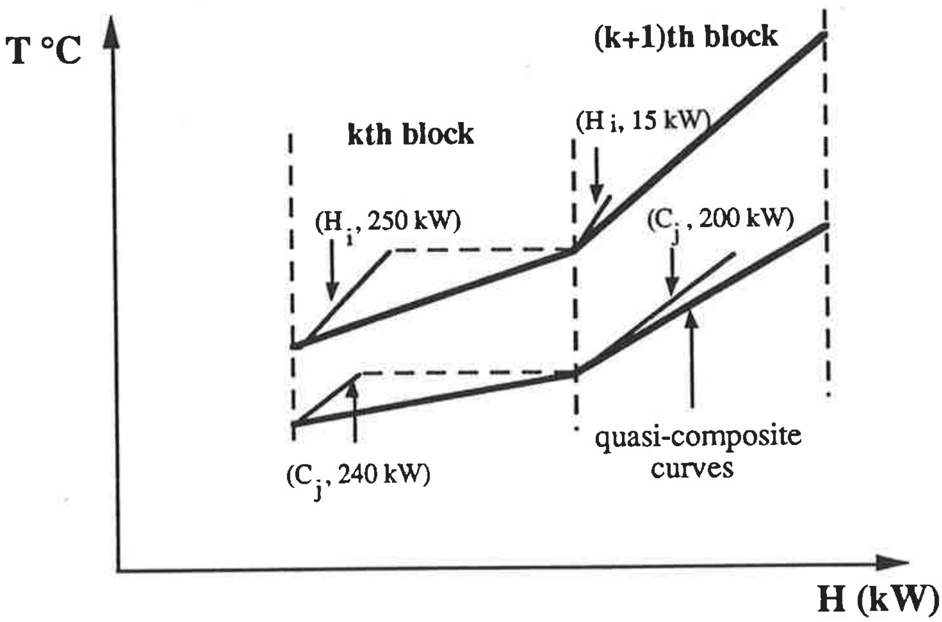


Figure 3.5: Diagram for illustrating the import/export rule

3.4.2.3 Rule 3: Stream Splitting

The selection of a good set of matches based on equation (3.10) or (3.11) may require some remaining stream section(s) to be split. The strategy for solving a splitting problem is presented in Section 3.8. The following formulae# is used to determine the split ratio of a single hot (cold) stream against two cold (hot) streams. For practical reasons splits are restricted to only two branches.

Simple formulae (Eqs. (3.8) & (3.9)) was suggested by a reviewer for the paper of Zhu et al (1993a).

Suppose a section of the hot stream H_i is to be split into branches to match cold streams C_j and C_k, the optimal split ratio of the branches, CP^1_{Hi} and CP^2_{Hi}, is determined by (see Appendix A)

$$\frac{CP^1_{Hi}}{CP^2_{Hi}} = \frac{CP_{Cj}}{CP_{ck}} \tag{3.8a}$$

$$CP^2_{Hi} = CP_{Hi} - CP^1_{Hi} \tag{3.8b}$$

Similarly, when a cold stream C_i is split into two branches to match the hot streams H_j and H_k, the optimal split ratio is determined by

$$\frac{CP^1_{ci}}{CP^2_{ci}} = \frac{CP_{Hj}}{CP_{Hk}} \tag{3.9a}$$

$$CP^2_{ci} = CP_{ci} - CP^1_{ci} \tag{3.9b}$$

Equations (3.8a) and (3.9a) are formulated based on the assumption that the three streams form a sub–set for optimal matching. The objective is to deduce the best fit to the composites of the sub-problem by the profiles of the two matches using stream splitting. Usually, the split ratio calculated as above yields a good solution with low area requirement.

3.4.3 Matching Matrix and the Selection of Matches in A 'Block'

For automated synthesis, a set of matches and their associated within–block minimum area penalties are selected to minimize an objective function such as the following:

$$\textit{minimize} \qquad \sum_{all\ i\&j} \frac{\Delta A_{ij}}{Q_{ij}} \tag{3.10}$$

where ΔA_{ij} represents an area penalty (–ve for benefit) for the match between the ith hot stream and the jth cold stream and Q_{ij} is the heat transferred by this match (ΔA_{ij} and Q_{ij} are defined in Section 3.4.4). Obviously, this criterion favours matches incurring small area penalties and transferring significant energy. In this manner, the resultant network features near minimum area coupled with a simple structure.

For hand computation, an alternative method for selecting the set of matches possessing minimum area is to minimize the alternative objective function:

$$\textit{minimize} \qquad \sum_{all\ i\&j} \frac{A_{ij}}{Q_{ij}} \tag{3.11}$$

where A_{ij} is the actual area required for a match between the ith hot stream and the jth cold stream.

The two criteria produce networks with similar topology and nearly identical area. The computation load is reduced by the use of equation (3.11).

The area penalties or benefits for any possible matches in a block can be calculated and tabulated in *matrix* form (such as Table 3.3) together with the corresponding heat loads. The matrix includes information relating to the area penalty (with '+' values) or benefit ('–' values) for each match. If equation (3.11) is employed as the matching criterion, then the matrix displays the heat load and area required for each possible match (Table 3.4).

By using the *matching matrix*, the total effect of all the matches on area in each block can be calculated, and the influence of any individual match on the area reported. Also, the cumulative progress of the design up to the current stage is available from the accumulating set of matching matrices. The network so developed is constrained to closely approach the area target. During development, the utility target may not be exactly satisfied because of the import/export of energy across the pinch.

Actually, selection of the best set of matches from a matching matrix by applying equations (3.10) or (3.11) is a mixed integer linear program. Usually, it can be done manually by examining a matching matrix. However, cases with large numbers of hot and cold streams involved for matches in a block, have a large sized matching matrix. Thus, selection of the best set of matches is not a simple task and mixed integer linear programming (MILP) may be required to solve this kind of problem. The detailed discussions about how to apply MILP program to solve the problem are given in Section 3.6. In addition, a matching matrix may be of a structure with equal numbers of columns and rows (square matrix) which means the number of hot and cold streams are identical, or may be non–square which corresponds to unequal populations of hot and cold streams in a block. How to handle these situations? In addition, with a non–square matching matrix, do some of streams require splitting and how to split streams? These complex issues are discussed in Section 3.8.

After a set of matches are selected based on above principles, a remaining problem may be solved requiring stream splitting. The strategy to determine the placement of parallel splits and their optimal ratio is given in Section 3.8.4. In some cases, it may also be worthwhile to try to avoid stream splitting. When is it possible to avoid stream splitting and how to determine the sequence for sequential matches? These issues will be addressed in Section 3.8.5.

3.4.4 Calculation of the Area Penalty ΔA_{ij}

With reference to Figure B1 (Appendix B), when 'ticking off' a hot stream H_i, specific match area penalties are calculated in the following manner:

- First, calculate the actual match area for the H_i, C_j match.

$$A_{ij,actual} = \frac{Q_{ij}}{U_{ij} \Delta T_{lm-ij}} \tag{3.12}$$

where
$$Q_{ij} = (T_b - T_a)\, CP_{Hi}$$

$$T_e = T_f + (T_b - T_a) \frac{CP_{Hi}}{CP_{Cj}}$$

and
$$\Delta T_{lm-ij} = \frac{(T_b - T_e) - (T_a - T_f)}{ln\left[\frac{(T_b - T_e)}{(T_a - T_f)}\right]}$$

- Second, calculate the quasi–composite based 'ideal area' for the match. The steps for calculating $A_{ij,quasi-ideal}$ are outlined in more detail in Appendix C. This is based on the computation of the ideal hot stream area $[A_{ij\ quasi\ ideal}]_{Hi}$ and the ideal cold stream area $[A_{ij\ quasi\ ideal}]_{Cj}$. These are then averaged to provide an estimate of $A_{ij,quasi\ ideal}$

$$A_{ij,quasi\ ideal} = \frac{[A_{ij\ quasi\ ideal}]_{Hi} + [A_{ij\ quasi\ ideal}]_{Cj}}{2} \tag{3.13}$$

The area penalty ΔA is then defined by the difference of the areas:

$$\Delta A_{ij} = A_{ij,actual} - A_{ij,quasi-ideal} \tag{3.14}$$

If $\Delta A_{ij} > 0$, then an area penalty is incurred. Likewise if $\Delta A_{ij} < 0$, an area benefit accrues.

3.4.5 EMAT

Most workers define a single minimum approach temperature (EMAT) for heat exchanger sizing in design (Gundersen and Naess, 1988). The choice of a single global EMAT for all exchangers in the network may result in topology traps (Gundersen and Grossmann 1990). For this method, all matches with EMAT larger than one third of the optimal HRAT are considered in the initial design. In the subsequent optimization procedure, this condition is expanded to consider all otherwise feasible matches with EMAT exceeding zero as the practical economic constraints governing temperature approaches are implicit in the optimization procedure.

3.4.6 Utility Streams

Often a single hot and cold utility is available for heating and cooling duties, respectively. These are supplied at the ends of the composite curves and are known as 'extreme utilities'. Utilities supplied at intermediate temperatures are likewise called 'intermediate utilities'. If intermediate hot and cold utilities are used, these are regarded in the same manner as process streams. Hence, an intermediate hot or cold utility can be matched with process streams at any stage provided the temperatures are appropriate. In this case, the balanced composite curves should be considered as the basis for block decomposition and subsequent design. For the normal situation employing a single hot and cold utility, the utility exchangers (if required) are placed at either end of the network and should be designed upon completion of the process–process exchangers.

3.5 The Procedures for HEN Synthesis

(i) Prediction of the Optimal HRAT

The optimal HRAT is predicted prior to design. The energy and capital targets are functions of HRAT. Clearly, the actual capital cost is affected by area distribution. However, at the targeting stage, the distribution of network area amongst the units in the network remains unknown. The assumption used in targeting is that the minimum area is distributed over the minimum number of units identically (Ahmad et. al., 1990). Upon specifying a plant lifetime and rate of return per annum, the annualized capital cost may be calculated. An optimal HRAT can be deduced from the total cost function. This optimization will be influenced by the process stream data and the associated cost data.

The optimization software is coded in C++, which provides utility target, unit target, shell target, and the area targets for networks with either counter–current heat exchangers or with 1–2 type of exchangers subject to a maximum area limit.

(ii) Determination of the blocks

Using the composite curves at the optimal HRAT, the number of blocks is determined by applying the strategy previously outlined in Section 3.4.1.

(iii) Calculation of the Area Penalties for Possible Matches

Following determination of the blocks, matches are considered employing the rules provided and area calculations are performed for possible matches with EMAT $\geq \frac{1}{3}$ HRAT. These calculations are summarized in the matching matrix.

(iv) Selection of a Set of Matches Featuring the Minimum Area Requirement / Penalty

For automated synthesis, the area penalty(benefit) for each match is available in the matching matrix and a good set of matches can be deduced *simultaneously* using equation (3.10) . For hand calculation, the area requirements for each match are summarized in the matching matrix and a set of matches with minimum area is determined using equation (3.11).

(v) Cost Optimization (see Section 3.7)

After network design, the total cost may be minimized using the non–linear optimization package MINOS 5.2 (Brook et al, 1988).

3.6 Mixed Integer Programming (MIP) for Match Selection

For large problems, the sizes of matching matrices could be quite large and the task for searching for the best set of matches is not simple. In this case, mathematical programming techniques may be required to solve the problem for match selection.

For example, there is a design problem that involves four hot streams and four cold streams. Assume that these streams all involve heat transfer within a certain block. After determining heat loads for possible matches, the matching matrix calculated by equation (3.11) can be expressed as

$$\begin{array}{c} \\ C_5 \\ C_6 \\ C_7 \\ C_8 \end{array} \begin{array}{c} \begin{array}{cccc} H_1 & H_2 & H_3 & H_4 \end{array} \\ \begin{bmatrix} 0.94 & 0.65 & 0.50 & 0.81 \\ 0.72 & 0.63 & 0.91 & 0.21 \\ 0.14 & 0.61 & 0.24 & 0.13 \\ 0.35 & 0.61 & 0.23 & 0.96 \end{bmatrix} \end{array}$$

where H_i represents the ith hot stream and C_j denotes the jth cold stream, respectively. Each element a_{ij} in the matrix represents $\frac{A_{ij}}{Q_{ij}}$. An obvious question arises: *how to select the best set of matches when applying equation (3.11).*

The general problem statement can be written as following. The total number of hot streams n is four which equals the number of cold streams in a block. Let a_{ij} be defined as $\frac{A_{ij}}{Q_{ij}}$ and assume each match ticks off two streams from this block. Let binary variables x_{ij} indicate the existence of a match between hot stream i and cold stream j. $x_{ij} = 1$ declares the existence of a match and $x_{ij} = 0$ non-existence of a match. Then, to select a set of matches to minimize the sum of $\frac{A_{ij}}{Q_{ij}}$, the following mixed integer programming problem can be defined:

$$\text{minimize} \quad \sum_{all\ i\&j} \frac{A_{ij}}{Q_{ij}} \quad <=> \quad \text{minimize} \quad \sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij}\, x_{ij}$$

$$\sum_{i=1}^{n} x_{ij} = 1 \qquad j = 1..n$$

$$\sum_{j=1}^{n} x_{ij} = 1 \qquad i = 1..n$$

$$x_{ij} = 0, 1 \qquad i, j = 1..\, n \tag{3.15}$$

The above integer problem has sixteen (16) binary (0–1) variables, and eight (8) constraints. This problem is actually soluble as a linear programming problem (Edgar & Himmelblau, 1988). In this work, the MIP solver in GAMS package (Brooke et al, 1988) is used to solve this problem. The results indicate that the set of matches (H_1–C_7, H_2–C_5, H_3–C_8, H_4–C_6) should be selected to achieve minimum area design as this set of matches achieves the smallest value of $\Sigma\frac{A}{Q}$.

The solution from the simultaneous matching approach defined in equation (3.15) always gives the best set of matches rather than a single best match. In other words, it is not necessary that a best single match be selected. For example, the above matching matrix indicates that the match of H_4–C_7 has the minimum $\frac{A}{Q}$ value of 0.13. However, this match does not appear in the best set of matches selected previously since any set of matches including H_4–C_7 match has a larger sum of $\frac{A}{Q}$ than the MIP solution.

If the total number of hot streams is not equal to that of cold streams, dummy elements with zero assignment are added to make a matrix square. To illustrate this, assume a problem has four hot streams and five cold streams. When constructing the matrix, a column is added into the matrix to make it square and revised matrix is given as

$$
\begin{array}{c} \\ C_5 \\ C_6 \\ C_7 \\ C_8 \\ C_9 \end{array}
\begin{array}{c}
\begin{array}{ccccc} H_1 & H_2 & H_3 & H_4 & H_d \end{array} \\
\begin{bmatrix}
0.94 & 0.65 & 0.50 & 0.81 & 0.00 \\
0.72 & 0.63 & 0.91 & 0.21 & 0.00 \\
0.14 & 0.61 & 0.24 & 0.13 & 0.00 \\
0.35 & 0.61 & 0.23 & 0.96 & 0.00 \\
0.84 & 0.45 & 0.92 & 0.32 & 0.00
\end{bmatrix}
\end{array}
$$

The results from solving the integer programming problem indicate that the hot streams (1, 2, 3, 4, d) should be assigned to cold streams (7, 9, 8, 6, 5) respectively. These matches are ranked in the order list by the $\frac{A}{Q}$ values, i.e.[H_1–C_7 (0.14), H_4–C_6 (0.21), H_3–C_8 (0.23), H_2–C_9 (0.45)]. Since the number of hot streams is one less than that of cold streams, one hot stream may be split to match two cold streams. In this case, the first three matches, i.e. [H_1–C_7, H_4–C_6, H_3–C_8] in the above order list are selected. Hot stream H_2 may need to be split to match cold streams C_5 and C_9 or a solution may exist with unsplit matches when the problem possesses wide composite curves. This issue will be addressed in detail in Section 3.8.

The above considerations can be similarly applied to equation (3.10). In this instance, the method will be same but the elements in the matching matrix are defined differently, i.e. a_{ij} defined as $\frac{\Delta A_{ij}}{Q_{ij}}$.

3.7 NLP Cost Optimization: Using either Units or Shells for Fixed Topologies

As stated, a good initial solution can be generated by applying the block method. After initial network design, a network featuring minimum total cost is deduced using non–linear optimization techniques. This involves the well known 'capital–energy' tradeoff. Two NLP models will be presented for cost optimization, one based on units and the other based on shells.

In the former model, it is assumed that each unit corresponds to a single counter-current exchanger. However, actual exchangers are often of the 1–2 type (1 shell pass–2 tube passes). These exchangers involve a mixture of counter–current and cocurrent flow. If such exchangers are employed then a match may require more than one shell. Thus, the second NLP formulation will be based on the application of 1–2 type of exchangers. The number of shells in series per unit may be calculated using the formula proposed by Ahmad and Smith (1989) and correction factor Ft for N shells in series may be determined from the relationships provided by Bowman et al (1940).

For each model, two approaches will be provided. The first is based on a general mathematical formulation and the other based on a specific formulation. Following the notation employed in the GAMS software package (Brook et al, 1988), parameters are indicated by upper–case characters whereas variables are denoted by lower–case characters.

3.7.1 The General Formulation

(i) Indices and Sets

I = {i| i denotes a process–process exchanger}

J = {j| j denotes a heater}

K = {k| k denotes a cooler}

(ii) Parameters

THU_{in} = supply temperature of a hot utility stream

THU_{out} = target temperature of a hot utility stream

TCU_{in} = supply temperature of a cold utility stream

TCU_{out} = target temperature of a cold utility stream

CP_H = heat capacity flow rate of a hot stream

CP_C = heat capacity flow rate of a cold stream

U = overall heat transfer coefficient

F = fixed cost in a cost model

B = coefficient in a cost model

. C = exponent in a cost mode

C_H = annual cost for a hot utility

C_C = annual cost for a cold utility

(iii) Variables

t_{i1} = hot inlet temperature in a process–process exchanger

t_{i2} = hot outlet temperature in a process–process exchanger

t_{im} = hot temperature after mixing

$\tilde{t}_{i1}$ = cold inlet temperature in a process–process exchanger

$\tilde{t}_{i2}$ = cold outlet temperature in a process–process exchanger

$\tilde{t}_{im}$ = cold temperature after mixing

$\tilde{t}_{j1}$ = cold inlet temperature in a heater

$\tilde{t}_{j2}$ = cold outlet temperature in a heater

t_{k1} = hot inlet temperature in a cooler;

t_{k2} = hot outlet temperature in a cooler;

cp = heat capacity flow rate of a branch of a process stream;

q_j = hot utility requirement for a heater;

q_k = cold utility requirement for a cooler;

$area_i$ = heat transfer area for a process–process exchanger;

$area_j$ = heat transfer area for a heater;

$area_k$ = heat transfer area for a cooler;

Δt_{mi} = logarithmical temperature difference of a process exchanger;

Δt_{mj} = logarithmical temperature difference of a heater;

Δt_{mk} = logarithmical temperature difference of a cooler.

(iv) Equations

Energy balance for each exchanger

$$CP_{Hi}(t_{i1} - t_{i2}) = CP_{Ci}(\bar{t}_{i2} - \bar{t}_{i1}) \tag{3.16}$$

$$q_j = CP_{Cj}(\bar{t}_{j2} - \bar{t}_{j1}) \tag{3.17}$$

$$q_k = CP_{Hk}(t_{k1} - t_{k2}) \tag{3.18}$$

Mass and energy balance for exchangers with stream splitting

As stated, splits are restricted only to two branches. Thus, the mass and energy balance equations for a hot and cold stream can be expressed as follows.

for a hot stream

$$cp^1_{Hi}(t_{i1} - t^1_{i2}) + cp^2_{Hi}(t_{i1} - t^2_{i2}) = CP_{Hi}(t_{i1} - t_{im}) \tag{3.19}$$

$$cp^1_{Hi} + cp^2_{Hi} = CP_{Hi} \tag{3.20}$$

for a cold stream

$$cp^1_{Ci}(\bar{t}^1_{i2} - \bar{t}_{i1}) + cp^2_{Ci}(\bar{t}^2_{i2} - \bar{t}_{i1}) = CP_{Ci}(\bar{t}_{im} - \bar{t}_{i1}) \tag{3.21}$$

$$cp^1_{Ci} + cp^2_{Ci} = CP_{Ci} \tag{3.22}$$

Heat transfer

$$area_i = \frac{CP_{Hi}(t_{i1} - t_{i2})}{U_i \, \Delta t_{mi}} \tag{3.23}$$

$$area_j = \frac{q_j}{U_j \, \Delta t_{mj}} \tag{3.24}$$

$$area_k = \frac{q_k}{U_k \, \Delta t_{mk}} \tag{3.25}$$

Logarithmic temperature differences

$$\Delta t_{mi} = \frac{(t_{i1} - \tilde{t}_{i2}) - (t_{i2} - \tilde{t}_{i1})}{ln\left[\frac{t_{i1} - \tilde{t}_{i2}}{t_{i2} - \tilde{t}_{i1}}\right]} \qquad (3.26)$$

$$\Delta t_{mj} = \frac{(THU_{in} - \tilde{t}_{j2}) - (THU_{out} - \tilde{t}_{j1})}{ln\left[\frac{THU_{in} - \tilde{t}_{j2}}{THU_{out} - \tilde{t}_{j1}}\right]} \qquad (3.27)$$

$$\Delta t_{mk} = \frac{(t_{k1} - TCU_{out}) - (t_{k2} - TCU_{in})}{ln\left[\frac{t_{k1} - TCU_{out}}{t_{k2} - TCU_{in}}\right]} \qquad (3.28)$$

To avoid the singularity inherent in the above logarithmic function when approach temperatures of both sides of the exchanger are identical, the following approximation for the lmtd term (Paterson, 1984) is employed:

$$\Delta t_{mi} = \frac{2}{3}\sqrt{(t_{i1} - \tilde{t}_{i2}) \times (t_{i2} - \tilde{t}_{i1})} + \frac{1}{3}\left[\frac{(t_{i1} - \tilde{t}_{i2}) + (t_{i2} - \tilde{t}_{i1})}{2}\right] \qquad (3.29)$$

Similar expressions may be written for Δt_{mj} and Δt_{mk}.

(v) Feasibility conditions

Constraints to ensure a monotonic decrease of temperature at each exchanger must be specified. Specification of positive temperature approaches ensures feasibility for heat transfer. If a minimum temperature approach is specified for an individual exchanger, the temperature approaches of an exchanger must not be less than the related minimum temperature approach. These conditions may be expressed as

$$t_{i1} \geq t_{i2}, \; \tilde{t}_{i2} \geq \tilde{t}_{i1}, \; \tilde{t}_{j2} \geq \tilde{t}_{j1}, \; t_{k1} \geq t_{k2} \qquad (3.30a)$$

and

$$t_{i1} - \tilde{t}_{i2} \geq \Delta T_{mini}, \; t_{i2} - \tilde{t}_{i1} \geq \Delta T_{mini},$$

$$THU_{out} - \tilde{t}_{j1} \geq \Delta T_{minj}, \; t_{k1} - TCU_{out} \geq \Delta T_{mink}. \qquad (3.30b)$$

(vi) Objective functions – minimizing total cost based on units or shells

In the models for total cost optimization, the situation with multiple utilities and alternative exchanger cost models is considered. Such considerations are important in practical terms because when multiple utilities are available, the trade–off between different energy costs and capital cost should be accounted for. In addition, streams with high temperature, pressure, or corrosion etc., require special materials of construction and it may be more economical and more reliable for some matches to use different types of exchangers, e.g. plate–fin exchangers. Thus, alternative exchanger cost models should also be considered.

Therefore, Two objective functions can be expressed as following:

Cost Optimization based on Units

$$\textbf{minimize} \quad \sum_{j\in I} C_{Hj}\, q_j + \sum_{k\in K} C_{Ck}\, q_k + R\Bigg[\sum_{i\in I}\left(F_i + B_i\, area_i^{C_i}\right) + \sum_{j\in J}\left(F_j + B_j\, area_j^{C_j}\right) + \sum_{k\in K}\left(F_k + B_k\, area_i^{C_k}\right)\Bigg] \tag{3.31}$$

Cost Optimization based on Shells

$$\textbf{minimize} \quad \sum_{j\in J} C_{Hj}\, q_j + \sum_{k\in K} C_{Ck}\, q_k + R\Bigg\{\sum_{i\in I} N_i\left[F_i + B_i\left(\frac{area_i}{N_i}\right)^{C_i}\right] + \sum_{j\in J} N_j\left[F_j + B_j\left(\frac{area_j}{N_j}\right)^{C_j}\right] + \sum_{k\in K} N_k\left[F_k + B_k\left(\frac{area_k}{N_k}\right)^{C_k}\right]\Bigg\} \tag{3.32}$$

where N is the number of shells and R is the annual recovery factor. Given plant life time n and annual interest rate r, R is defined as

$$R = \frac{r\,(1+r)^n}{(1+r)^n - 1} \tag{3.33}$$

The above model (3.32) assumes that the area for a unit is evenly distributed over the shells comprising the unit. If the area per shell in a unit is larger than the maximum allowable area per shell, the number of shells in this unit is incremented by one in the optimization process. Given an exchanger cost model with an exponent less than unity, the cost optimization normally favours a small number of units and shells in the final optimized network.

It should be noted that the Eq (3.32) displays discontinuities associated with shells and requires iterative loops to solve such discontinuous problems which may be unable to be handled by GAMS (Brook et al, 1988). The problem may be solved by writing a program implemented with an iterative searching technique.

(vii) Constraints

The previous formulation involves no imposed constraints. In practice, constraints are often present and hence must be considered in design. Such restrictions on a network are readily incorporated into the problem specification. Possible constraints include:

Area bounds on required matches

$$Area_i^L \leq area_i \leq Area_i^U \tag{3.34}$$

$$Area_j^L \leq area_j \leq Area_j^U \tag{3.35}$$

$$Area_k^L \leq area_k \leq Area_k^U \tag{3.36}$$

Prohibition of stream splitting

$$\begin{aligned} cp_{Hi}^1 = 0 \quad or \quad cp_{Hi}^2 = 0 \\ cp_{Ci}^1 = 0 \quad or \quad cp_{Ci}^2 = 0 \end{aligned} \tag{3.37}$$

Specified total number of matches

The total number of matches in a HEN may be specified. The constraint fixing the total number of exchangers is:

$$\sum_{i \in I} x_i \ \$(area_i \geq Area_i^L) + \sum_{j \in J} x_j \ \$(area_j \geq Area_j^L) + \sum_{k \in K} x_k \ \$(area_k \geq Area_k^L) \ \leq N_t \tag{3.38}$$

where x_i, x_j, and x_k are binary variables and are used to indicate the existence of process-process exchangers, heaters and cooler respectively. $ is the symbol in GAMS denoting an 'if' condition.

3.7.2 The Specific Formulation

The general formulation can be directly coded into a GAMS program. It may be applied to any exchanger networks; only the initial values differ. However, it involves a large number of variables and equations which may affect solution quality. In order to solve the problems, a specific formulation for cost optimization is proposed. With this formulation, some variables (dependent variables) in a network are represented by the other variables (independent variables) by means of energy balance equations. Thus these dependent variables can be removed from the optimization model. Thus, the number of variables and equations can be reduced significantly. Obviously, the corresponding hypersurface of this optimization program is greatly simplified. As a result, the efficiency and solution quality may be improved. However, the major disadvantage of this formulation is its speciality. In other words, one formulation only applies to a specific network.

The key element of the formulation will be illustrated using the example presented in Figure 3.6. This network involves five independent variables, i.e. (t_1, t_2, t_3, t_4, cp_{C4}^1) and seven dependent variables, i.e. (t_5, t_6, t_7, t_8, t_9, t_{10}, cp_{C4}^2). The mass and energy balance equations for this network can be derived as follows:

$cp_{C4}^{1} + cp_{C4}^{2} = CP_{C4}$	cold stream C4;	(3.39)
$CP_{H3}\,(343 - t_4) = CP_{C5}\,(t_9 - t_{10})$	exchanger 1;	(3.40)
$CP_{H2}\,(267 - t_2) = CP_{C4}\,(t_5 - t_6)$	exchanger 2;	(3.41)
$CP_{H1}\,(159 - t_1) = CP_{C5}\,(t_{10} - 118)$	exchanger 3;	(3.42)
$CP_{H2}\,(t_2 - t_3) = cp_{C4}^{1}\,(t_7 - 26)$	exchanger 4;	(3.43)
$CP_{H3}\,(t_4 - 90) = cp_{C4}^{2}\,(t_8 - 26)$	exchanger 5;	(3.44)
$CP_{C4}\,(t_6 - 26) = CP_{H3}\,(t_4 - 90) + CP_{H2}\,(t_2 - t_3)$	exchangers 4 & 5.	(3.45)

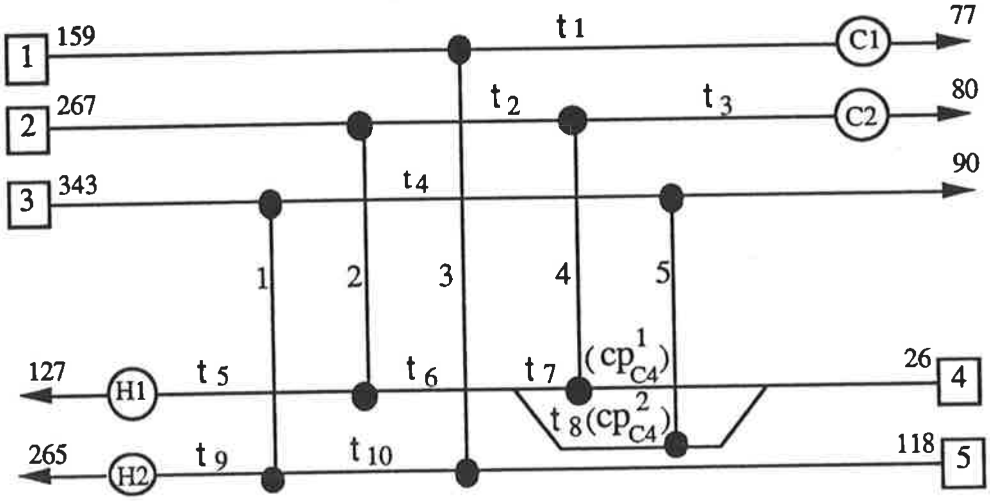


Figure 3.6: Example network for illustrating specific formulation

Rearranging of above seven equations yields:

$$cp_{C4}^{2} = CP_{C4} - cp_{C4}^{1} \tag{3.46}$$

$$t_{10} = \frac{CP_{H1}}{CP_{C5}}(159 - t_1) + 118 \tag{3.47}$$

$$t_9 = \frac{CP_{H3}}{CP_{C5}}(343 - t_4) + t_{10}$$

$$= \frac{CP_{H3}}{CP_{C5}}(343 - t_4) + \frac{CP_{H1}}{CP_{C5}}(159 - t_1) + 118 \qquad (3.48)$$

$$t_8 = \frac{CP_{H3}\,(t_4 - 90)}{CP_{C4} - cp^{1}_{C4}} + 26 \qquad (3.49)$$

$$t_7 = \frac{CP_{H2}}{cp^{1}_{C4}}(t_2 - t_3) + 26 \qquad (3.50)$$

$$t_6 = \frac{CP_{H2}}{CP_{C4}}(t_2 - t_3) + \frac{CP_{H3}}{CP_{C4}}(t_4 - 90) + 26 \qquad (3.51)$$

$$t_5 = \frac{CP_{H2}}{CP_{C4}}(267 - t_2) + t_6$$

$$= \frac{CP_{H2}}{CP_{C4}}(267 - t_3) + \frac{CP_{H3}}{CP_{C4}}(t_4 - 90) + 26 \qquad (3.52)$$

Clearly, logarithmic temperature differences, heat transfer areas and feasible conditions for each exchanger in this network may be derived in terms of the five independent variables (t_1, t_2, t_3, t_4, cp^{1}_{C4}). As a result, this program only involves five independent variables (t_1, t_2, t_3, t_4, cp^{1}_{C4}) and 18 dependent variables (these are the logarithmic temperature differences and heat transfer areas). The program comprises a sole equation for the objective function, eighteen (18) equations for logarithmic temperature differences and heat transfer areas, six (6) constraints to ensure feasibility and fourteen (14) constraints for monotonic temperature decrease. This provides a total of thirty-nine (39) equations for the NLP solver in GAMS. By comparison, the general formulation for this network requires thirty-eight variables and sixty-seven (67) equations. Therefore, the numbers of variables and equations are almost halved for this problem by resorting to the specific formulation.

Obviously, the advantage of the specific formulation is the simplicity. In other words, it involves less variables and equations. However, the major drawback is the complexity in constituting the optimization model. Derivation of the required equations is tedious work. On the contrary, the advantage of the general formulation is the generality but at the expense of more variables and equations compared to the specific formulation.

3.7.3 Suggestions for Practical Implementation

(i) The generality associated with the general formulation suggests its application to all problems. However, the general formulation normally involves a more complex hypersurface for the objective function containing many more inferior local optimal solutions. If a resultant solution appears to be unsatisfactory compared to targets, then the specific formulation should be applied.

(ii) Despite the block method's capability of generating good initial solutions for NLP optimization, the global optimum is not guaranteed. In some cases, a local optimal solution may include one or more very small units which are not practical. In this instance, these small units should be removed and the network re–optimized.

(iii) Following Saboo and Morari (1986), dummy heaters and coolers with zero initial heat loads are provided for cold and hot streams without such units. This enlarges the available search space and provides the possibility of replacing process–process exchangers with utility exchangers. If some of the additional utility exchangers are retained in the optimized design then the controllability of the network may be improved.

3.8 Match Alternative with & without Splitting

Three possible matching cases exist. First, the number of hot and cold streams may be identical in a block providing a square matching matrix (Case 1). Second, the number of hot streams may not be the same as that of cold streams (Case 2). Third, a single hot/cold stream may need to match with many streams of other type (Case 3). The latter two cases result in non–square matching matrices. The objective function is identical for all. Namely, to find a matching scheme which results in low overall area requirement and simple network structure. As well, wide–spaced composite curves and narrow spaced composite curves may require different treatment. The general rules applying to these situations will be given and the intelligent application of these heuristics is necessary in the solution of specific problems.

3.8.1 Case 1: Square Matching Matrix

In this case, a matching matrix is square and usually a set of unsplit matches featuring minimum area requirement can be found. As well, minimum number of units is achieved because at least one of the pairing streams can be 'ticked off' and in some cases two streams can be 'ticked off' by a match. Normally, a pair of streams providing a promising match is unlikely to contain identical enthalpies in a block, thus energy import/export will be required for this match.

However, in instances where a stream(s) has (have) excessively large heat capacity flow rate compared to other streams, (even though the numbers of hot and cold streams are identical), it may be impossible to recover the bulk of the energy in a simple acyclic network. In such cases, stream splitting may provide a possible solution. If the problem features tight composite curves, the situation is more severe and stream splitting is more desirable. However, if the associated composite curves have wide-spaced profiles, stream splitting may be avoidable since a wide latitude is available for stream shifting or criss-crossing.

3.8.2 Case 2: Unequal Numbers of Hot and Cold Streams

Usually, the optimal set of matches (in terms of area) is simultaneously determined as stated above. The remaining problem then usually involves multiple streams of one type against a single stream of the other type (Case 3). However, a problem with multiple small streams of one type versus more than one large stream of the other type is not uncommon. Again for this case, split match(es) may be necessary in situations with tight composite curves and stream splits may be avoidable in situations with wide composite curves.

3.8.3 Case 3: Multiple Hot/Cold Stream vs A Single Cold/Hot Stream

This is a basic case. Three possibilities exist for match selection, namely no stream splits or partially-split matches or all split matches. These situations are shown in Figure 3.7. Again for wide-spaced composite curves, it may be possible to avoid stream splitting partially or completely.

(a)

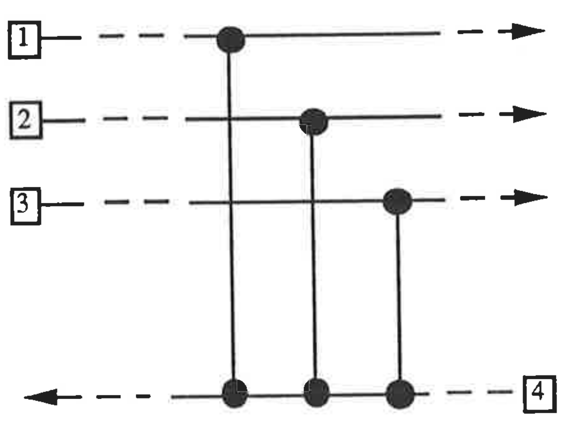


Figure 3.7 — Caption on next page

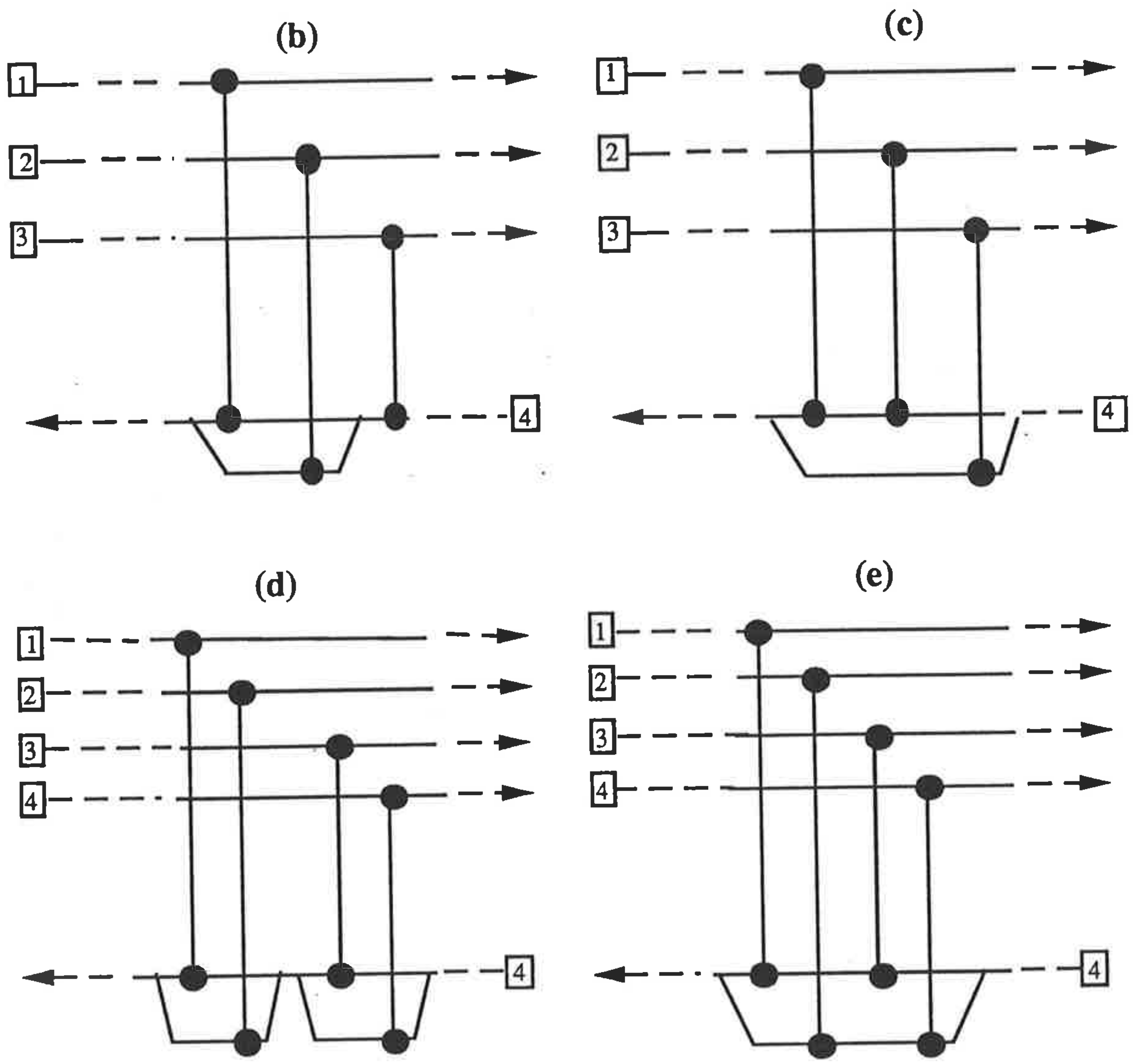


Figure 3.7: Possible alternative match scheme for a problem

3.8.4 Strategy for Stream Splitting

After a set of matches is selected by applying the block method, stream splitting may be required to reduce both area requirement and the number of units.

Linnhoff and Hindmarsh (1983) have stated the conditions for stream splitting, which must be satisfied in the vicinity of pinch point. However, the conditions do not provide any guidelines as to which stream should be split to achieve minimum area. Actually, there are two problems to be considered for solving a splitting problem. The first problem is how to determine the placement of matches with stream–splitting and the second one is how to determine the split ratio. The objective of these considerations is to achieve a minimum area design. It is these two problems that this section addresses. As stated previously, split is restricted to two branches.

It has been proved by Linnhoff and Ahmad (1990) that if the temperature profile of a match can follow the related part of the composite curves, this match usually achieves minimum or near minimum area requirement when streams have similar film coefficients. For a match to mimic the composite curves, the necessary and sufficient condition is to have the match ratio equal or approximately equal to the ratio of the composite curves, i.e.

$$\left.\frac{CP_H}{CP_C}\right|_{match} = \left.\frac{\Sigma CP_H}{\Sigma CP_C}\right|_{composite} \tag{3.53}$$

This condition was presented by Linnhoff and Ahmad (1990) as the criterion used for selecting matches in the vicinity of pinch points. Applying this condition, an approach is proposed to solve splitting problems. The idea is to determine the placement of matches and split ratio such that the temperature profiles of these matches can achieve a good overall fit to the composite curves.

Suppose the split ratio is determined as suggested in Eq (3.8a) or (3.9a). For the ease of discussions, assume there are two hot streams (i and k) to match one cold stream (j). Applying Eq (3.9a) yields

$$\frac{CP^1_{Cj}}{CP^2_{Cj}} = \frac{CP_{Hi}}{CP_{Hk}} \quad \text{or} \quad \frac{CP_{Hi}}{CP^1_{Cj}} = \frac{CP_{Hk}}{CP^2_{Cj}} \tag{3.54}$$

The fitness of the profiles of parallel splits to the composite curves can be expressed as

$$\delta_{ij} = \frac{CP_{Hi}}{CP^1_{Cj}} - \frac{\Sigma CP_H}{\Sigma CP_C}$$

or

$$\delta_{ij} = \frac{CP_{Hk}}{CP^2_{Cj}} - \frac{\Sigma CP_H}{\Sigma CP_C} \tag{3.55}$$

If Eq. (3.54) is satisfied, these two δ_{ij} values in Eq.(3.55) are identical. Clearly, δ values indicate the closeness that a match mimics the composite curves and thus it can be used to compare the suitability of different matches. Coming to the situation of a block, since it may span several enthalpy intervals (in which ΣCP_H and/or ΣCP_C may vary) the equivalent expression to (3.55) for the block method is

$$\delta_{ij} = \frac{CP_{Hi}}{CP^1_{Cj}} - \left.\frac{\Sigma CP_H}{\Sigma CP_C}\right|_{quasi\text{–}omposite}$$

or

$$\delta_{ij} = \frac{CP_{Hk}}{CP^2_{Cj}} - \left.\frac{\Sigma CP_H}{\Sigma CP_C}\right|_{quasi\text{–}omposite} \tag{3.56}$$

To give a clear illustration, consider a problem containing four hot streams with relatively small capacity flowrates and two cold streams with relatively large capacity flowrates (Figure 3.8a).

For this problem, the optimal placement of matches and the split ratio are not obvious. To achieve an optimal solution, we need to consider and compare as many possibilities for matches as possible and then chose one from them. First, consider all the possibilities for splitting cold stream 1 to match any two of four hot streams and then calculate associated δ values. For instance, consider hot streams 1 and 3 to match cold stream 1. Applying Eq (3.9), the splits of cold stream 1 can be calculated as

$$CP^1_{C1} = \frac{CP_{C1}\frac{CP_{H1}}{CP_{H3}}}{1+\frac{CP_{H1}}{CP_{H3}}} = \frac{130\frac{25}{45}}{1+\frac{25}{45}} = 46.4 \text{ (kW/K)}$$

$$CP^2_{C1} = CP_{C1} - CP^1_{C1} = 83.6 \text{ (kW/K)}$$

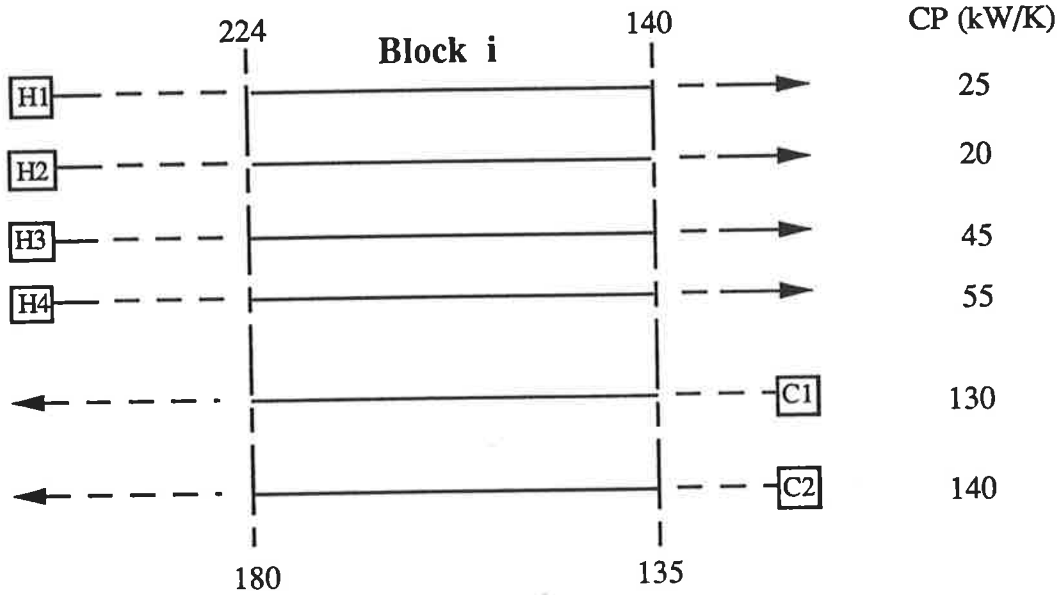


Figure 3.8a: Determining splits placement and split ratio using area targeting principle

Thus, the match ratio $\frac{CP_{H1}}{CP^1_{C1}}$ is 0.54. The ratio of the composite curves calculated is 0.54 as well. Hence, the δ value for this parallel splits equals zero which indicates perfect matches between these two hot streams and cold stream 1. By contrast, if cold stream 1 is split to match hot streams 1 and 2, a large δ value of 0.22 results which indicates a relatively poor matching. The similar calculations are carried out for all possible matches with cold stream 1 and δ values are summarized in the matrix as

for splitting cold stream 1:

$$\begin{array}{c} \\ H_1 \\ H_2 \\ H_3 \\ H_4 \end{array} \begin{array}{cccc} H_1 & H_2 & H_3 & H_4 \end{array} \\ \begin{bmatrix} M & 0.19(72.2) & 0.00(46.4) & 0.08(40.6) \\ 0.19(72.2) & M & 0.04(40.0) & 0.04(34.7) \\ 0.00(46.4) & 0.04(40.0) & M & 0.23(58.5) \\ 0.08(40.6) & 0.04(34.7) & 0.23(58.5) & M \end{bmatrix}$$

Any matrix element a_{ij} indicates the δ value for the match between cold stream 1 and hot streams i and j, and the value in brackets gives the capacity flowrate of one branch of cold stream 1. This matrix is symmetrical and diagonal elements are all assigned to a large integer (M) indicating an improper match between a hot stream and cold stream 1 without splitting cold stream 1, otherwise such an unsplit match would have been determined at the previous stage.

Similarly, the matrix for the case of splitting cold stream 2 is obtained as following

for splitting cold stream 2:

$$\begin{array}{c} \\ H_1 \\ H_2 \\ H_3 \\ H_4 \end{array} \begin{array}{cccc} H_1 & H_2 & H_3 & H_4 \end{array} \\ \begin{bmatrix} M & 0.22(77.8) & 0.04(50.0) & 0.03(43.8) \\ 0.22(77.8) & M & 0.07(43.1) & 0.00(37.3) \\ 0.04(50.0) & 0.07(43.1) & M & 0.18(63.0) \\ 0.03(43.8) & 0.00(37.3) & 0.18(63.0) & M \end{bmatrix}$$

As stated, the objective is to achieve an overall best fit to the composite curves. This objective can be expressed for the current problem as

$$minimize \quad \delta_{ij} + \delta_{i'j'} \quad (i \neq i' \text{ and } j \neq j') \tag{3.57}$$

where δ_{ij} is associated with the first matrix and $\delta_{i'j'}$ with the second matrix. The result of this optimization indicates that the cold stream 1 should be split to match hot streams

1 and 3, and that cold stream 2 is split to match hot streams 2 and 4. Both these parallel splits exactly mimic the composite curves. The related design is shown in Figure 3.8b. If an identical film coefficient for all streams is assumed, these matches achieve minimum area design.

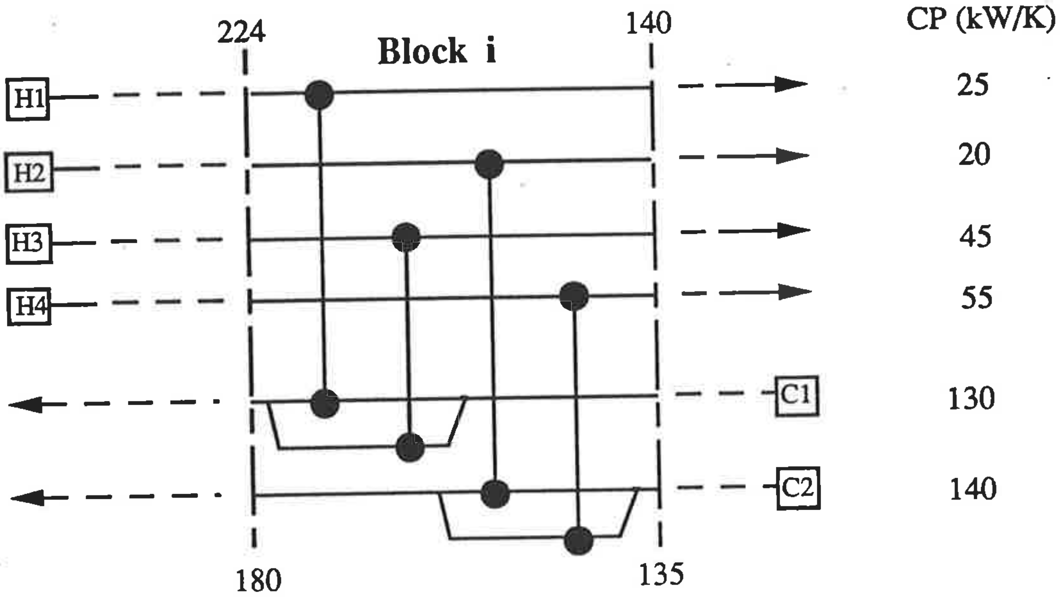


Figure 3.8b: Solution to the splitting problem shown in Figure 3.8a

In cases where the number of hot (cold) streams is more than twice the number of cold (hot) streams, a mixture of parallel and sequential matches may be required. Figure 3.9 displays two such possible instances, due to the limitation of splitting into only two branches. In Figure 3.9a, one pair of splitting matches follows the other pair of splitting matches. In this case, first consider and place the matches at the tighter boundary as it is more liable to incur a more severe area penalty if matches are placed improperly. In the case indicated as Figure 3.9b, first consider parallel splits at the more narrow-spaced boundary and the unsplit match follows. This is because the narrowly-spaced regions are very sensitive to the improper use of driving forces and they should be given first priority and designed with care. It should be noted that when exploring unsplit matches, the match selection is done by minimizing $\Sigma\frac{A}{Q}$. While determining splitting matches, the criteria for match selection is to minimize the δ value as stated above.

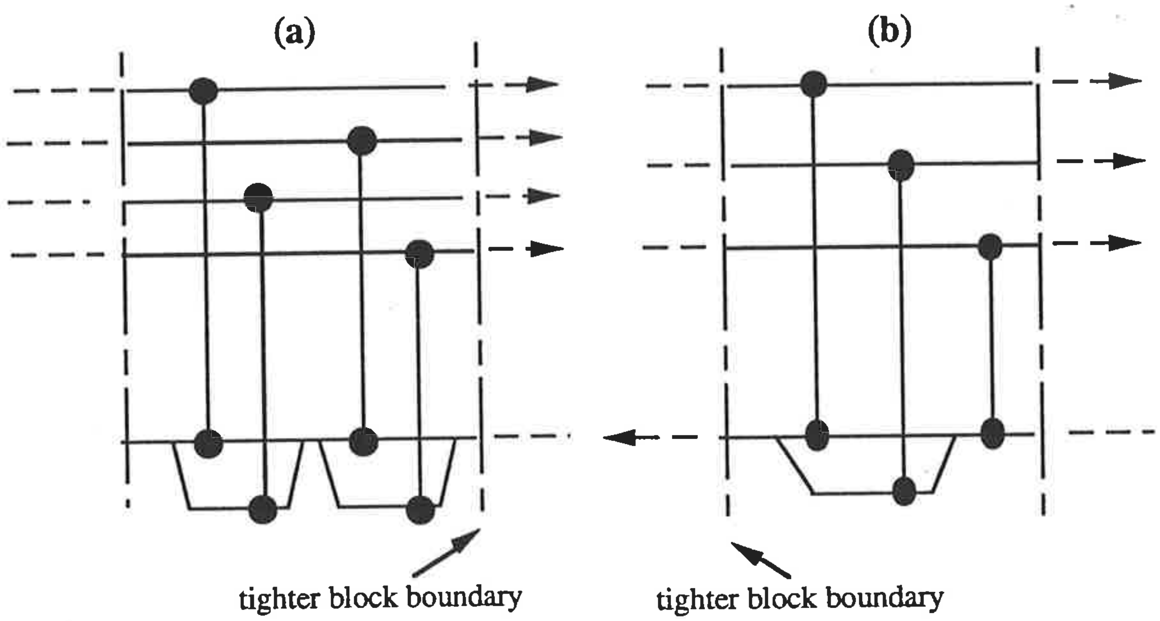


Figure 3.9: Two possible instances for splits

3.8.5 Strategy for Sequential Matches

As stated, for widely-space composite curves, it may be possible to avoid stream splitting. However, the question may be raised: how to determine the sequence of matches? Again, the minimum area principle is used to determine the sequence. The order of sequential matches is ranked using the $\frac{A}{Q}$ values (applying equation (3.11) or $\frac{\Delta A}{Q}$ values (employing equation (3.10)). In other words, matches are selected based on finding the smallest values for $\frac{A}{Q}$ or $\frac{\Delta A}{Q}$ and continuing sequentially. For a section where there are more than one hot and cold streams, $\Sigma\frac{A}{Q}$ or $\Sigma\frac{\Delta A}{Q}$ should be minimized for this section. This has been found to give reasonably low area requirements for the network as a whole. Again, the match selection for a relatively narrow–spaced region should be done first as such a region is more sensitive to the improper use of driving forces.

The following example (Figure 3.10–see Case Study 5 for more detail) is used to illustrate the use of above rules to determine match sequences. In block 1, there are six hot streams and two cold streams. The cold stream 8 has large heat capacity flow rate in the hottest section (397.4 kW/K) as compared with other streams. However, since this problem has a rather wide composite curves, it may be possible to find an unsplit solution.

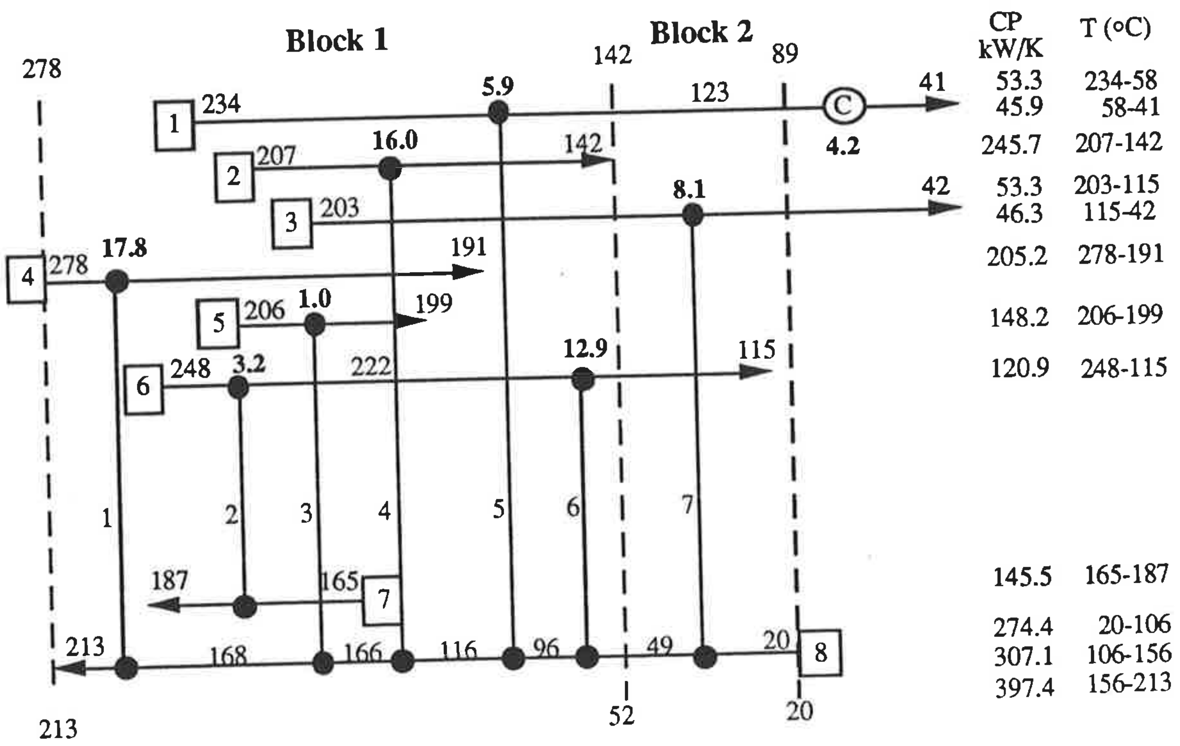


Figure 3.10: Determining match sequence using area targeting principle

To avoid the use of hot utility, the design starts from the hottest part. Possible matches exist between hot streams 1 or 4 or 6 and cold stream 8. From the calculation of area requirement for each match, it is found that the match 4–8 (match 1 in Figure 3.10) has minimum $\frac{A}{Q}$ value and thus is most appropriate match and selected. After this match is selected, there are two cold streams with similar terminal temperatures to be matched. Five remaining hot streams (1,2,3,5,6) are eligible to match these two cold streams. By determining proper heat loads for any possible matches, the matches 6–7 and 5–8 (matches 2 and 3) are selected since they have minimum $\Sigma \frac{A}{Q}$ value. From these two matches onwards, the remaining problem is of multi-hot streams against a single cold stream (a Case 3 situation as stated in Section 3.8.3). The match choice is determined sequentially and the match with minimum $\frac{A}{Q}$ is always selected. It can be seen in Case study 5 that this approach can produce a network with low area and shell requirement.

In summary, the above two approaches are deterministic in selecting matches and the solutions feature a minimum area requirement and small number of matches. Thus, the block method is consistent through a design. For cases with streams having significantly different film coefficients, minimum area may favour large criss–crossing matches. However, there may be too many alternatives to search for the best criss–crossing matches. In order to handle this problem and make the block method consistent with both the cases having similar film coefficients and the situations with variable film coefficients, the diverse pinch approaches (Rev and Fonyo, 1991, Zhu et al, 1994) are used to shift streams according to their film coefficients, and thus the block method, including above two approaches, can still be applied. The details for the extension of the block method to handle problems with variable film coefficients is given in Chapter 4.

3.9 Discussions and Comparison: the Sequential Approach versus the Simultaneous Approach for Match Selection

As mentioned above, the match selection by using either equations (3.10) or (3.11) is carried out in a simultaneous manner which systematically considers a set of matches to achieve minimum area and near minimum number of units. This is different from the sequential match choice used in the PDM which selects a single match at a time. The nature of the sequential approach is of the best first search. The best first search only focuses on the current stage and does not view the generation of a node (e.g. a match) at any stage as a part of the whole problem. Although this approach can usually select a best node at any stage of the design evolution, it may not find a best solution for the whole problem.

This can be explained more clearly by using the two networks (Figures 2.2 and 2.3 but also reproduced here), the one in Figure 3.11a produced by the DFP and the other one (Figure 3.11b) by applying the RPA (Linnhoff and Ahmad, 1990). The match 1 in Figure 3.11a has a lower area penalty (0.1%) than that of the match 1 (6.1%) in Figure 3.11b. According to the sequential match choice (best first search), the match 1 in Figure 3.11a is selected and design continues using the sequential match choice until the network in Figure 3.11a is produced. As an alternative, the match 1 in Figure 3.11b is selected though it has a relatively large area penalty. The selection of match 1 opens up a different path of design. As a result, the better design (Figure 3.11b) is obtained.

In addition, the sequential match approach may need to back track in design when some match incurs a large area penalty. Consider Figure 3.11a again. After the match 1 is determined, the design continues until it is found that the match 4 in Figure 3.11a incurs a large area penalty (11.1%). At this point, the design should go back track to the stage where a match causes the severe condition for the match 4 and start the design from this point again. It is found that match 1 causes the problem and the design restarts from the very beginning.

From above discussions, it may be seen that though the match selected by the sequential match choice (best first) has the least area penalty at one stage, the subsequent sequence of matches may not have the least overall area penalty. When some latter match is detected having a large area penalty, a design has to back track. It is not usually a easy task to identify which match(es) causes a problem. Even if all matches selected have a tolerable area penalty, however, whether the set of matches selected is the best solution in terms of area is still uncertain. Thus, it can be concluded that the sequential approach may not always produce near optimal solutions.

However, the disadvantages of the sequential approach can be overcome by the simultaneous approach because this approach considers all possible alternative paths of a design and aims for a minimum overall area requirement instead of searching for a single match with minimum area. For the problem above, the same network as that in Figure 3.11b is achieved by using the simultaneous match choice with a three block decompositions. However, when using a two block decomposition, a better design (Figure 3.3b) with a lower area requirement and simple structure can be obtained.

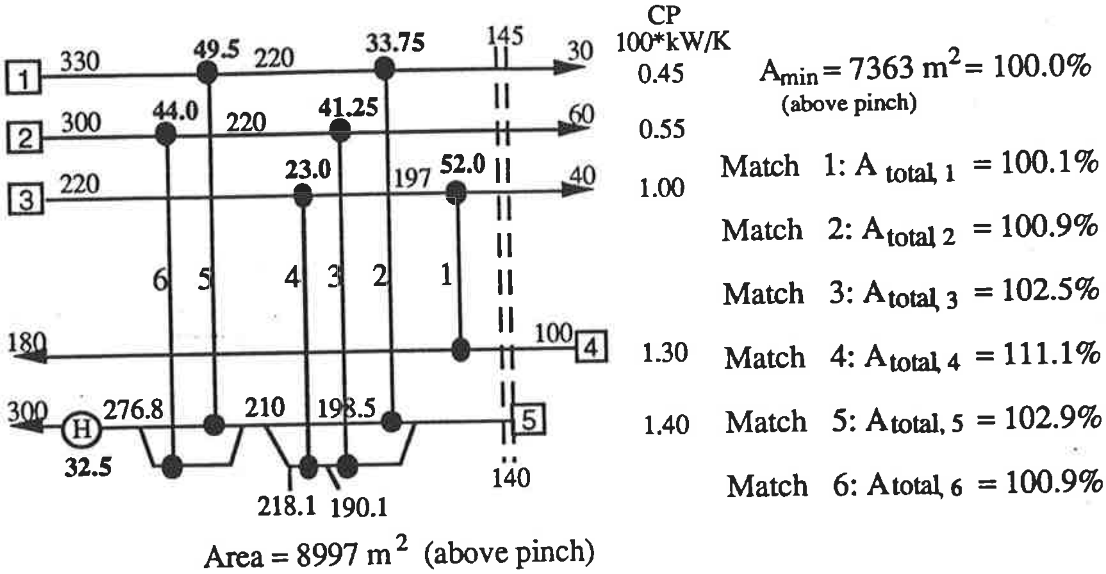


Figure 3.11a: Network produced using the DFP (Linnhoff & Ahmad, 1990)
– The RPA shows the significant area penalty incurred by match 4

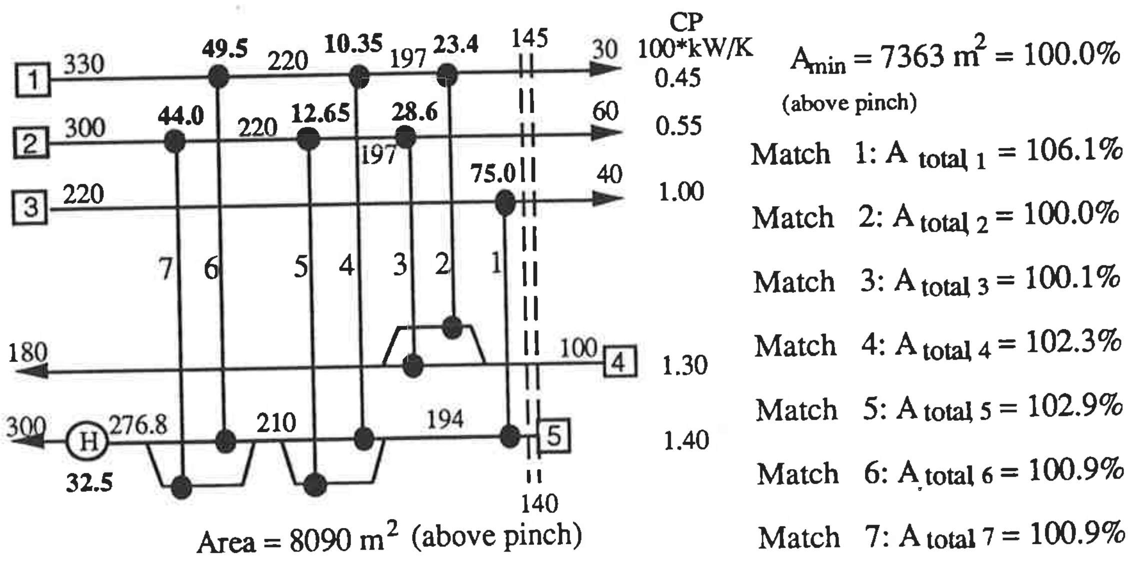


Figure 3.11b: Network produced using the RPA (Linnhoff & Ahmad, 1990)

3.10 Case Studies Based on Units

To illustrate the principles and the procedures of the proposed design method, a series of case studies are presented.

3.10.1 Case Study 1

Consider the following four stream problem (Table 3.1). The stream data and cost data were introduced by Linnhoff and Ahmad (1990) and Ahmad et al (1990) respectively.

For this example, the minimum total cost target occurs at HRAT = 10 K (Figure 3.12a). The corresponding composite curves and targets are given in Figure 3.12b and Table 3.2 respectively.

TABLE 3.1 STREAM DATA FOR CASE STUDY 1

Stream	Heat Capacity Flowrate kW K^{-1}	Supply Temperature °C	Target Temperature °C
1	200	150	50
2	100	170	40
3	300	50	120
4	500	80	110

UTILITY DATA

Hot utility: Saturated steam: 180 °C

Cold utility: Supply temperature: 20 °C; Target temperature: 40 °C

$U = 100\ W\ m^{2}K^{-1}$ for all matches

COST DATA

Installed heat exchanger cost: Cost ($) = $30{,}800 + 750\text{Area}^{0.81}$

Plant lifetime = 6 years; Rate of interest = 10 % per annum

Cost of hot utility = $110 \frac{\$}{\text{kW}\cdot\text{yr}}$, Cost of cold utility = $10 \frac{\$}{\text{kW}\cdot\text{yr}}$

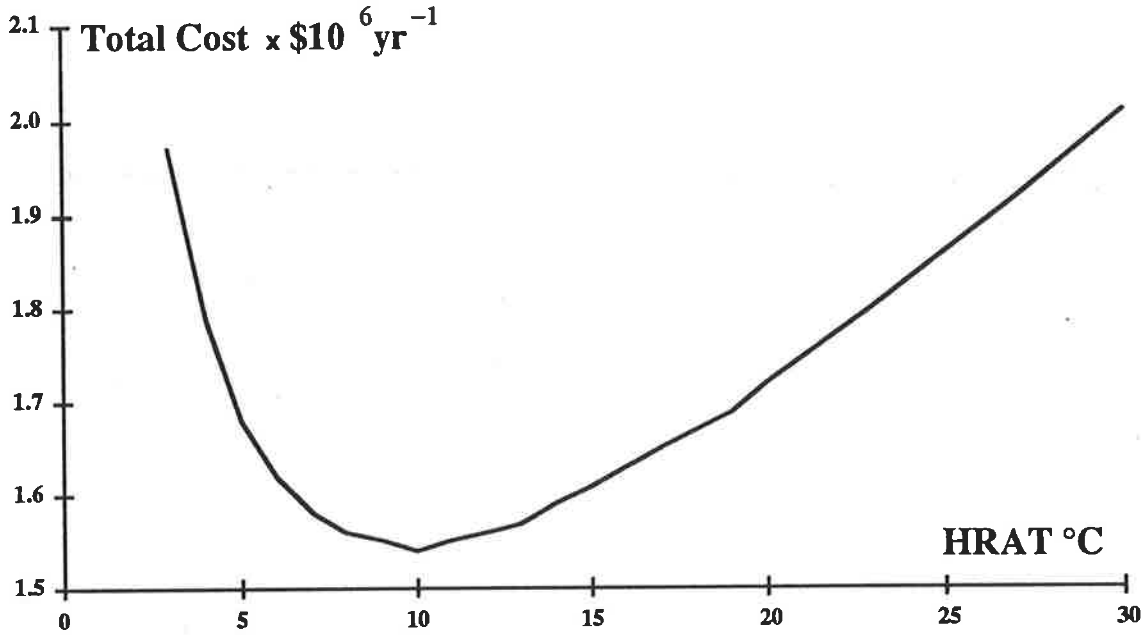


Figure 3.12a: Total Cost Target as function of HRAT - Case Study 1

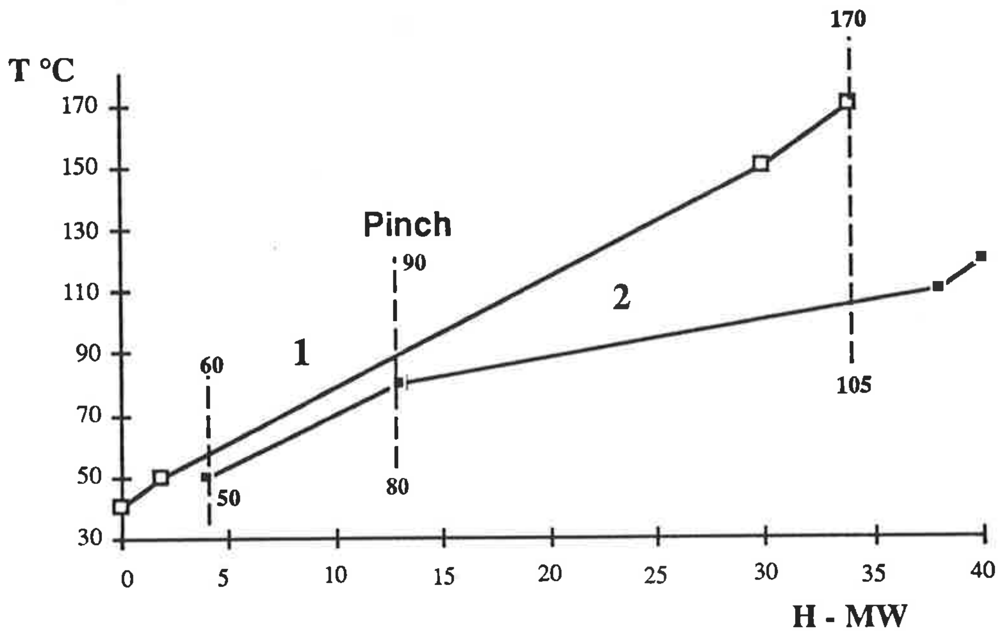


Figure 3.12b: Composite curves – Case Study 1

TABLE 3.2: TARGETS FOR HRAT = 10 K (CASE STUDY 1)

Hot utility kW	Cold utility kW	Area above pinch m^2	Area below pinch m^2	Units	Total cost $\frac{\$}{yr}$
7000	4000	8852	10785	5	1.55×10^6

By inspection of the composite curves, the minimum number of blocks equals two. In this example, this is identical to the pinch decomposition. Above the pinch, the quasi–composites are calculated as:

$$
\begin{array}{lll}
\text{Hot quasi–composites:} & T\,^{\circ}C = 90 + 0.0037q \quad [kW] & \\
\text{Cold quasi–composites:} & T\,^{\circ}C = 80 + 0.00125q \quad [kW] & \\
q = H - 13{,}000; & H \quad [kW] \in [13{,}000\ .\ .\ 33{,}000] & (3.58)
\end{array}
$$

where the enthalpy interval of this block is from 13,000 kW to 33,000 kW and H represents any enthalpy in this interval. The reciprocals of the slopes of equation (3.58) yield $CP_{\text{hot quasi–composite}} = 270\ kW\ K^{-1}$ and $CP_{\text{cold quasi–composite}} = 800\ kW\ K^{-1}$, respectively.

The quasi–composites below the pinch are determined in an identical manner. For this problem, a single enthalpy interval (not including the cold utility) occurs below the pinch, and the quasi–composites are co–incident with the true composite curves.

The predicted areas (equation (3.7)) for the quasi–composites including heaters and coolers are 8260 m^2 above the pinch and 10785 m^2 below the pinch. The replacement of the composite curves by the quasi–composites results in a 3 % difference in area which satisfies the given area deviation constraint (e.g. $\leq 5\%$). The two blocks are the minimum number of blocks achieving the area deviation. Hence, the optimal number of blocks for this problem equals two.

As an illustration of the calculation of area penalties or benefits for a feasible match, consider a potential match between the hot stream 1 and the cold stream 4 in the block above pinch (Figure 3.13). Initially, blocks are considered without employing the import/export rule.

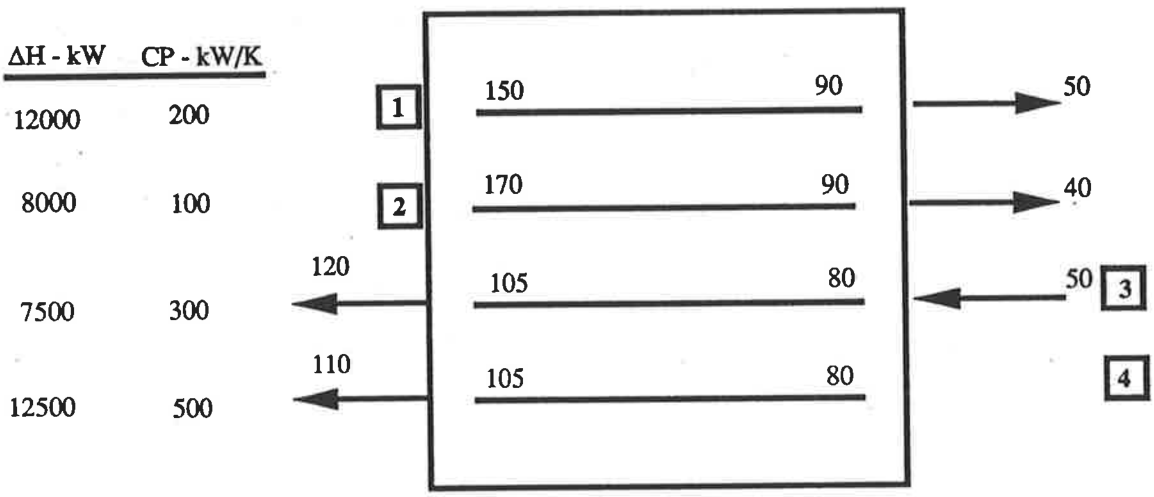


Figure 3.13: Energy balance for the block 2 – Case Study 1

As energy import is not employed, the maximum energy transfer for this match is 12,000 kW. To transfer this energy, the temperature of Stream 1 falls from 150 °C to 90 °C and the temperature of the corresponding section of Stream 4 rises from 80 °C to 104 °C. The area required for this exchanger is 5087 m^2. The 'ideal area' for this match can be calculated from the quasi–composites as 4646 m^2 (Appendix C). Hence for this match, the area penalty is 441 m^2 (5087 m^2 – 4646 m^2). Other matches may provide area benefits, i.e. the actual matches require less area than the ideal calculated from the quasi–composites. An example of this is readily provided. Consider the match between the streams 2 and 4 in the block above the pinch. This match requires an actual area of 2502 m^2 for transferring 8000 kW of energy and the ideal area of 3200 m^2 is calculated from the quasi–composites. Thus for this match, the area benefit is 698 m^2. After the area calculations for all feasible matches in this block are completed, the matching matrix may be drawn up as shown in Table 3.3.

TABLE 3.3: MATCHING MATRIX – ABOVE THE PINCH (CASE STUDY 1)

Q kW, $\Delta A^{\dagger}$ m^2, $\frac{\Delta A}{Q}$ m^2kW^{-1}	1	2
3	(7500, 1625, 0.217)	(7500, –20, –0.003)
4	(12000, 441, 0.037)	(8000, –698, –0.087)

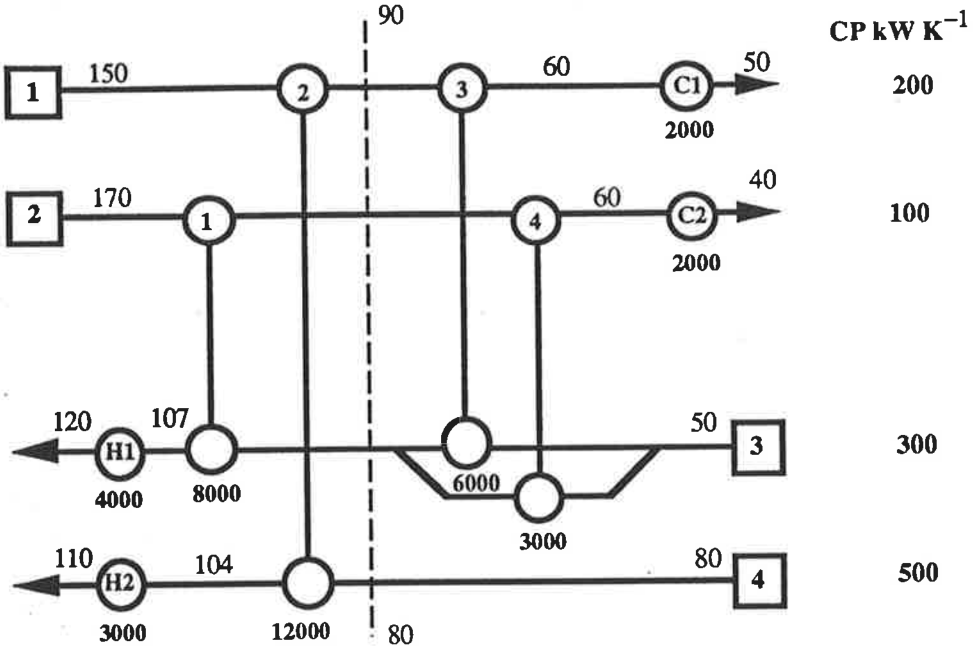
† – negative sign indicates a benefit

Alternatively, if equation (3.11) is employed as the basis for calculation , then the following matching matrix (Table 3.4) results:

TABLE 3.4: MATCHING MATRIX – ABOVE THE PINCH (CASE STUDY 1)

Q kW, A m^2, $\frac{A}{Q}$ m^2kW^{-1}	1	2
3	(7500, 4870, 0.65)	(7500, 2688, 0.36)
4	(12000, 5087, 0.42)	(8000, 2502, 0.31)

Utilizing the matching matrix, the set of matches may be determined based on either equation (3.10) or (3.11). The sum of $\frac{\Delta A}{Q}$ in Table 3.3 (or the sum of $\frac{A}{Q}$ in Table 3.4) for the matches 1–4 and 2–3 is 0.034 m^2kW^{-1} (0.78 m^2kW^{-1}) which is much smaller than 0.130 m^2kW^{-1} (0.96 m^2kW^{-1}) for the matches 1–3 and 2–4. Hence, the preferred matches are 1–4 (load = 12,000 kW) and 2–3 (load = 7500 kW subsequently this is adjusted to 8000 kW to simplify the network). These matches are presented in Figure 3.14.



Q_H = 7000 kW Area = 19690 m^2 Total cost = $\$1.60 \times 10^6\ yr^{-1}$

Figure 3.14: Initial design 1 – Case Study 1

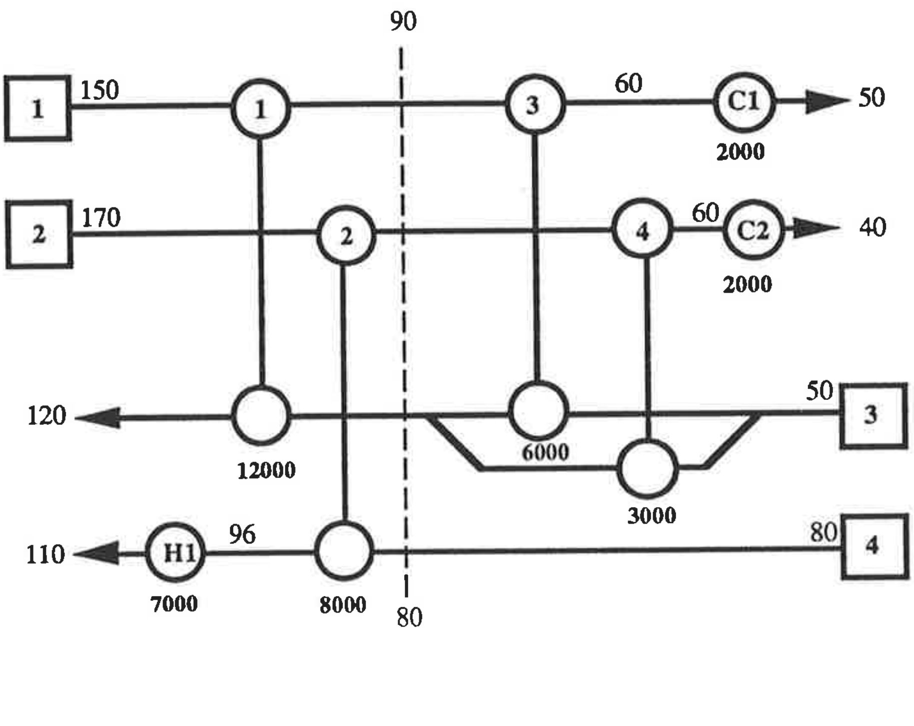
The above synthesis is conducted in a defined block without permitting the import or export of energy from neighboring blocks. The design is severely restricted. A simpler network may be achieved by permitting the import or export of energy from neighboring blocks.

For all streams within the block $CP_{Hi} < CP_{Cj}$ hence the conditions for the import/export rule are satisfied as $CP_{hot\ quasi\text{-}composite} < CP_{cold\ quasi\text{-}composite}$. Energy may be imported to provide a total heat load of 12000 kW for the match 1–3, 12500 kW for match 1–4 and 8000 kW for the match 2–3. With these maximum loads for all possible matches in this block, the revised matching matrix may be obtained (Table 3.5). For simplicity, this calculation is based on equation (3.11).

TABLE 3.5: MATCHING MATRIX (IMPORT/EXPORT) – ABOVE THE PINCH (CASE STUDY 1)

Q kW, A m^2, $\frac{A}{Q}$ m^2kW^{-1}	1	2
3	(12000, 6592, 0.55)	(8000, 2770, 0.35)
4	(12500, 6438, 0.52)	(8000, 2502, 0.31)

The sum of $\frac{A}{Q}$ for the matches 1–3 and 2–4 is 0.86 m^2kW^{-1} compared with 0.87 m^2kW^{-1} for the matches 1–4 and 2–3. These sums are quite close and it remains unclear as to which constitutes the best option. In this case, both alternative sets of matches should be considered. Selection of the second pair produces the network very similar to that shown earlier (Figure 3.14). The first pair produces the alternative network shown as Figure 3.15 (containing one less unit).



Q_H = 7000 kW Area = 20816 m^2 Total cost = $\$1.63 \times 10^6$ yr^{-1}

Figure 3.15: Initial design 2 – Case Study 1

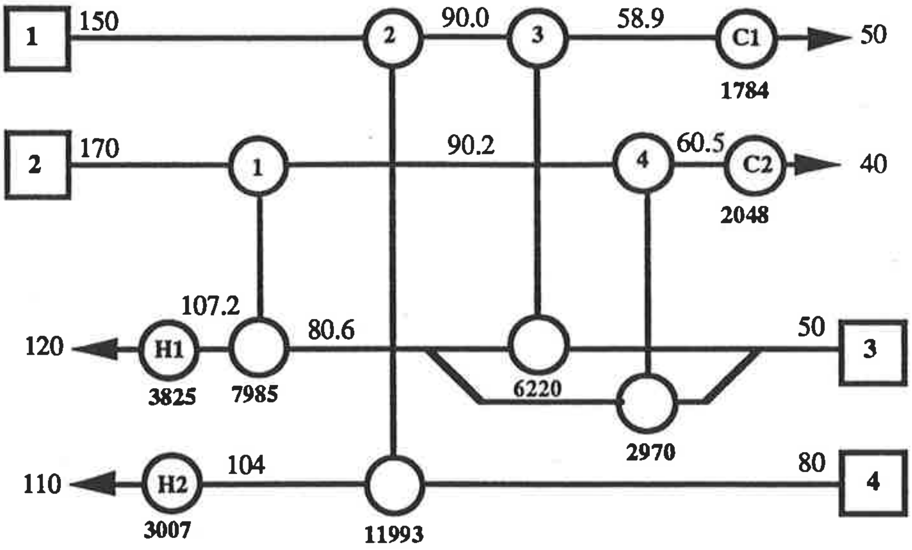
For the block below the pinch, two hot streams (1, 2) and one cold stream (3) exist. To fully utilize the available driving force, it is necessary to split stream 3 to match with streams 1 and 2. The split ratio of cold stream 3 is determined using equation (3.8a). The remaining process stream requirements are provided by utilities after all matches in the two blocks are selected. The initial design is summarized in Figures 3.14 (Design 1) and 3.15 (Design 2), respectively. The performance details of the network are summarized in Table 3.6.

Design 2 (Figure 3.15) does not get very close to the area target, but both designs achieve the energy target and approach the cost target closely. The number of units is reasonably close to the desired target. Design 2 is a little simpler as a consequence of applying the import/export rule. This simplification has been achieved at the expense of additional area.

TABLE 3.6: INITIAL DESIGN RESULTS (CASE STUDY 1)

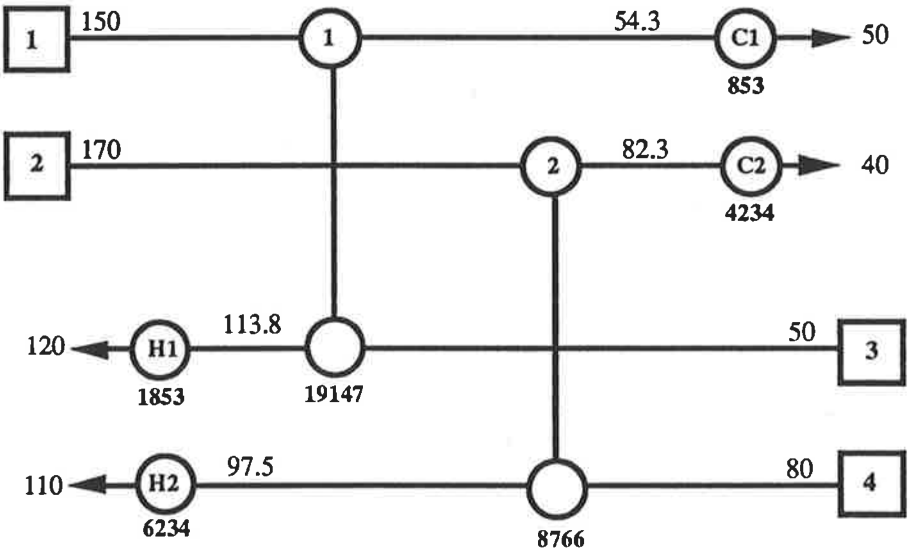
	Hot utility kW	Cold utility kW	Area m^2 above pinch	Area m^2 below pinch	Units	Total cost $\frac{\$}{yr}$
Design 1 Fig.3.14	7000	4000	8880	10810	8	$1.60x10^6$
Design 2 Fig.3.15	7000	4000	10005	10811	7	$1.63x10^6$

After optimizing these networks using MINOS 5.2, final optimal designs are derived (Figure 3.16 – Design 1 and Figure 3.17 – Design 2). The Design 2 (Figure 3.17) has a very simple structure and consists of two disconnected subnetworks which may provide benefits in terms of operability. Table 3.7 summarizes the optimal conditions.



Q_H = 6832 kW Area = 20394 m^2 Total cost = 1.59×10^6 yr^{-1}

Figure 3.16: Optimized design 1 –Case Study 1



Q_H = 8087 kW Area = 19830 m^2 Total cost = 1.63×10^6 yr^{-1}

Figure 3.17: Optimized design 2 –Case Study 1

TABLE 3.7: OPTIMAL SOLUTIONS FOR CASE STUDY 1

	Hot utility kW	Cold utility kW	Area m^2	Units	Cost: \$ $annum^{-1}$
Design 1 Fig.3.16	6832	3832	20394	8	1.59×10^6
Design 2 Fig.3.17	8087	5087	19830	6	1.63×10^6

Interestingly, the optimized design presented in Figure 3.17 requires 20% more energy than the energy target. It might be expected that the well–known area–energy tradeoff would mean that this network would require substantially less area. However, this design requires 193 m^2 more area than the area target at HRAT = 10 K. The reason is that this design results from an overall cost optimization rather than area optimization. As the exponent on area in the cost model is 0.81, the optimization performs the tradeoff between area, units and energy and does not solely focus on minimizing exchanger area. For this reason, the exchanger driving forces are extremely tight (exchanger 1 – 4.3 K and exchanger 2 – 2.3 K).

3.10.2 Case Study 2

The stream data relevant to this problem is summarized in Table 3.8. The problem is taken from the study of Rev and Fonyo (1991). The exchanger cost equation in Table 3.8 is similar to that used by Ahmad et al (1990) but is modified so that for the size of exchangers used here the constant exchanger cost is about 20–25% of the total cost of an average exchanger.

This example demonstrates how differing block structures influence the initial designs and determine the final designs. Using this data, an optimal HRAT equal to 30 K may be deduced. This HRAT and its associated targets determine the design conditions. The results are presented in Table 3.9. The composite curves for the problem are provided as Figure 3.18. Three distinct regions may be identified and these are each used to define a block. The initial design based on these parameters is shown in Figure 3.19. In summary, the energy consumption is less than the target by 4.3%, the total area required exceeds the area target by 7.0% and there are nine units – five process–process exchangers and four utility exchangers.

TABLE 3.8 STREAM DATA (CASE STUDY 2)

Stream	Supply Temperature °C	Target Temperature °C	Heat Capacity Flowrate kW K^{-1}	Film Coefficient W $m^{-2}K^{-1}$
1	159	77	2.285	100
2	267	80	0.204	40
3	343	90	0.538	500
4	26	127	0.933	10
5	118	265	1.961	500
Steam	300	300	–	50
Water	20	60	–	200

COST DATA

Installed heat exchanger cost: Cost ($) = $3{,}800 + 750A^{0.83}$

where A = exchanger area m^2

Plant lifetime = 6 years

Rate of interest = 10 % per annum

Cost of hot utility = $110 \frac{\$}{\text{kW}\cdot\text{yr}}$

Cost of cold utility = $10 \frac{\$}{\text{kW}\cdot\text{yr}}$

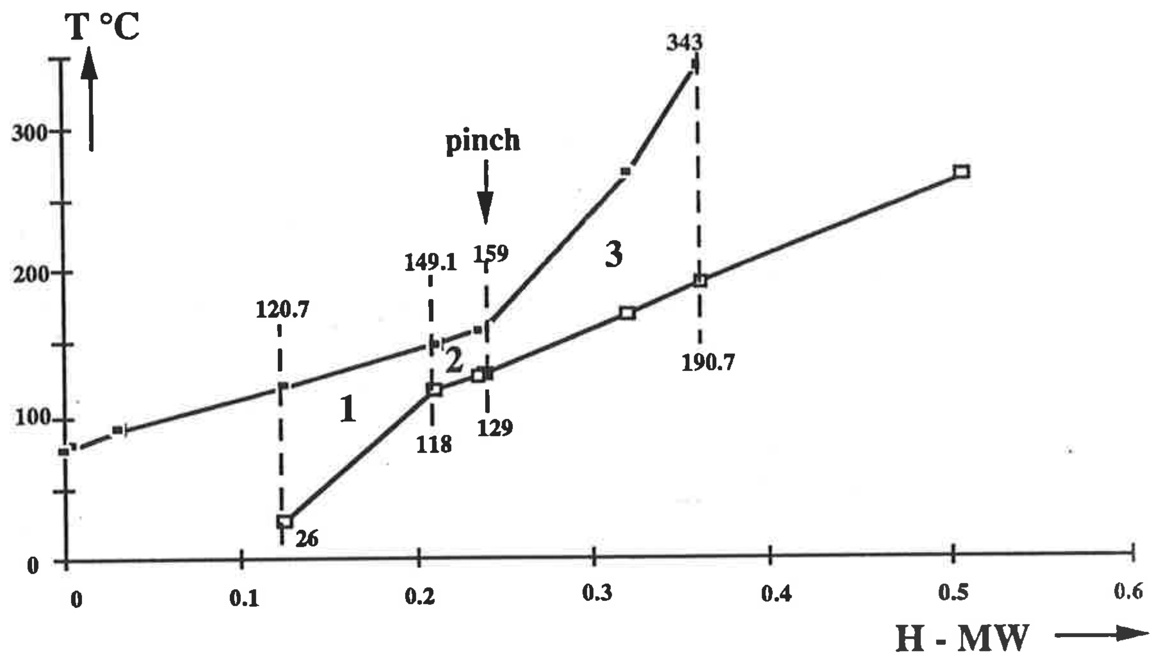
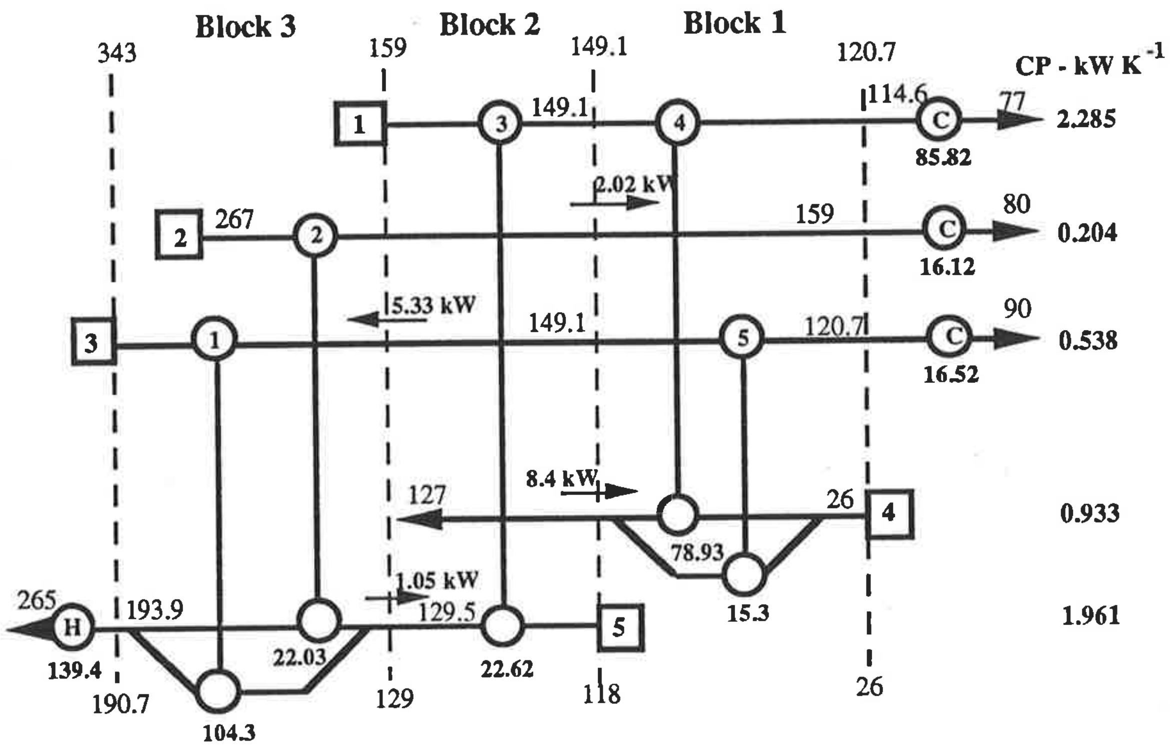


Figure 3.18: Composite curves for Case Study 2



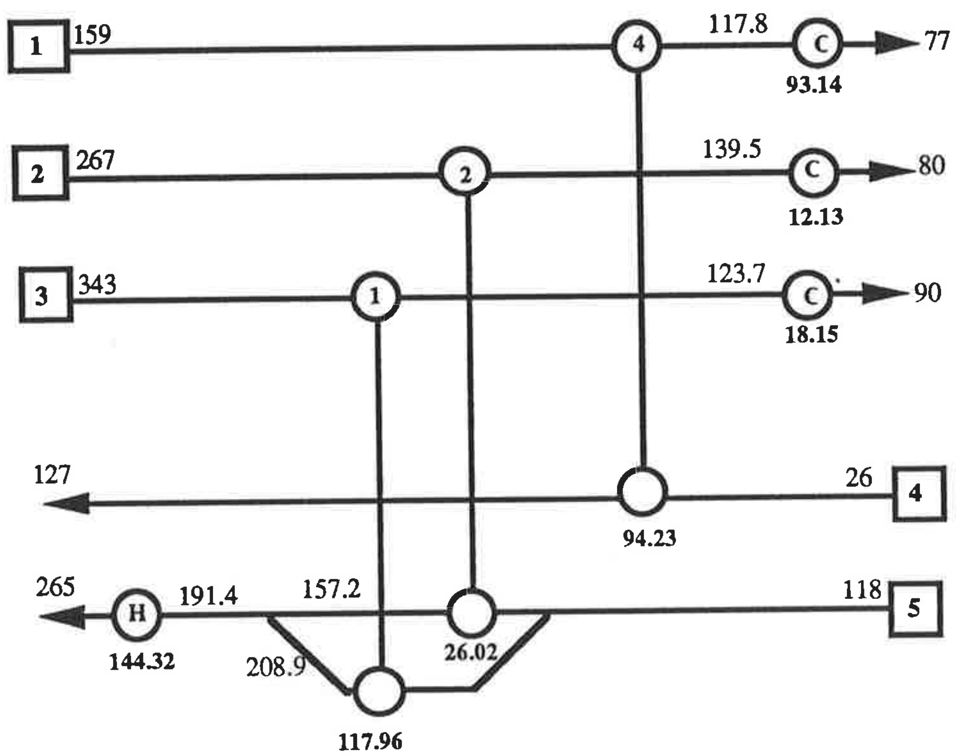
Q_H = 139.4 kW Area = 320 m^2 Total cost = \$51188 yr^{-1}

Figure 3.19: Initial design 1 for Case Study 2

The network is deduced by applying the import/export rule. Consider block 2, this block includes sections of the three hot streams (1–3) and the two cold streams (4–5). The enthalpy of hot stream 1 (22.62 kW) dominates the remaining hot streams' contribution (stream 2 – 2.02 kW and stream 3 – 5.33 kW). Likewise, the content of cold stream 5 (21.57 kW) is much greater than that of stream 4 (8.4 kW). To remove all the energy from stream 1 in this block necessitates a import of 1.05 kW for stream 5. To deal with the residual energy within the block requires the addition of two small exchangers (i.e. transfer of 7.35 kW from hot streams 2 & 3 to heat cold stream 4 (8.4 kW available)). To avoid introducing these small units, energy may be exported to neighboring blocks. The relatively small amount of enthalpy associated with stream 2 is exported to block 1 because this block has closer temperature approaches than block 3. However, as stream 3 has relatively large enthalpy it may be exported to block 3. These transfers are illustrated on Figure 3.19. The next step is to apply a non–linear optimizer to the network to seek an optimum design. Matches 3 and 5 in the initial network are removed (result zero heat loads after the cost optimization) producing a simple but low–cost network (Figure 3.20). This network has seven units (one more than the unit target) and its total cost is 4.5% below the cost target.

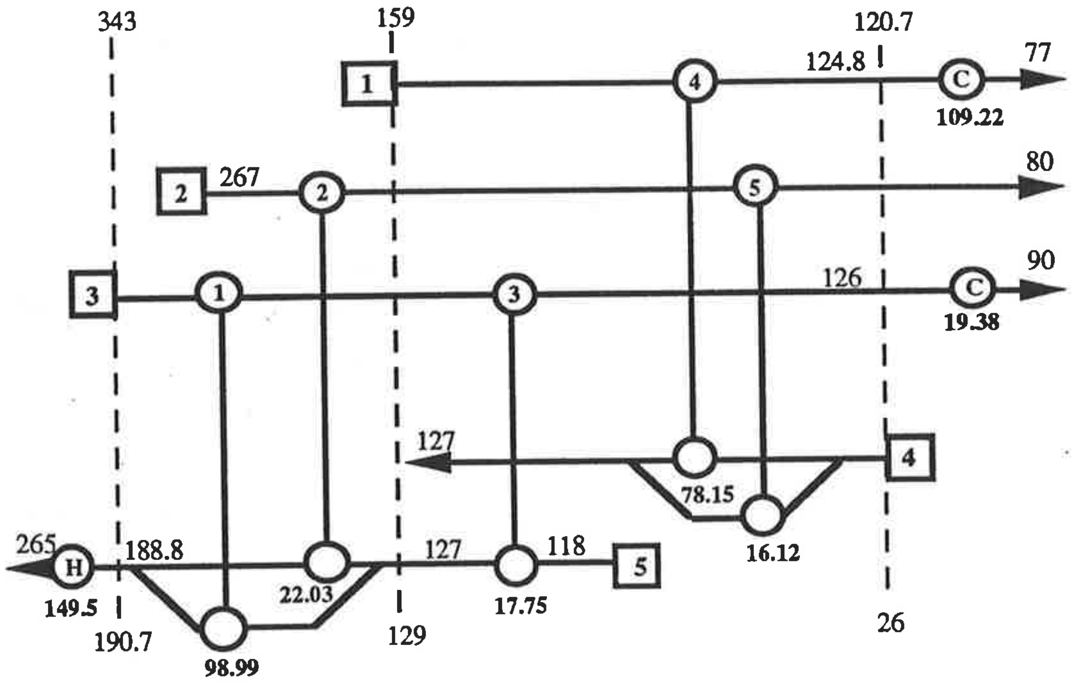
Suppose a different block configuration is employed, then alternative designs will result. Consider the composite curves, the energy contained in the middle section (region 2) is small relative to that of the remaining two sections. Clearly, it is possible to reduce the number of blocks (from three to two) by combining this region with either of the remaining regions. The composite curves in region 2 resembles those in region 1 more closely than the curves of region 3. Hence, it is logical to combine 1 & 2 to produce a single block in order to reduce the area penalty. Based on the two new blocks, an alternative initial design is produced (Figure 3.21). Following optimization, a final network is presented as Figure 3.22. This network achieves the unit target and its total cost is 4.7% lower than the cost target. A detailed comparison of the targets and designs is summarized in Table 3.9.

This example illustrates how differing block decomposition results in alternative initial and optimized designs. It may be possible to define a variety of initial block structures. These will produce a variety of final designs which should be investigated to determine the optimal solution.



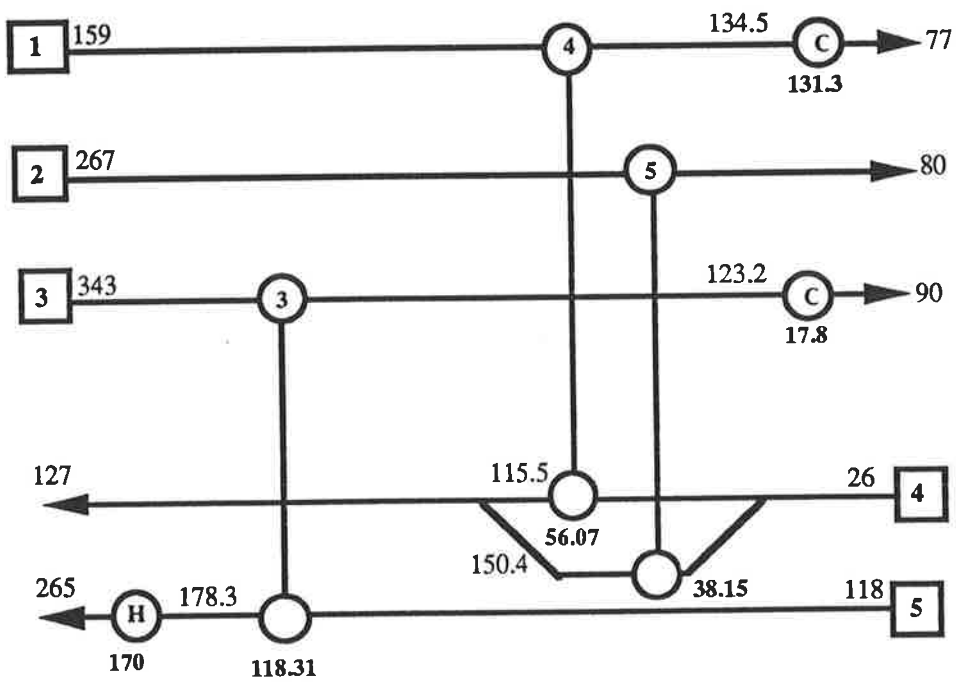
Q_H = 144.3 kW Area = 289 m^2 Total cost = \$46786 yr^{-1}

Figure 3.20: Optimized design 1 for Case Study 2



Q_H = 149 kW Area = 293 m^2 Total cost = \$49603 yr^{-1}

Figure 3.21: Initial design 2 for Case Study 2



Q_H = 170 kW Area = 243 m^2 Total cost = \$46686 yr^{-1}

Figure 3.22: Optimized design 2 for Case Study 2

TABLE 3.9: PERFORMANCE STUDY OF DESIGNS FOR CASE STUDY 2

	Hot Utility kW	Cold Utility kW	Area m^2	Units	Cost $ $annum^{-1}$
Targets HRAT = 30 K	145.7	124.8	299	6	48975
Initial Design 1 (Fig.3.19)	139.4	118.5	320	9	51188
Final Design 1 (Fig.3.20)	144.3	123.4	289	7	46786
Initial Design 2 (Fig.3.21)	149.0	128.1	293	8	49603
Final Design 2 (Fig.3.22)	170.0	149.1	243	6	46686

3.10.3 Case Study 3: The Aromatics Plant

This problem (Table 3.10) has been investigated using the pinch technology (Linnhoff and Ahmad, 1990). The cost data provided by Linnhoff and Ahmad (1990) is employed for comparison. The optimal HRAT equals 25 K. However, Linnhoff used 26 K as the HRAT in their designs. For comparison purposes, this HRAT will be employed in the design study. The composite curves for a HRAT of 26 K are presented as Figure 3.4a.

As mentioned in the example 3 in Section 3.3.1, two blocks are employed for this problem. Block 1 spans the pinch point. Employing the rules and methods discussed previously, two initial designs (Figure 3.4b and Figure 3.4c) were produced. Final optimal designs derived from these networks are presented as Figures 3.23 and 3.24, respectively.

TABLE 3.10 STREAM DATA (CASE STUDY 3)

Stream	Supply Temperature °C	Target Temperature °C	Heat Capacity Flowrate kW K^{-1}	Film Coefficient kW $m^{-2}K^{-1}$
1	327	40	100	0.5
2	220	160	160	0.4
3	220	60	60	0.14
4	160	45	400	0.3
5	100	300	100	0.35
6	35	164	70	0.7
7	85	138	350	0.5
8	60	170	60	0.14
9	140	300	200	0.6
Hot oil	330	250	–	0.5
Water	15	30	–	0.5

COST DATA

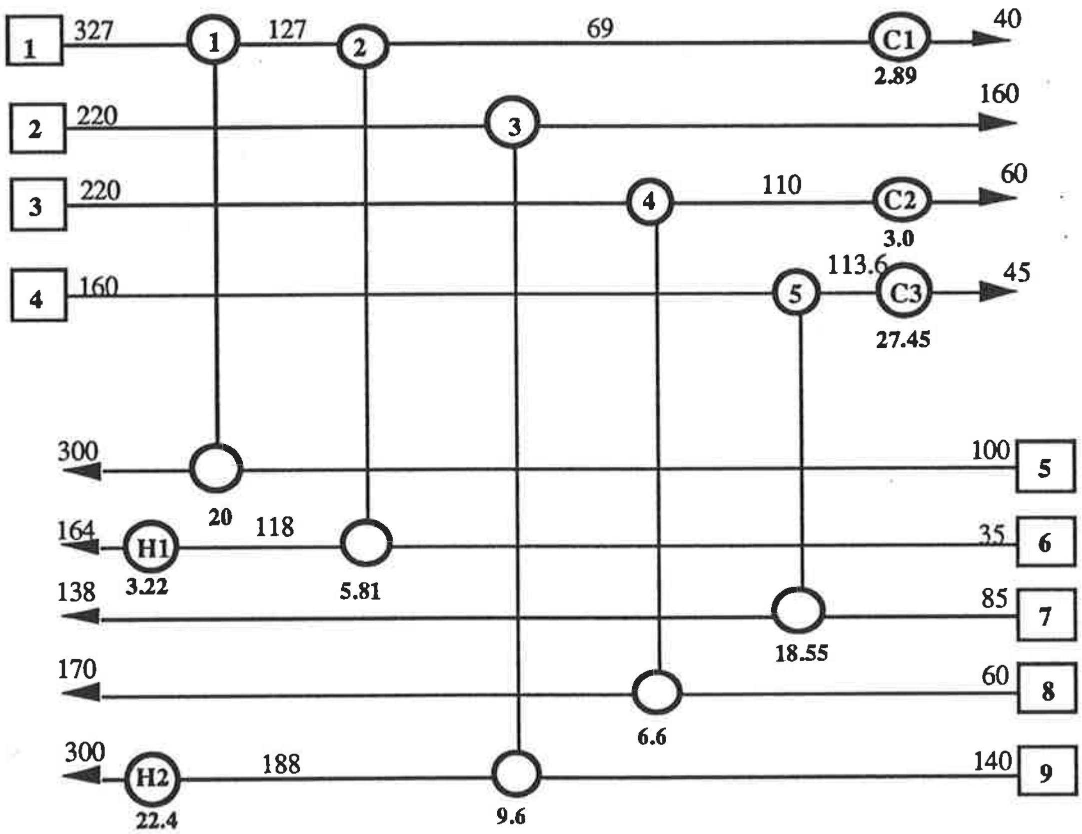
Installed heat exchanger cost: Cost ($) = 10,000 + 350Area ($m^2$)

Plant lifetime = 5 years

Rate of interest = 0 % per annum

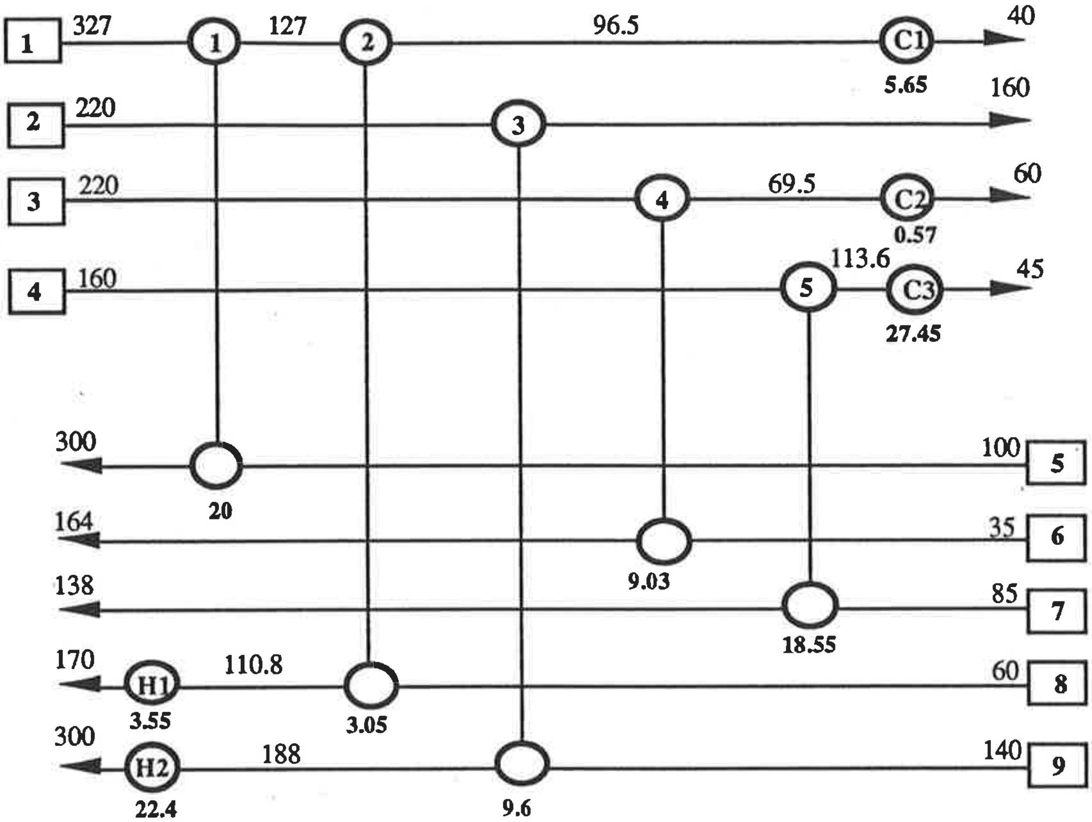
Cost of hot utility = $60 \frac{\$}{kW \cdot yr}$

Cost of cold utility = $6 \frac{\$}{kW \cdot yr}$



Q_H = 25.62 MW Area = 17464 m^2 Total cost = $2.98x10^6 yr^{-1}$

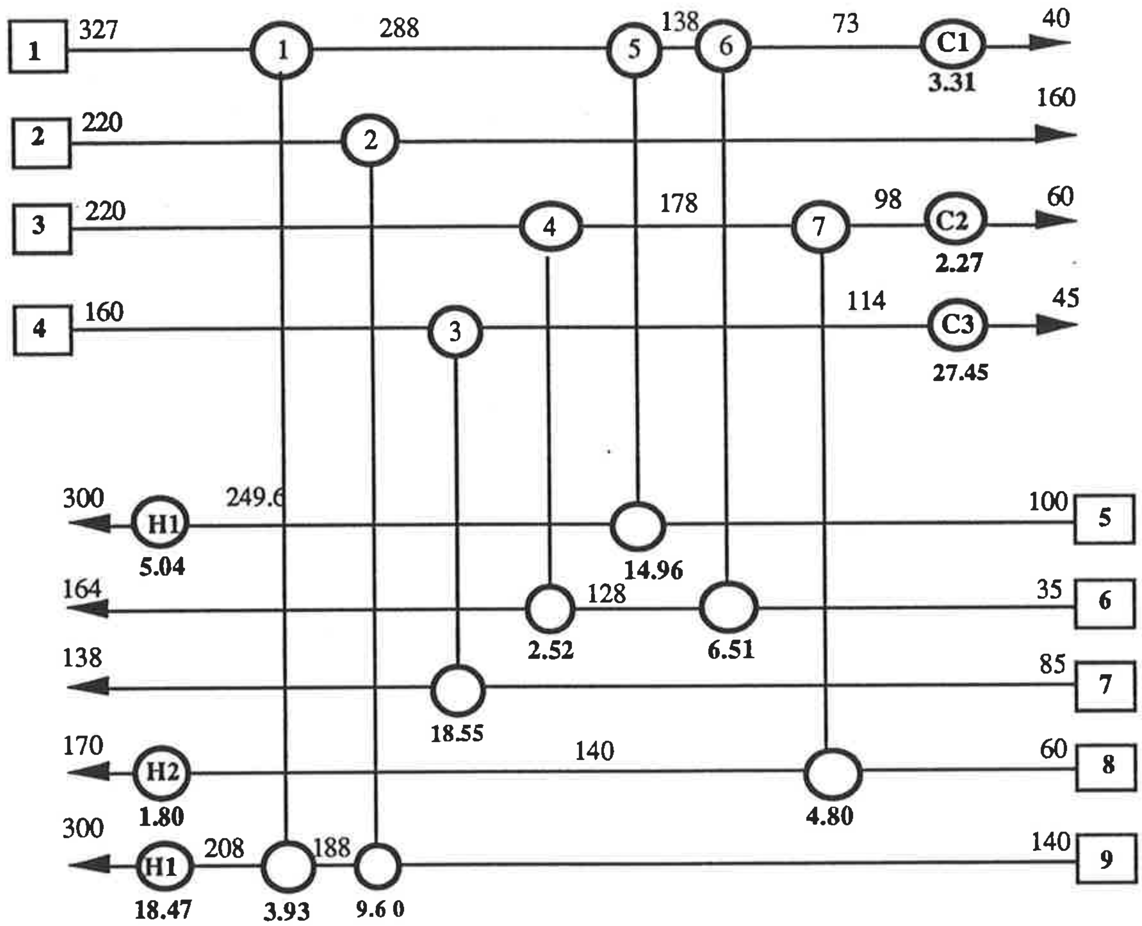
Figure 3.23: Final optimized design 2 for aromatics plant – Case Study 3



Q_H = 25.95 MW Area = 17395 m^2 Total cost = $\$2.99\text{x}10^6\ yr^{-1}$

Figure 3.24: Final Optimized Design 3 for Aromatics Plant –Case Study 3

In Figure 3.24, the dummy heater added to stream 8 is required in the optimal design but the heater on stream 5 is deleted by the optimization process as compared to the network in Figure 3.4c. The designs are compared with the design produced using the improved pinch method (Figure 3.25 – produced by Linnhoff and Ahmad (1990)). This is the optimal final design based on the initial design presented in Figure 3.4d. Both networks (Figures 3.23 and 3.24) produced by the block method satisfy the unit target and achieve a low overall cost. Comparing these two two designs with the pinch design (Figure 3.25), reveals that the pinch design achieves a marginally lower total cost (1% saving) but it employs three more units. If a non-linear cost model is used, then the block designs are likely to be favoured. A comparison between targets and designs is listed in Table 3.11.



Q_H = 25.31 MW Area = 17398 m^2 Total cost = $\$2.96 \times 10^6\ yr^{-1}$

Figure 3.25: Optimized Design 1 for aromatics plant – Case study 3 (Linnhoff & Ahmad, 1990)

TABLE 3.11: TARGETS & DESIGNS FOR CASE STUDY 3

	Hot Utility MW	Cold Utility MW	Area m^2	Units	Cost $/yr
Targets HRAT = 26 K	25.04	32.76	16984	10	$2.91x10^6$
Initial Design 1 (Fig.3.4d) (Linnhoff et al 1990)#	25.04	32.76	17716	17	$2.97x10^6$
Final Design 1 (Fig 3.25) (Linnhoff et al 1990)*	25.31	33.03	17398	13	$2.96x10^6$
Initial Design 2 (Fig.3.4b)	29.30	37.02	15762	11	$3.11x10^6$
Final Design 2 ** (Fig.3.23)	25.62	33.34	17464	10	$2.98x10^6$
Initial Design 3 (Fig.3.4c)	29.20	36.92	16166	10	$3.13x10^6$
Final Design 3 (Fig 24)	25.95	33.67	17395	10	$2.99x10^6$

Linnhoff & Ahmad (1990) did not provide the area calculation for their initial design (Figure 3.4d). This figure was provided by a reviewer for the paper of Zhu et al (1993a).

* Linnhoff and Ahmad (1990) presented the total cost as $2.89x10^6 yr^{-1}$ for the optimized network (Figure 3.25). The authors (Zhu et al, 1993a) were unable to reconcile this value with their calculations. The values for the area and total cost used (17398 m^2 and $2.96x10^6 yr^{-1}$) were provided by the reviewer for the paper of Zhu et al (1993a). The calculation provided by the reviewer required that the hot utility be split for two of the heaters with third in series following the split. This arrangement is not suggested in the paper of Linnhoff and Ahmad (1990). The arrangement is important as it avoids the very low driving force (0.4 K) for the heater on cold stream 5.

** To avoid splitting the hot utility, the heaters in Figures 3.23 and 3.24 are arranged in series.

3.11 Designs Based on Shells

The composite curves represent the widest overall distribution of temperature differences for a set of streams (Nishimura, 1980; Townsend and Linnhoff, 1984). Consequently, any network which can satisfy exactly this temperature distribution in the minimum number of matches is expected to have the minimum number of shells (Ahmad and Smith, 1989). Actually, the number of shells is targeted solely based on the composite curves (Shiroko and Umeda, 1983; Trivedi et al, 1987; Johns, 1987; Ahmad and Smith, 1989). As discussed above, in the block method, the composite curves are approached by block decomposition and quasi–composite curves. As a direct consequence, a network designed by the block method approaches not only the area, energy and unit targets but also the shell target. Again, the energy target at optimal HRAT predicted is relaxed in the design which may provide more flexibility and opportunity to achieve simple network structure while approaching all targets. Following examples show how a network can directly approach all targets with small number of units and shells using the block method.

3.11.1 Case Study 4

This case study is adopted from a realistic petrochemical process which is part of one of the largest aromatics complexes in Europe. This case was originally discussed by Linnhoff et al (1982). More recently, Ahmad and Smith (1989) studied a modified version (Table 3.12) of this problem (which is similar to Case Study 3) using the driving force plot and the remaining problem analysis based on shell considerations.

This problem has four hot process streams and five cold process streams and hot oil and cooling water as hot and cold utilities respectively. As can be seen from Figure 3.26, this problem has a tight composite curves. Ahmad and Smith (1989) pointed out that in cases with tight composite curves, minimum area can become difficult to approach with the minimum number of units. To achieve the units target usually requires each match to satisfy the full enthalpy change for one of its streams (on each side of the pinch). This tick–off heuristic may not be consistent with obtaining a good fit to the driving force plot (Ahmad, 1985). This observation was illustrated and demonstrated by the solution (Figure 3.27) to the problem by Ahmad and Smith (1989).

TABLE 3.12 STREAM DATA (CASE STUDY 4)

Stream	Supply Temperature °C	Target Temperature °C	Heat Capacity Flowrate kW K^{-1}	Film Coefficient kW $m^{-2}K^{-1}$
1	327	30	100	1.0
2	220	160	160	1.0
3	220	60	60	1.0
4	160	45	200	1.0
5	100	300	100	1.0
6	35	164	70	1.0
7	80	125	175	1.0
8	60	170	60	1.0
9	140	300	200	1.0
Hot oil	330	329	–	1.0
Water	15	40	–	1.0

HRAT = 20 K; Xp = 0.90 (ensure minimum $F_T \geq 0.75$); Maximum area per shell = 550 m^2

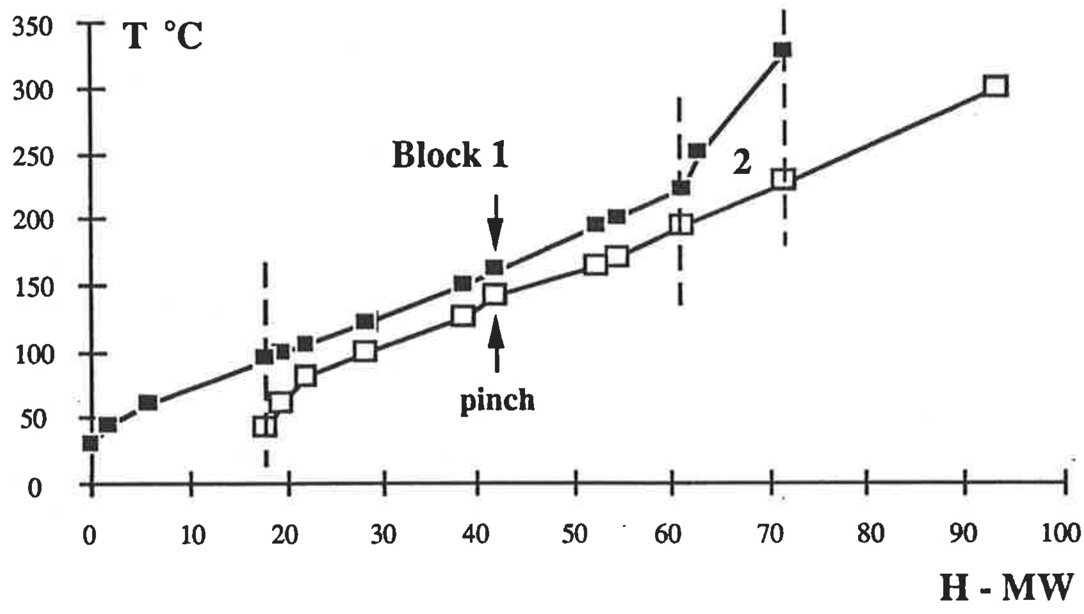
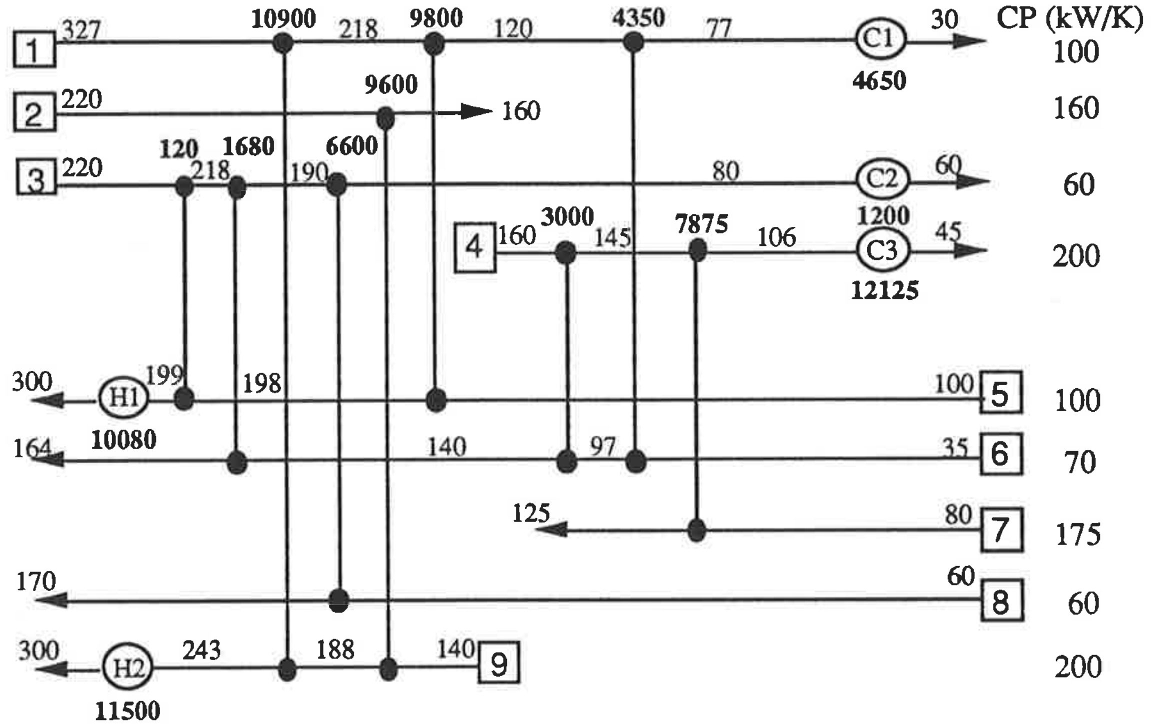


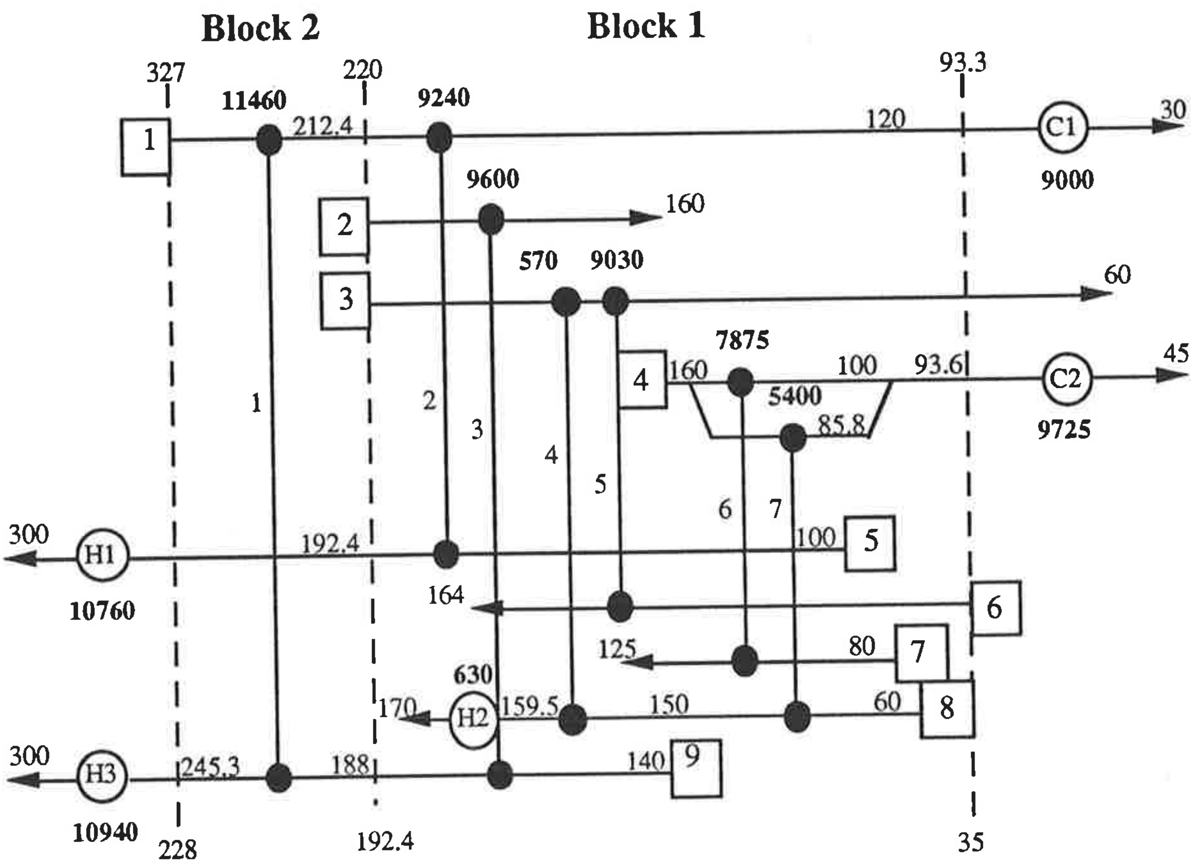
Figure 3.26: composite curves (HRAT = 20 K) for Case Study 4 – tight profiles



Q_H = 21580 kW (0%); $Area_{1\text{-}2}$ = 6537 m^2 (13.3%); shells = 27; Units = 14.

Figure 3.27: Network designed on shell basis by Ahmad & Smith (1989) – Case Study 4

This problem can also be solved by applying the block method and a better solution can be produced. For this problem, two blocks are determined and the pinch is included in the block 1 because the middle of the composite curves displays a rather parallel profile. The initial design (Figure 3.28) based on these two blocks is easily obtained. This network requires 750 kW (3.5%) more hot utility requirement, 696 m^2 (12.1%) more area and 4 shells less than the corresponding targets with only two more units than the unit target. By contrast, the network in Figure 3.27 achieves the energy target and needs 4 less shells than the shell target but requires 767 m^2 (13.3%) more area and 4 more units than the corresponding targets.



Q_H = 22330 kW (3.5%); $Area_{1\text{-}2}$ = 6466 (12.1%); Shells = 27; Units = 12.

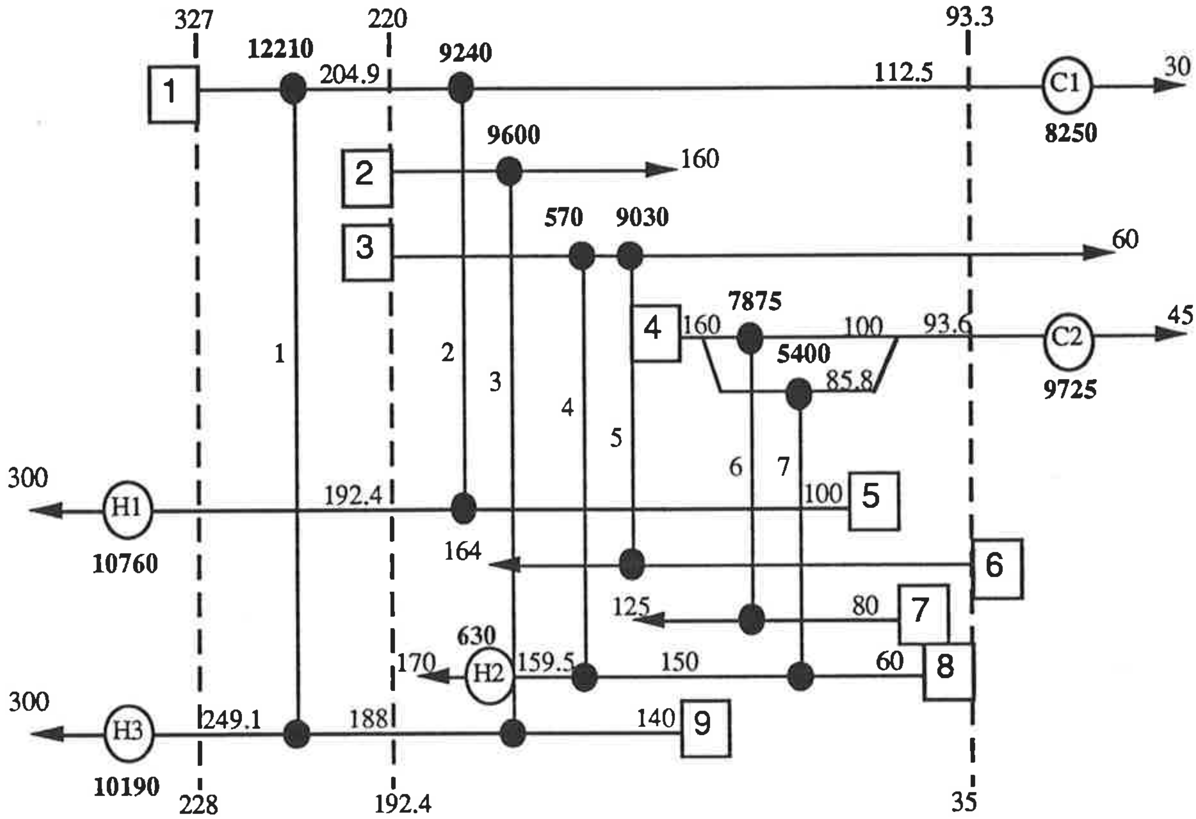
Figure 3.28: Network designed on shell basis – Case Study 4

This case study shows that besides near minimum area requirement, near maximum energy recovery and simple network structure, a low shell requirement is also the feature of the block method. As well, this example reveals an important observation that allowing small energy relaxation provides a great flexibility and opportunity in searching for a simple network while approaching all targets. In comparison, for cases with tight composite curves, with a fixed energy consumption, the situation becomes more severe for finding a simple design . That is one of the reasons why the network (Figure 3.28) obtained by allowing energy relaxation is simpler than that in Figure 3.27 designed with a fixed utility consumption.

To reveal the drawbacks with the constraint of fixed energy for design, the problem is analyzed using the block method with fixed energy constraint. This network (Figure 3.29) is designed with two block decomposition and has identical structure to that in Figure 3.28 but achieves the energy target. However, it requires 1580 m^2 (27.4%) more area than the target and 3 more shells than the network in Figure 3.28. The detail comparison is summarized in Table 3.13. The reason why the network in Figure 3.29 incurs such a large area penalty is related to the improper application of the import/export rule, as some matches benefit from excess driving forces and may themselves require a low number of shells and area, but will cause subsequent matches to have small temperature differences. The large net penalty in area and shells is the result. Thus, when a problem has a severe condition of tight composite curves, one should import or export energy with care. On the other hand, to avoid a large penalty in area and shells while still fixing the energy, a large number of units may be needed since in cases of tight composite curves, the freedom for achieving minimum area design is very much restricted. However, by allowing small relaxation in energy constraint, the severe conditions in driving forces can be improved, while still retaining the benefit of simple structures from the import/export rule.

TABLE 3.13: DESIGN COMPARISON FOR CASE STUDY 4

	Hot Utility kW	Area$_{1-2}$ m^2	Units	Shells
Targets HRAT = 20 K	21580	5770	10	31
Figure 3.27	21580	6537 (13.3%)	14	27
Figure 3.28	22330 (3.5%)	6466 (12.1%)	12	27
Figure 3.29	21580	7350 (27.4%)	12	30



Q_H = 21580 kW (0%); Area$_{1-2}$ = 7350 m^2 (27.4%); Shells = 30; Units = 12.

Figure 3.29: Network designed on shell basis with fixed energy consumption– Case Study 4

3.11.2 Case Study 5

The crude oil preheat train from a Shell refinery in Australia was discussed by O'Neill et al (1989). This problem involves six hot process streams and two cold process streams. The actual heat capacities vary as a function of temperature. In order to handle the real process conditions, the safe side linearization technique proposed by Linnhoff et al (1982) was applied. The stream data and economic bases are presented in Table 3.14. The composite curves are shown in Figure 3.30 which have wide open profiles. The composite curves indicate it is a threshold problem as the fired heater duty (with the furnace having a different costing) has been omitted.

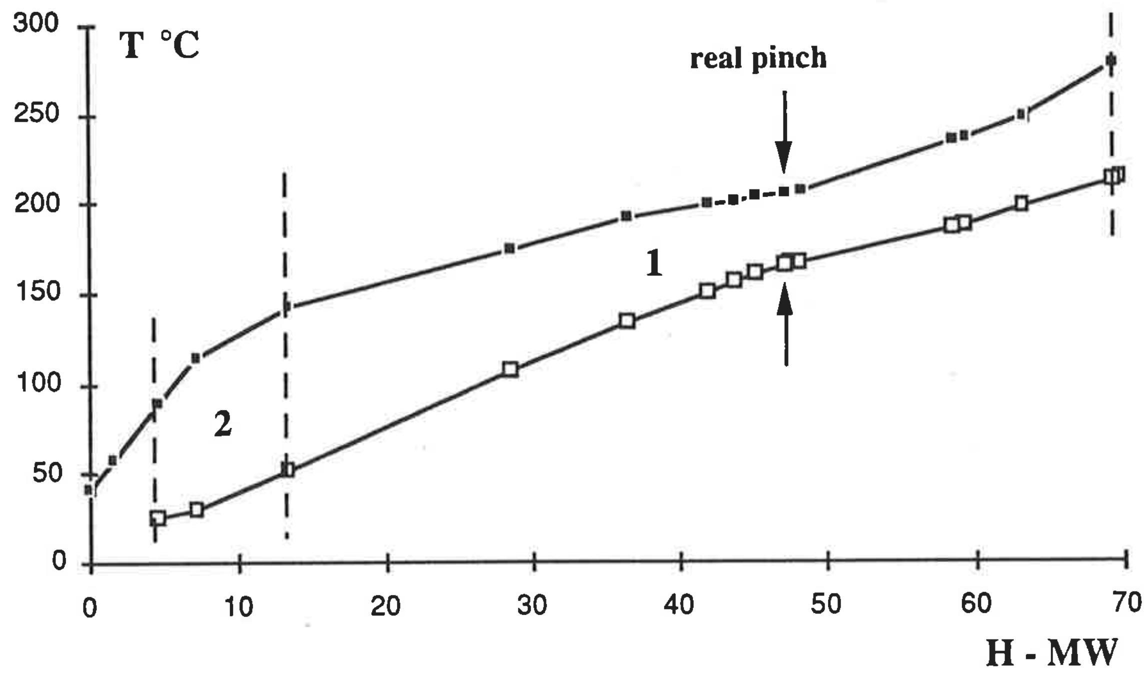


Figure 3.30: Composite curves (HRAT = 40 K) for Case 5 – wide profiles

TABLE 3.14 STREAM DATA (CASE STUDY 5)

Stream	Supply Temperature °C	Target Temperature °C	Heat Capacity Flowrate kW K^{-1}	Film Coefficient kW $m^{-2}K^{-1}$
1	234.0	58.4	53.3	1.5
	58.4	41.0	45.9	1.5
2	207.0	142.0	245.7	2.1
3	203.0	114.7	53.5	1.6
	114.7	41.8	46.3	1.6
4	278.0	191.0	205.2	2.3
5	206.0	199.0	148.2	7.6
6	248.0	114.7	120.9	0.6
7	165.0	187.0	145.5	2.9
8	19.5	106.6	274.4	1.3
	106.6	156.3	307.1	1.3
	156.3	213.4	397.4	1.3
Water	15	25	–	1.05

HRAT = 40 K

Xp = 0.90 (ensure minimum $F_T \geq 0.75$)

Maximum area per shell = 500 m^2

COST DATA

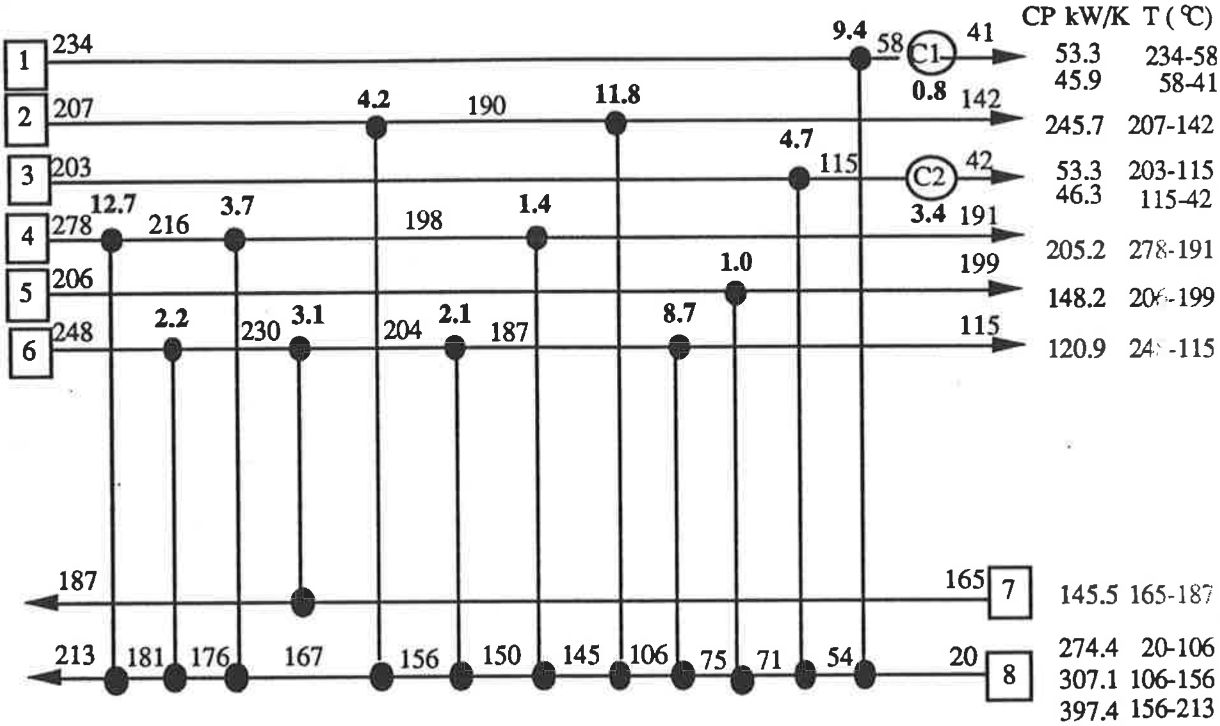
Installed heat exchanger cost: Cost (\$) = 989Area$^{0.6}$ (m^2)

Annual recovery factor = 0.28;

Cost of cold utility = $6.4 \frac{\$}{kW \cdot yr}$

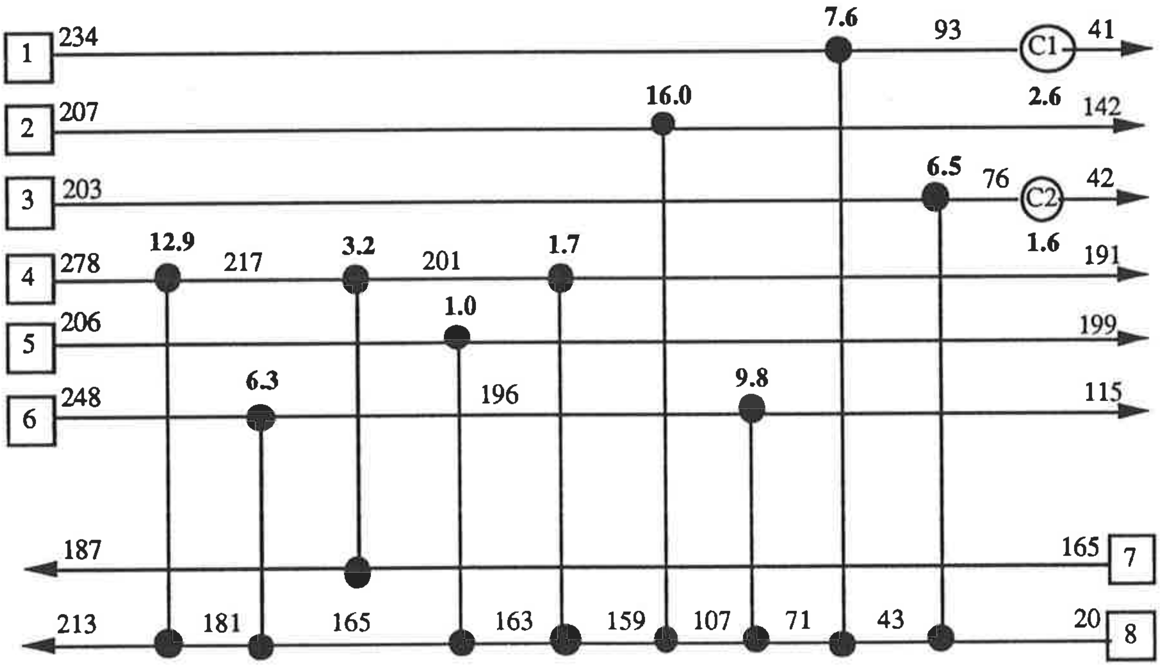
The design (Figure 3.31–O'Neill et al (1989)) based on the dual–approach temperature method (DATM) was generated using HEXTRAN and O'Neill et al (1989) presented their design (Figure 3.32) using pseudo pinch method to compare with the design by DATM in Figure 3.31. Clearly, their design improved on the design by the DATM. Recently, Suaysompol (1991) studied this problem applying the flexible pinch method and presented further improved designs, one (Figure 3.33) obtained by free hand calculation and the other (Figure 3.34) produced using the expert system (FLEXNET).

However, by applying the block method to this problem, the design can be improved. The problem is decomposed with two blocks. Again, the pinch is not used as a block boundary. In each block, there are more hot streams than cold streams, particularly in block 1. As stated in Section 3.8, in situations with tight composite curves and uneven stream population in a block, stream splits may be necessary. However, this problem has wide spaced composite curves and stream split can be avoided even with a fixed energy consumption. The match selection is carried out in a sequential manner according to the rules stated in Section 3.8. For example, the hottest section of the cold stream 8 can be feasibly matched by hot streams 1, 4 and 6. By area assessment for each possible match with a desirable heat load, the match between the hot stream 4 and cold stream 8 has lowest $\frac{A}{Q}$ value and thus this match is selected. This approach applies to the selection of all other matches and the resultant network is shown in Figure 3.35. As pointed out previously, the match selection in the block method is done using area assessment when considering network simplification, so a resultant network usually features low area requirement and simple structure. In the meantime, since a close approach to the composite curves is embedded in block determination, the low shell requirement is implied automatically. For this problem, the network shown in Figure 3.35 has the lowest number of shells and units and a lowest total cost either on a unit basis or a shell basis compared to the other designs presented above. The detail comparison is summarized in Table 3.15.



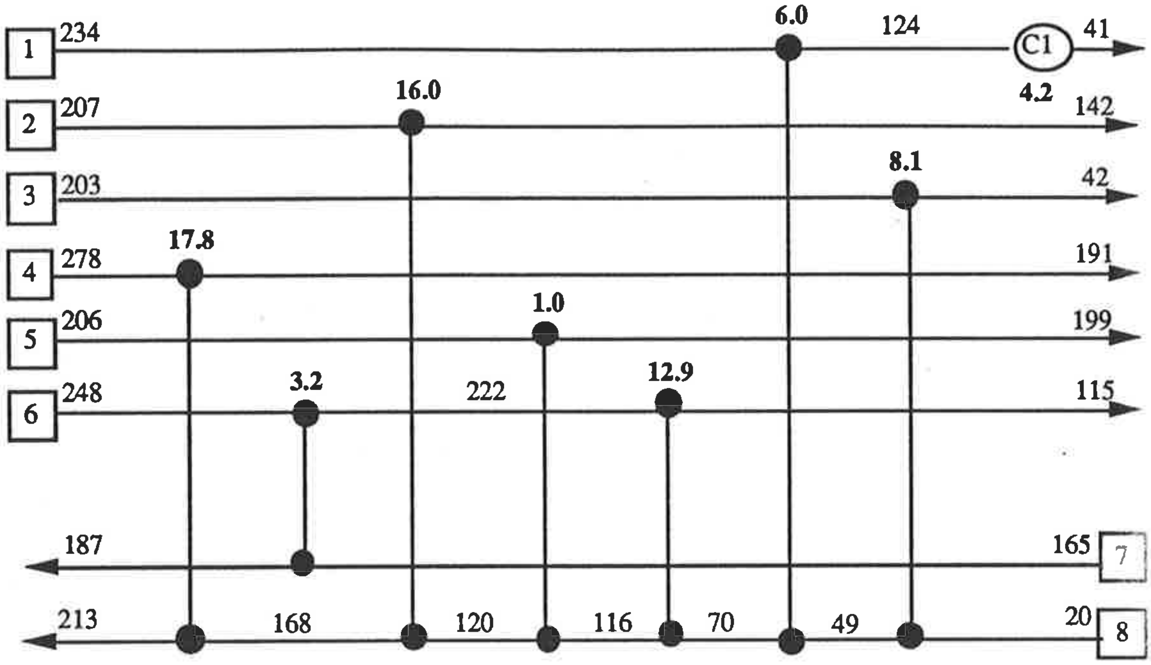
Q_H = 4.2 MW; $Area_{1\text{-}2}$ = 2359 m^2; Shells = 15; Units = 14;
Total cost (unit) = 105 k\$/yr; Total cost (shell) = 107 k\$/yr.

FIGURE 3.31: Dual Approach Temperature Design using HEXTRAN for Case Study 5 (O'Neill et al, 1989)



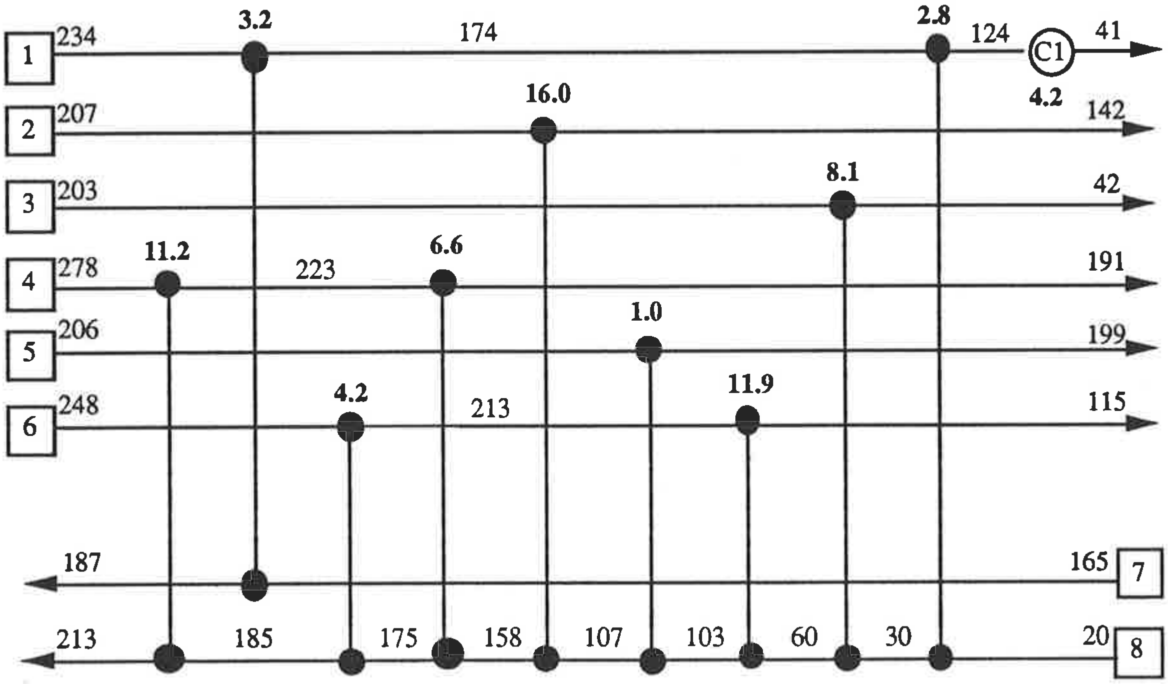
Q_H = 4.2 MW; $Area_{1\text{-}2}$ = 2252 m^2; Shells = 12; Units = 11;
Total cost (unit) = 96 k\$/yr; Total cost (shell) = 100 k\$/yr.

FIGURE 3.32: Pseudo Pinch Design for Case Study 5 (O'Neill et al, 1989)



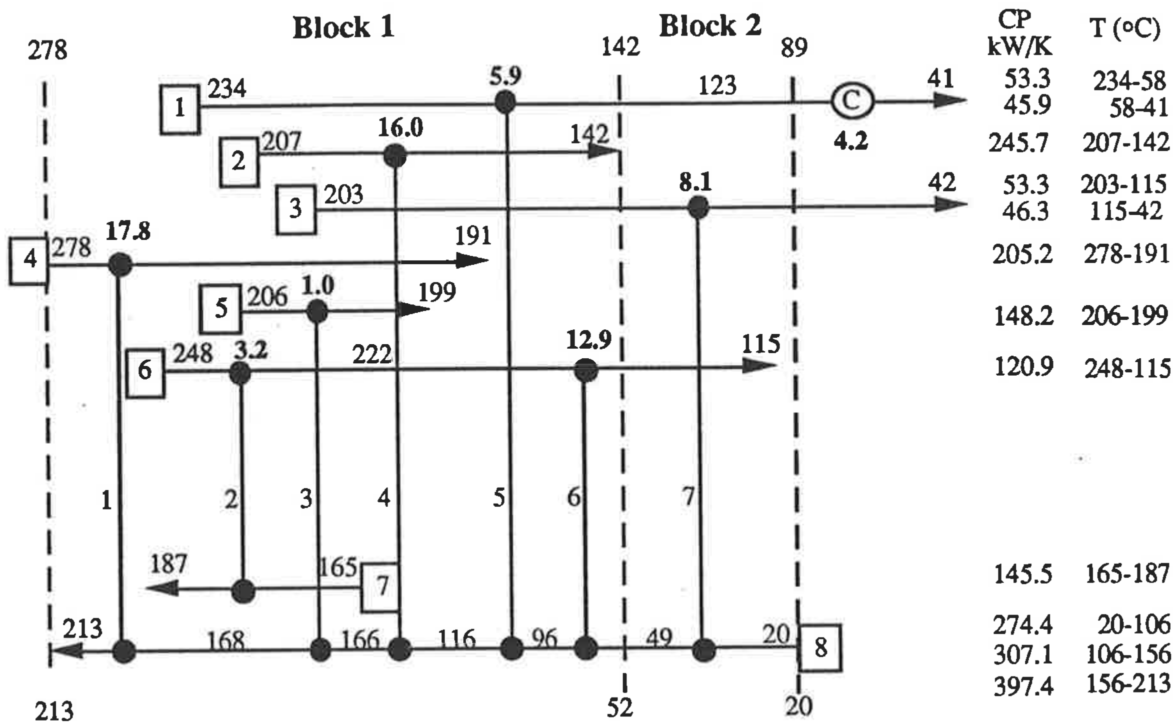
Q_H = 4.2 MW; $Area_{1-2}$ = 2476 m^2; Shells = 12; Units = 8;
Total cost (unit) = 89 k$/yr; Total cost (shell) = 104 k$/yr.

FIGURE 3.33: Flexible Pinch Design for Case Study 5 (Suaysompol, 1991)



Q_H = 4.2 MW; $Area_{1-2}$ = 2231 m^2; Shells = 13; Units = 10;
Total cost (unit) = 94 k$/yr; Total cost (shell) = 102 k$/yr.

FIGURE 3.34: Flexible Pinch Design using FLEXNET for Case Study 5 (Suaysompol, 1991)



Q_H = 4.2 MW; $Area_{1-2}$ = 2283 m^2; Shells = 11; Units = 8;
Total cost (unit) = 87 k\$/yr; Total cost (shell) = 98 k\$/yr.

FIGURE 3.35: Block Method Design for Case Study 5

TABLE 3.15: DESIGN COMPARISON FOR CASE STUDY 5

	Energy (MW)	$Area_{1-2}$ (m^2)	Units	Shells	Total cost (unit) k\$/yr	Total cost (shell) k\$/yr
Targets HRAT=40K	4.2	1927	8	12	89	97
DATM (Fig.3.31)	4.2	2359	14	15	105	107
PPDM (Fig 3.32)	4.2	2252	11	12	96	100
FPDM (Fig 3.33)	4.2	2476	8	12	89	104
FPDM (Fig 3.34)	4.2	2231	10	13	94	102
BDM (Fig 3.35)	4.2	2283	8	11	87	98

3.12 Conclusions and Discussions

A number of useful new concepts namely blocks, quasi–composites and the matching matrix have been introduced. They provide excellent tools for designing networks featuring near–minimum network area and small numbers of units and shells. The design process is based upon information about the area penalty (benefit) or area requirement for all matches. The effect of an individual match on total area can be rapidly deduced and the influence of simultaneous matches on total area can be considered. Since the area penalty (benefit) or area requirement for any match can be calculated, the method provides a rigorous and deterministic guide for approaching the area target in general network design. Since the cost target is obtained from the area, units or shells and utility targets, cost optimal networks normally closely approach these targets.

The block concept provides an efficient method for approaching the area and utility targets. Network simplification is achieved by use of the 'tick–off' rules, and the import/export rules as well as the use of blocks. The initial network obtained using the proposed method may contain more units than the unit target. This network can then be evolved and optimized using conventional NLP. The final design parameters locate the optimal network which may be a subset of the initial structure (i.e. some initial matches may carry zero heat loads after optimization). As a result, a network closely approximating the cost target is achieved. In summary, the concept is simple to understand, readily implemented and it yields a low cost and simple solution.

When the exchanger capital cost exponent is close to unity, little reduction in annual cost can be achieved during the optimization phase as the cost optimization, in this case, is not sensitive to unit numbers. However, greater benefits can be shown when a network cost exponent is smaller. In such situations, there is more potential for cost reduction through network simplification. The assumption of identical distribution of heat transfer area in the network cost targeting program is an over–simplification. To avoid this possible problem, a more rigorous cost target model (see Chapter 5) can be employed. This should yield a cost target taking into consideration the reality of a network associated with a cost target and incorporating practical constraints, including constrained matches, no stream splits and specified number of units allowed for a network etc.

At present, the method does not systematically consider streams with significantly different film heat transfer coefficients. However, the method can be extended to cope with this difficulty by considering the individual stream ΔT contribution as proposed by Rev and Fonyo (1991). The main idea is to shift stream temperatures using individual ΔT contributions, the composite curves from the modified stream temperatures are processed using blocks, quasi–composites and the matching matrix and the design is guided by area calculations. The detailed analysis and development of the extended block method is given in Chapter 4.

CHAPTER 4

EXTENSION OF THE BLOCK METHOD FOR CASES OF UNEQUAL FILM COEFFICIENTS

SUMMARY

A new approach (Zhu et al, 1994) has been developed for the synthesis and design of heat exchanger networks featuring streams with variable film heat-transfer coefficients. The methodology couples the new block method (Chapter 3; Zhu et al, 1993a) with the concept of individual stream ΔT contributions as introduced by Rev and Fonyo (1991). It generates improved solutions to problems involving unequal film coefficients compared with currently available methods.

In this new approach, different stream structures can be screened and compared prior to detailed design. This enables the designer to determine an attractive stream structure featuring low area for subsequent analysis. Potentially good matches are readily identified and topology traps can be effectively avoided. As a consequence, good initial designs are generated and available for subsequent cost optimization using non-linear programming. The likelihood of identifying a globally optimal design is substantially increased.

4.1 Introduction

In Chapter 3, an efficient new method for synthesis of heat exchanger networks using area-targeting principles is presented. The method is known as the 'block' method. The key feature of an initial design generated using this procedure is the close approach to both the energy target and the area target coupled with a small number of units. After cost optimization, the network is easily evolved to a final network with near-optimum total cost and with the number of units close to the units target.

The initial development of the block method focussed on problems involving streams with constant or similar film heat transfer coefficients. The case for the synthesis for streams possessing significantly different film coefficients was not systematically addressed. However, the block method can be readily extended to this situation. The diverse-pinch concept pioneered by Rev and Fonyo (1991) has been employed to determine the ΔT-contributions resulting from the differing film coefficients. The streams in the initial problem are then shifted by their respective ΔT-contributions and a new set of composite curves are generated. The block method is then applied to these modified curves to synthesize an initial network. In this manner, the differences in the stream film coefficients can be exploited and initial networks featuring a low area requirement and small number of units are readily devised.

In this new approach, different stream structures can be screened and compared prior to detailed design. This enables the designer to determine an attractive stream structure featuring low area for subsequent analysis. Potentially good matches are readily identified and topology traps can be effectively avoided. As a consequence, good initial designs are generated and available for subsequent cost optimization using non-linear programming. The likelihood of identifying a globally optimal design is substantially increased.

4.2 Review of Related Works

The general approach for dealing with different film coefficients was suggested by Nishimura (1975, 1980). According to Nishimura, such a system can achieve the minimum area requirement if the temperature differences are related to the overall heat transfer coefficients as follows:

$$(T_1-t)\sqrt{U_1} = (T_2-t)\sqrt{U_2} = \cdots = (T_n-t)\sqrt{U_n} \tag{4.1}$$

where t = temperature of the single stream of one type (hot or cold).
T_j = temperature of stream j of the other type (cold or hot).
U_j = overall heat transfer coefficient between T_j and t.

Unfortunately, equation (4.1) is only applicable when considering potential matches of a single hot (or cold) stream with a number of cold (or hot) streams. Based on this work, a general design heuristic for match selections was proposed by Umeda et al (1978), namely: energy should be exchanged between streams possessing the closest film coefficients. This heuristic avoids an excessive area penalty associated with a mismatch of streams with widely-differing film coefficients. The rule provides no guide as to selection of the best matching between streams with similar film coefficients and can lead to sub-optimal solutions.

Townsend (1989) extended Nishimura's result to the case of multiple hot streams matching multiple cold streams by defining stream individual "ΔT-contributions" as follows

$$\Delta T_i \sqrt{h_i} = \text{constant} = \alpha \tag{4.2}$$

where ΔT_i = the ΔT-contribution from the stream i.
h_i = film coefficient of the stream.

This study provided the basis of the approach adopted by Ahmad et al (1990). In their work, α is defined such that the ΔT-contributions maintain the energy balance at the shifted enthalpy boundary and the set of linear equations are formulated as

$$\Delta T_j \sqrt{h_j} = \alpha \qquad j = 1 \cdot\cdot S_i$$
$$\sum_{j=1}^{S_i} CP_j\,(\Delta T_j - \Delta T_k) = 0 \tag{4.3}$$

where S_i = the number of streams at the ith enthalpy interval boundary.
CP_j = heat capacity flowrate of stream j.
k = the stream responsible for the ith boundary.

The ΔT-contributions calculated from equation (4.3) are used only at the pinch interval provided that the composite curves do not closely approach each other elsewhere. Otherwise, they are also adopted at those enthalpy intervals possessing small temperature differences. Based on individual stream shifts determined as above, Ahmad (1985) proposed a pseudo-BATH formula and it was demonstrated that this approach normally provides a lower prediction of the area target.

However, Rev and Fonyo (1991) argued that the extrapolation of Nishimura's results to general problems involving multiple heat sources and sinks was questionable and concluded that the determination of ΔT-contributions using equation (4.3) was ambiguous.

To avoid this ambiguity in determining ΔT-contribution and to preserve the ΔT-contribution for each stream, Rev and Fonyo proposed a new approach (the diverse pinch). The ΔT-contribution for stream i was defined by:

$$\Delta T_i = \kappa h_i^{-z} \qquad z \in [0.5, 1.0] \tag{4.4}$$

Hot or cold streams are vertically shifted by subtracting or adding a ΔT correction based on equation (4.4) and then cascading is performed to determine κ which fulfils the same role as the uniform HRAT. A modified set of composite curves is generated from the individually-shifted streams.

Clearly, equations (4.3) and (4.4) will provide different individual ΔT-contributions. The main difference between these two approaches is that the diverse pinch approach applies individual shifting at the very beginning while the Ahmad's method applies individual shifts at a latter phase of the design while maintaining the original (uniform) pinch and corresponding vertical intervals. The diverse pinch approach results in the unambiguous treatment of the diversity problem (Rev and Fonyo, 1993). In this study, the diverse-pinch approach is adopted. The major advantage of equation (4.4) is that no ambiguity exists in the determination of ΔT contribution and that coding into a targeting program is straightforward. It should be noted that equation (4.4) for z = 1.0, is based on the concept of a minimum heat flux (Fraser, 1989a), an idea derived from and demonstrated by industrial practice (Fraser, 1989b). The objective of Fraser's work was to avoid the need for multi-variable optimization, when considering individual ΔT–contributions, by using the minimum heat flux as the global variable (the minimum heat flux Q_{minf} is related to the κ with $\kappa = 2Q_{minf}$). The ΔT_{min} concept was usefully extended by Colbert (1982) and subsequent workers, it seems probable that a single value for the minimum heat flux should not be used as an absolute constraint for all streams. Therefore in order to increase the search space, both κ and z, are regarded as variables whose optimum values are to be determined at the targeting stage so long as the combination of κ and z satisfies the thermodynamic conditions. As will be shown, the extra freedom so allowed by this choice, does allow a greater range of possible stream structures to be examined. This makes it more probable that one of the best possible structures can be chosen as the starting point for the design. Network design is then based on the set of composite curves corresponding to these parameters. The network is then produced using the block method (Chapter 3; Zhu et al, 1993a).

4.3 Motivating Example

Gundersen and Grossmann (1990) demonstrated that the heat transfer area may be affected significantly when the film coefficients vary considerably. This is typically the case in plants possessing a mixture of liquid and vapor streams, where it is common to have from one to two orders of magnitude difference in film coefficients. They employed a simple example (Table 4.4 in Case Study 2) to reveal the drawbacks of using a single uniform ΔT_{min} or HRAT for synthesis when film coefficients vary considerably. Applying the PDM to this problem produces the vertical design illustrated in Figure 4.1.

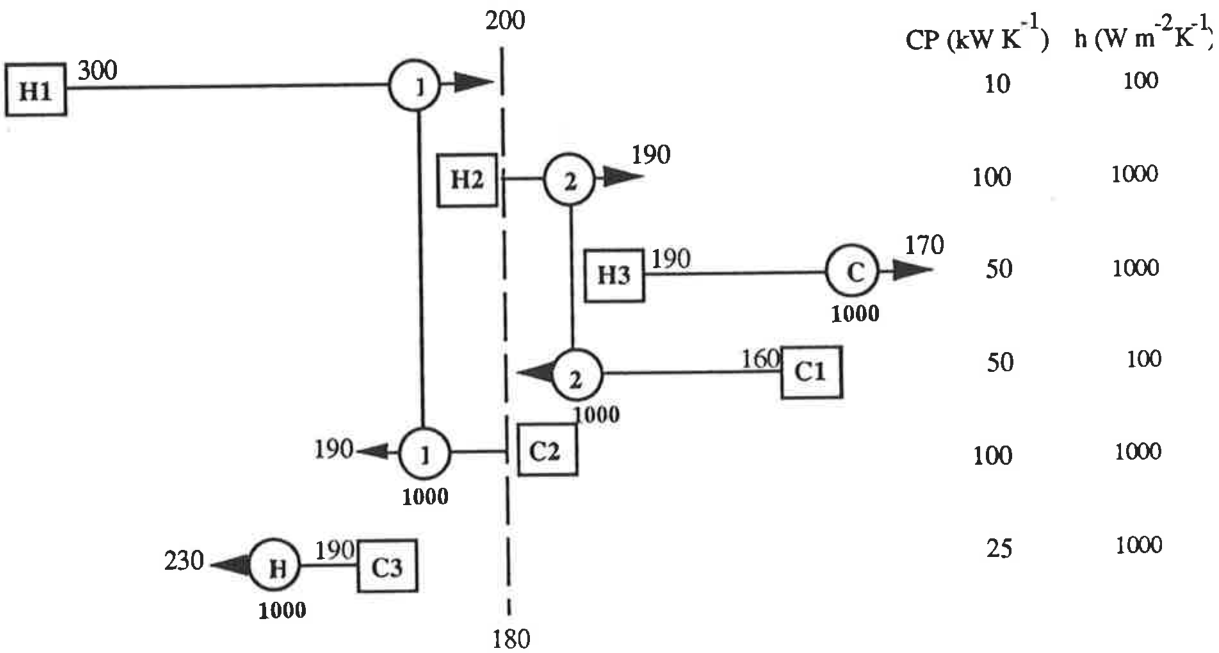


Figure 4.1: Pinch design with HRAT = 20°C
(Gundersen and Grossmann, 1990)

The PDM will always produce vertical designs at the pinch, due to its strict pinch decomposition. Normally, however, criss-crossing is introduced away from pinch by employing the 'tick-off' heuristic which is employed to minimize the number of units. In this case, the strict vertical design is the only feasible four-unit design when using a uniform ΔT_{min} (HRAT) of 20 K (Gundersen and Grossmann, 1990). Clearly, there is no possibility for H1 (low h) to match with C1 (low h) and H2 (high h) to match with C2 (high h) as H1 and C2 are located above pinch whilst H2 and C1 appear below pinch.

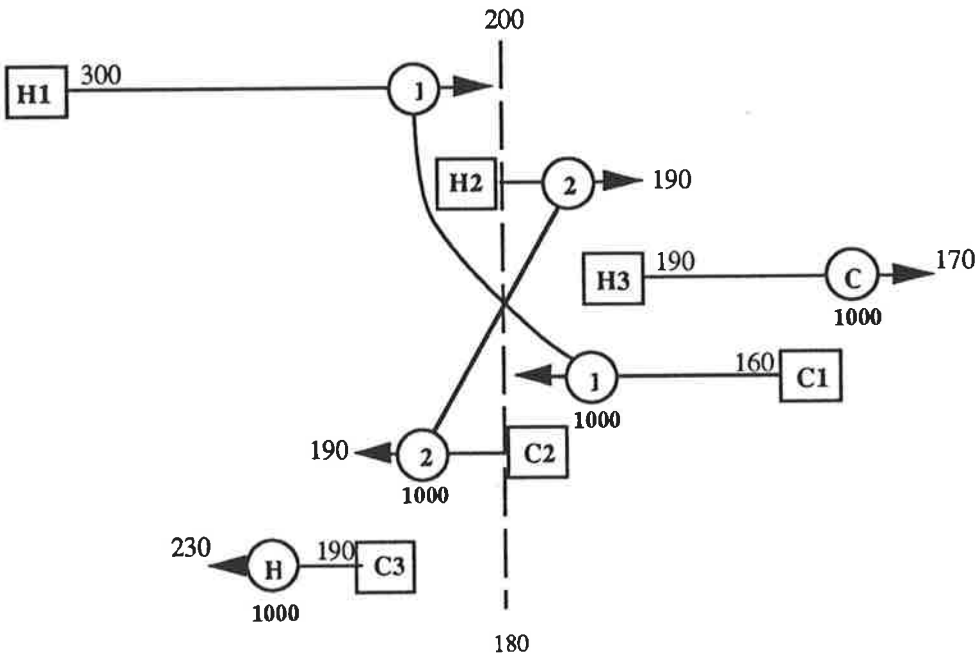


Figure 4.2: Criss-cross design with HRAT = 20°C
(Gundersen and Grossmann, 1990)

However, permitting heat transfer across pinch provides the optimal design of Figure 4.2 which includes matches of H1-C1 and H2-C2. These two matches follow the general rule: "Match streams with *low film coefficients* in order to isolate area deterioration" (Umeda et al, 1978, Ahmad, 1985). The criss-cross design is superior in both area (27.5% less) and cost (20% less). Therefore, Gundersen and Grossmann suggested that a better design may be found by systematic criss-crossing through the pinch point. The violations of the pinch rule in the two directions are balanced; hence no extra energy is needed.

Rev and Fonyo (1991) noted that this systematic violation can be extremely complicated in complex cases and suggested that it is unnecessary if the effect of different film coefficients can be considered at the early stage of design.

In this work, the difference of film coefficients is accounted for at the targeting stage and it results in an optimal stream-shifting scheme. The effect of matches is taken into account at the design stage by employing the block method. The following two sections address these two issues respectively.

4.4 Total Cost Targeting – Searching for Optimal κ and z

Rev and Fonyo (1991) proposed the following formula (diverse Bath formula) to estimate the minimum area requirement for the shifted composite curves:

$$A_{min} = \sum_{k}^{interval} \frac{1}{\Delta T_{lm_k}} \sum_{j} \frac{q_j}{h_j} \tag{4.5}$$

where the log mean temperature difference ΔT_{lm_k} is calculated from the mean temperature differences ΔT_m at borders of kth enthalpy interval as:

$$\Delta T_m = \Delta T_{sf} + \frac{1}{q_k} \sum_{j} |q_j \Delta T_{j,sf}| \tag{4.6}$$

where ΔT_{sf} is the temperature difference between shifted hot and cold composite curves at the border of the kth interval,

$\Delta T_{j,sf}$ is the individual ΔT shift contribution of stream j,
q_k is the sum of heat loads from streams of one type (i.e. hot or cold)
and q_j represents the heat load of the stream j in the interval.

An alternative approach is to formulate the minimum area calculation as a LP problem as follows:

$$A_{min} = \textbf{minimize} \sum_{k}^{interval} \sum_{all\ i\ \&\ j} \frac{Q_{ijk}}{\Delta T_{lm_{ijk}} U_{ij}} \quad (4.7)$$

where Q_{ijk} is the heat load between ith hot stream and jth cold stream in the kth interval,
U_{ij} is the overall heat transfer coefficient between the ith hot stream and the jth cold stream.
and $\Delta T_{lm_{ijk}}$ is the logarithmic temperature difference of this match in kth interval.

Q_{ijk} and $\Delta T_{lm_{ijk}}$ can be expressed by following simple balance equations:

$$(T_{1i,k} - T_{2i,k})\, CP_i = \sum_j Q_{ijk} \quad (4.8a)$$

$$(T_{1j,k} - T_{2j,k})\, CP_j = \sum_i Q_{ijk} \quad (4.8b)$$

$$\Delta T_{lm_{ijk}} = \frac{(T_{1i,k} - T_{1j,k}) - (T_{2i,k} - T_{2j,k})}{\ln\left[\dfrac{(T_{1i,k} - T_{1j,k})}{(T_{2i,k} - T_{2j,k})}\right]} \quad (4.8c)$$

where CP_i and CP_j are the capacity-flow rates of the hot and cold streams, respectively.
$T_{1i,k}$ and $T_{2i,k}$ are the shifted border temperatures of the ith hot stream in the kth interval.
$T_{1j,k}$ and $T_{2j,k}$ are the shifted border temperatures of the jth cold stream in the kth interval.

Equation (4.7) normally provides a more precise area estimate than equation (4.5). However, its complexity renders it impractical to implement in a targeting program as a set of linear equations is required for each enthalpy interval. Hence, the simpler equation (4.5) is used to estimate minimum area and the capital cost can be calculated based on the cost data provided. It has been demonstrated by Rev and Fonyo (1991) that the minimum area calculation using the diverse Bath formula (equation (4.5)) is at least as good as that obtained by employing the Bath formula (Townsend and Linnhoff (1984)) for problems with unequal film coefficients.

Rev and Fonyo (1991) found that the effect of exponent z on the minimum area calculation to be slight and they suggested that z be fixed at unity. In this study, the areas for different z based on same energy consumption varied by approximately 10%. This difference is small but it probably should be considered. As well, changes in z affect the stream structures prior to design. This effect may provide opportunities for the discovery of very simple networks which approach the area target. This matter will be discussed in detail in Section 4.5.2. Therefore, z remains as an optimization variable. The range of feasible values for κ and z are defined such that their values are sufficient to make a stream shift feasible i.e. no overlap permitted on the shifted composite curves. The z bounds are set such that $0 < z \leq m$. Values greater than m will render the shift infeasible. Typically, m is less than 2.

With the minimum area calculated by using equation (4.5), the total cost target can be calculated based on the cost data provided. Thus, for a fixed z, a curve of total cost (energy + capital) versus κ can be deduced and the optimal κ determined (κ_{opt}). This procedure may be repeated for the set of z's providing a set of associated optimal κ_{opt}'s. If the total costs corresponding to the set of κ_{opt}'s differ significantly, the globally-optimal κ_{opt} and z providing the lowest cost are selected (Figure 4.3a) and used to calculate the ΔT-contributions for streams. The composite curves defined using these two optima form the basis for network synthesis. In some cases, the total costs associated with the set of κ_{opt}'s exhibit only marginal differences. The cost curves from the example (Table 4.1) show this feature (Figure 4.3b). For such situations, one needs to investigate the variations in stream structures and select κ and z values which provide the simplest initial stream structure. Normally, a simpler initial stream structure yields a simple initial network which may be subsequently optimized to an improved final design.

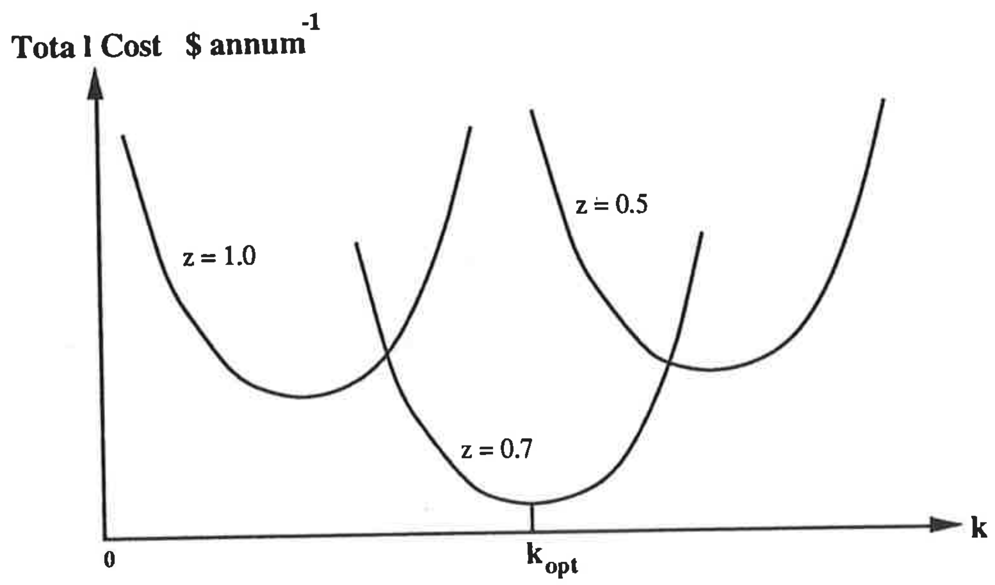


Figure 4.3a: A family of cost curves

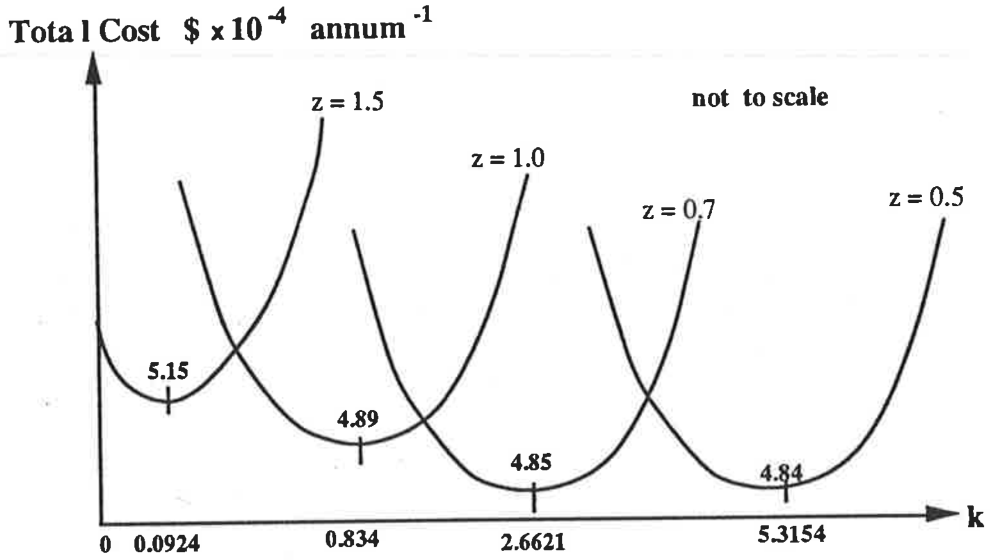


Figure 4.3b: The family of cost curves (not to scale) for the example (Table 4.1)

The optimal energy consumptions differ considerably between the simple vertical model (Bath formula of Townsend and Linnhoff (1984)) and diverse Bath model (equation (4.5)) for the area target. Consider the example (Table 4.1) presented for illustration. Targeting using the vertical model produces an optimal HRAT of 30 °C with a minimum hot utility of 145.7 kW and a total cost target of 48975 \$/yr based on the assumed cost data. By contrast, if one uses the individual ΔT-contributions, the optimal κ equals 5.3154 when $z = 0.5$ with the minimum hot utility of 167.0 kW which is corresponding to a uniform HRAT = 38 °C and a total cost target of 48393 \$/yr. Clearly, for $z = 0.5$ the optimal minimum approach temperatures differ by 8 K. Furthermore, the optimal energy consumptions predicted when z is varyed may also differ. Changing z to 1 alters the optimal energy consumption to 161.2 kW for the hot utility and 140.3 kW for the cold utility. This consumption corresponds to a uniform HRAT = 36 °C. As well, the corresponding total cost target is changed to 48915 \$/yr. In this case of $z = 1.0$, the minimum heat flux can be calculated as suggested by Fraser (1989a). As the optimal $\kappa = 0.834$ kW/m^2, it is equivalent to the minimum heat flux of 417 W/m^2 ($Q_{minf} = (0.834 \times 1000)/2 = 417$ W/m^2).

Table 4.1: Stream data for example 1

Stream	T_s °C	T_t °C	CP kW K^{-1}	h W $m^{-2}K^{-1}$
H1	159	77	2.285	100
H2	267	80	0.204	40
H3	343	90	0.538	500
C1	26	127	0.933	10
C2	118	265	1.961	500
Steam	300	300		50
CW	20	60		200

Cost Data:

Cost of hot utility: \$110 $kWyr^{-1}$; Cost of cold utility: \$10 $kWyr^{-1}$;

Exchanger cost model: \$ = 3,800 + $750A^{0.83}$;

Plant life: 6 yr; Interest rate: 10%.

These observations suggest that during the targeting stage, the optimal values of κ and z must be located in a family of cost profiles. This procedure contradicts the suggestion by Ahmad et al (1990), who observed that while the capital costs calculated by the simple vertical model (Townsend and Linnhoff, 1984) and the linear programming model (equation (4.3)) may differ, the optimum ΔT_{min} (HRAT) remains roughly constant. They recommend that the optimum ΔT_{min} (HRAT) be calculated using the simple vertical model.

The previous code for targeting using the vertical model was written using object-oriented programming techniques and has been re–used in this instance. The efficiency of the search techniques to find global optimal κ and z was improved by adopting a one-dimensional search strategy. First, for a fixed initial value of z, a small interval containing the optimal κ is identified by a rough pattern search. The exact optimal κ is then located using the Fibonacci algorithm. This procedure is then repeated for varying z (range specified by user) to locate the globally optimal values of κ and z. As a consequence, the searching process for global optimal κ and z is rapid (approximately one minute on IBM 386 PC).

4.5 Synthesis for Handling Unequal Film Coefficients

4.5.1 The Block Decomposition

The composite curves based on the individual ΔT contributions form the basis for synthesis using the block method. The composite curves corresponding to the globally optimal values of κ and z, can be decomposed into a number of blocks using the method suggested in Chapter 3. After block decomposition, the temperatures of the hot streams and cold streams are adjusted at all block boundaries using their ΔT-contributions . The method is illustrated using an example stream data by Rev and Fonyo (1991) who modified the original data of Ahmad et al (1990) which is given in Table 4.1. This data does contain some inconsistencies, such as the uneconomically high temperature for steam and low film coefficients for both steam and cooling water, but is used uncorrected, so that comparisons may be made with the results of these other workers.

Figure 4.4 presents the shifted composite curves derived after targeting using the diverse pinch approach. The optimal values of κ and z are 5.3154 and 0.5, respectively. The utility requirements are hot utility = 167 kW and cold utility = 146.1 kW. Three blocks can be defined as shown on Figure 4.4. The block-boundary temperatures are then shifted using equation (4.4) and Figure 4.5 summarizes the resulting stream structure after stream shifting. Clearly, energy is balanced in each block but the border temperatures for streams of one type (hot or cold) differ. Hot or cold streams possessing low (high) film coefficients have high (low) temperatures. This implies that streams with poor transfer potential are matched at larger ΔT (and vice versa). Boundary temperatures of one type (hot or cold) though not identical are equivalent when the differences in film coefficients are accounted for.

These adjustment ensure a network with reduced area.

Following block decomposition, synthesis may be undertaken block by block. If the matches are constrained within each block, a minimum area network may result but the network structure will be complex. To simplify the network structure, the import/export rule can be invoked and a set of improved matches can be selected following the area-targeting principles outlined previously in Chapter 3.

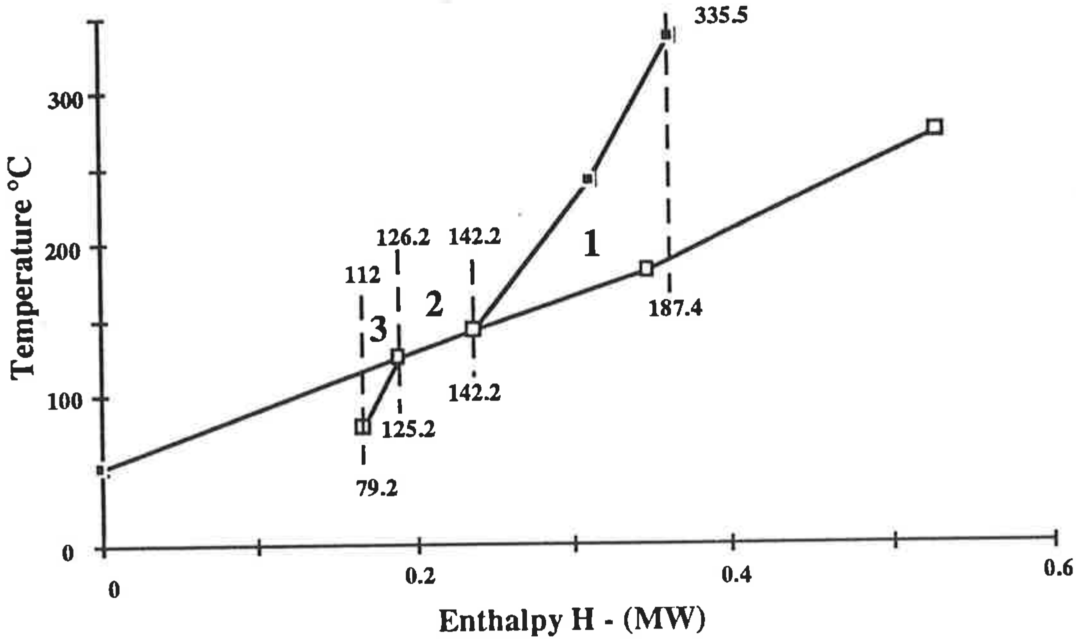
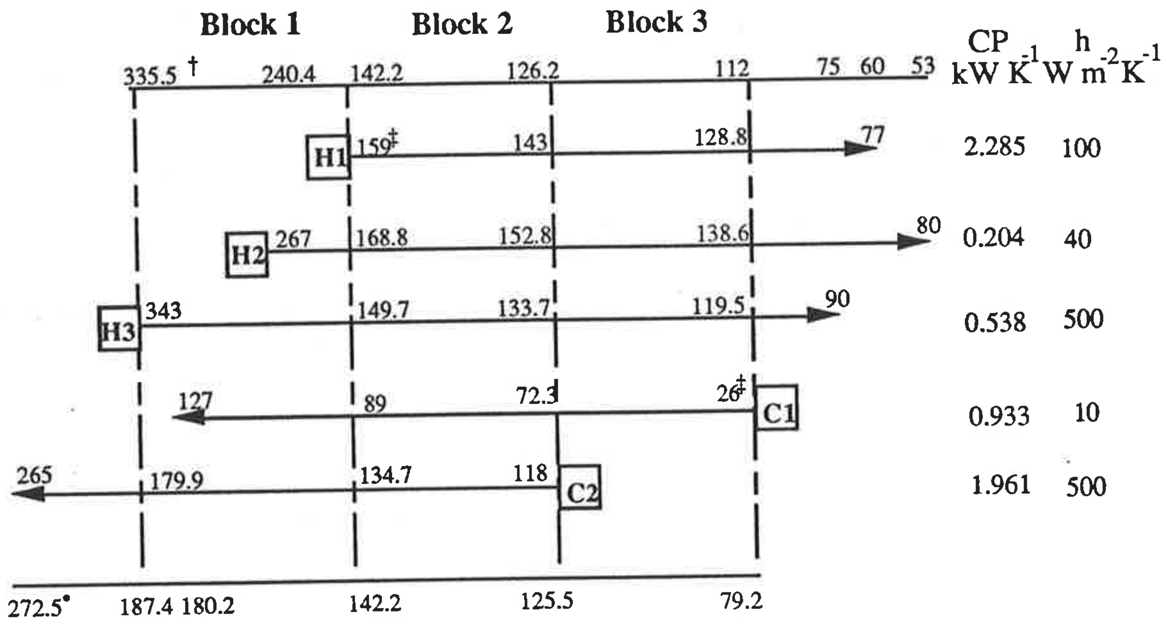


Figure 4.4: Composite curves when $\kappa = 5.3154$ and $z = 0.5$

(the utility consumption corresponds to HRAT = 38 K)

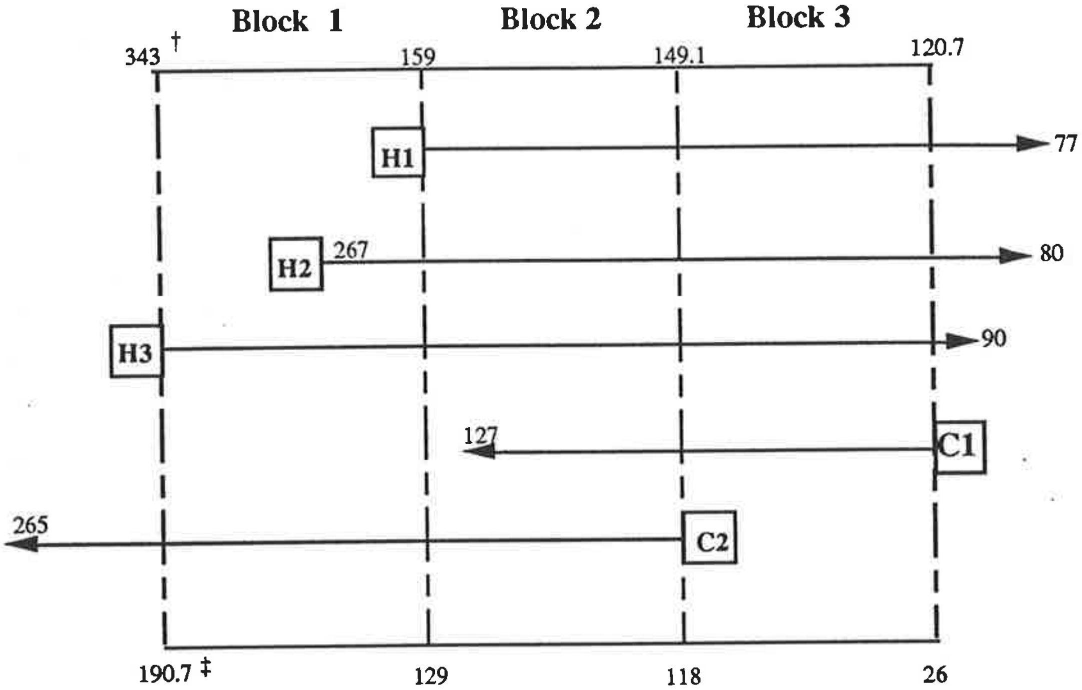


† Temperatures on the hot shifted composite curve.
• Temperatures on the cold shifted composite curve.
‡ Hot border temperature = temperature on composite curve + individual ΔT contribution
Cold border temperature = temperature on composite curve - individual ΔT contribution

Figure 4.5: Stream Structure for $\kappa = 5.3154$ and $z = 0.5$
(the utility consumption corresponds to HRAT = 38 K)

4.5.2 The Significance of z in Changing Stream Structures

As mentioned previously, the major effect of a variation in z is to alter the stream structures prior to design. The example (Table 4.1) demonstrates this point. Four possible stream structures (Figures 4.5, 4.6, 4.7, & 4.8) satisfy the optimal energy consumptions predicted by the targeting program. The predicted total minimum costs for each case are similar. An obvious question is: *"which stream structure provides the best starting point for synthesis?"*.



† Temperatures on hot composite.
‡ Temperatures on cold composite.
For the case of uniform ΔT contribution, the temperatures on the hot(cold) composite curves equal the hot(cold) border temperatures.

Figure 4.6: Stream Structure for HRAT = 30°C for example 1

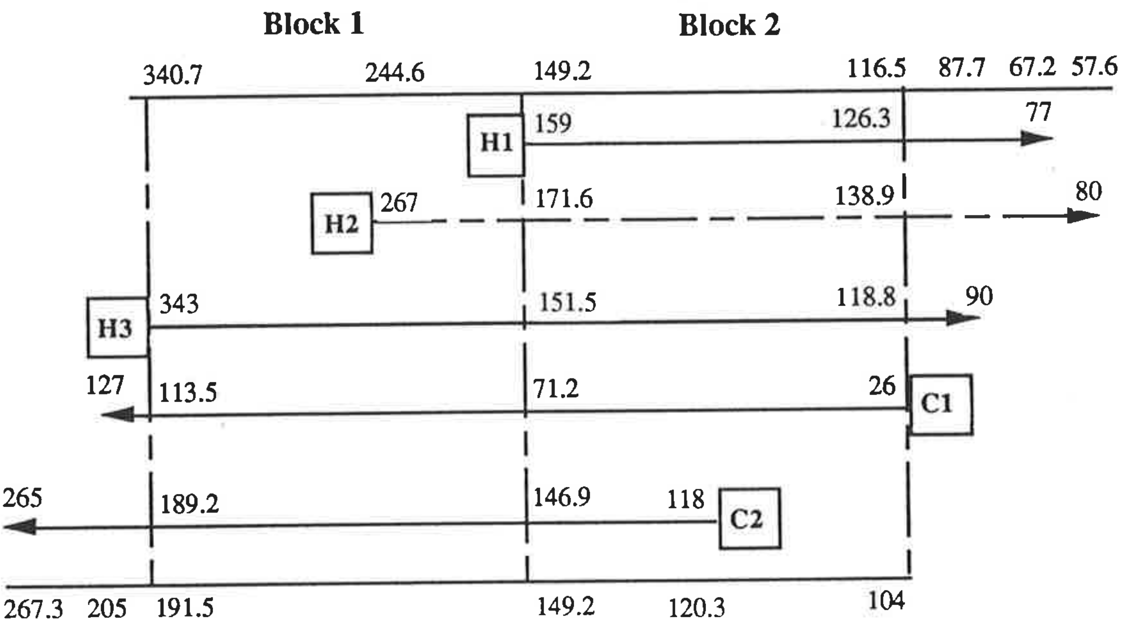


Figure 4.7: Stream Structure for $\kappa = 1.2356$ and z = 0.9 for example 1

(the utility consumption corresponds to HRAT = 36 K)

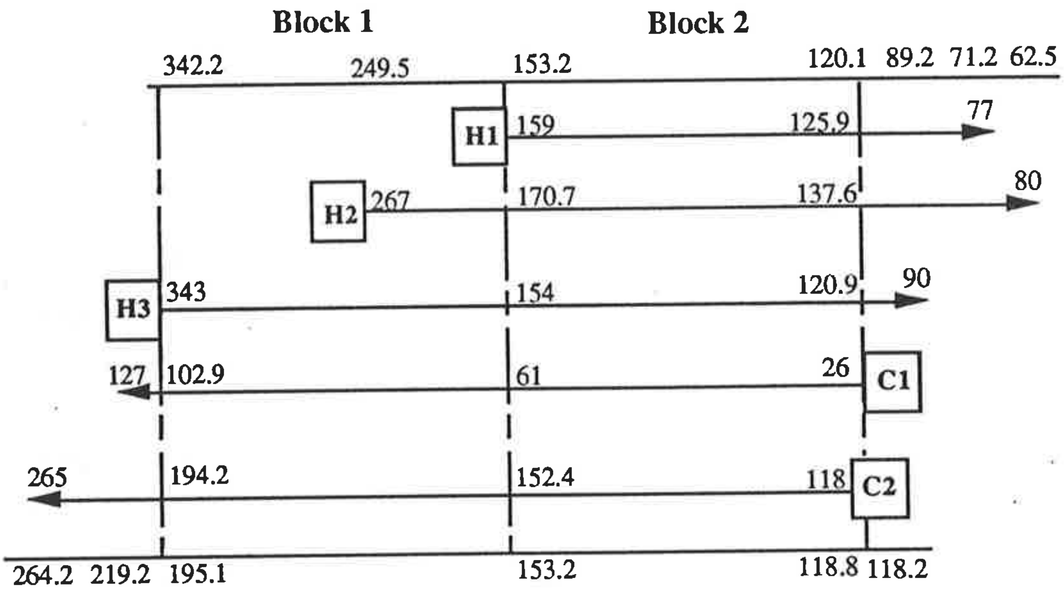


Figure 4.8: Stream Structure for $\kappa = 0.36696$ and $z = 1.2$ for example 1 (the utility consumption corresponds to HRAT = 36 K)

Figure 4.6 displays the stream structures of HRAT = 30 °C and the stream structure for $\kappa = 5.3154$ and $z = 0.5$ is provided in Figure 4.5. Three blocks may be defined for each situation. Clearly, the subsets of streams at the boundaries and the situations in each block differ significantly. In particular, stream Cl in Figure 4.5 (lowest film coefficient) is assigned the largest ΔT-contribution producing an equivalent target temperature of 180.2 °C (approximately equal to the border temperature of 187.4 °C). Obviously, this change affects the network structure. The stream structure of $\kappa = 1.2356$ and $z = 0.9$ is illustrated in Figure 4.7 with two blocks defined. Clearly, changing z, alters the number of blocks (three for $z = 0.5$ and two for $z = 0.9$) and the boundary temperatures. For example, stream Cl remains within block 1 for $z = 0.5$ (Figure 4.5) but when $z = 0.9$ it crosses the first-block border suggesting a requirement for hot utility. When z is increased to 1.2, the related stream structure is shown in Figure 4.8. The stream population in each block is similar to that of Figure 4.7 ($z = 0.9$). The major difference is that stream C2 (Figure 4.8) moves towards the border of the block 2 and its equivalent supply temperature approximately equals that of Cl. Hence, this stream can match any hot streams in this block providing a better vertical heat transfer pattern compared with z = 0.9. This may provide a lower area during synthesis. As well, the stream structure requires one fewer block than z = 0.5. This change may yield a simpler initial network structure. The twin considerations of area minimization and a simpler stream structure favour the stream structure in Figure 4.8 (z = 1.2). The effect of these differing stream structures on both the initial designs and the optimized networks are further considered in section 4.6.

Clearly, variations in z provide a number of good starting points for synthesis. Even though the associated predicted minimum total costs may be similar, the block decomposition and stream structures can be quite different. Hence, a decision is required to select the optimal starting point for synthesis. This starting point should incorporate a good stream structure and require few blocks. Pre-optimization for stream structures prior to design is necessary in addition to the pre-optimization to determine optimal κ and z trading-off energy and capital. The first optimization determines how minimum total cost can be approached by exploiting a simple initial network structure.

4.5.3 A Proposed Procedure

For problems with streams having significant differences in film coefficients, individual ΔT-contributions should be considered to produce lower area networks. Ahmad (1985) and Townsend (1989) showed that provided film coefficients differ by less than one order of magnitude, the area computation using the Bath formula normally provides a reasonable approximation (within 10%) compared with more sophisticated approaches. Hence, Ahmad et al (1990) suggest that one order of magnitude differences in film coefficients provides a threshold test for potential area reduction. This suggestion was based solely on area considerations. However, another important factor worthy of consideration is the stream structure prior to design. Figure 4.9 provides an algorithm for improved design. It considers both areas (i.e. capital costs) and stream structures prior to design.

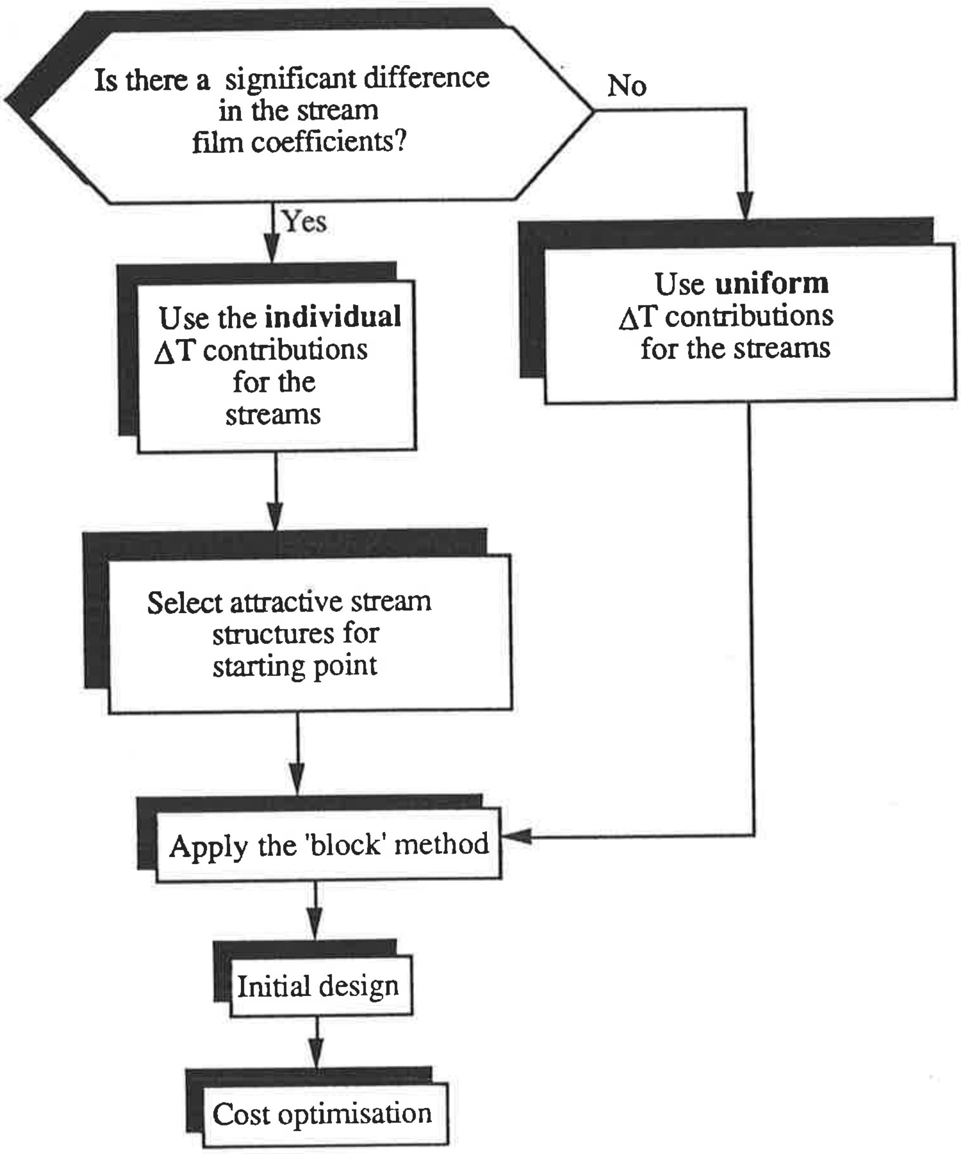


Figure 4.9: Procedure for testing to determine if ΔT contributions are required

The improved Pinch algorithm (Ahmad et al, 1990) and the block method differ significantly in their handling of the situation featuring closely approaching-composite curves including the pinch. In the former method, the ΔT-contributions derived from equation (4.3) are used for each enthalpy interval in the narrow region and a design proceeds one interval at a time in this region. By contrast, the block method may combine the enthalpy intervals in this narrow region into a single block when the hot (cold) composite segments have similar profiles. ΔT-contributions are used only at the block boundaries. Synthesis is performed in this block rather than based on the enthalpy intervals. Exploiting the block for synthesis rather than several enthalpy intervals greatly reduces the number of matches. The area target is likewise approached quite closely with a simple network structure. A small violation of the energy target may be incurred as energy may cross the pinch. The reason for allowing a small violation of the energy target is very simple. The optimal HRAT (ΔT_{min}) or optimal κ and z is based on an approximate trade-off between energy and capital. In addition, the initial design will be subsequently optimized using a cost objective. Hence, maintaining the energy target, if this requires a complicated network structure, is inappropriate.

Multiple pinches can be handled in a similar manner. In this case, a single block may span a number of pinches. This treatment avoids the pinch decompositions and solves the problem of how to design networks between pinches.

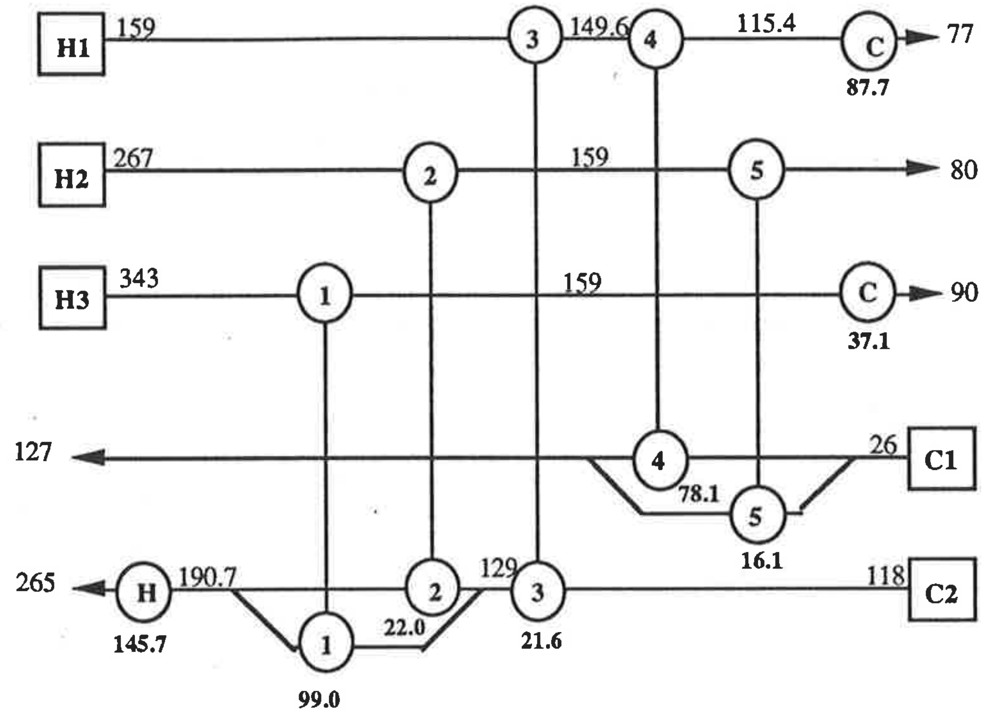
The Pseudo Pinch Method (Trivedi et al, 1989) and Flexible Pinch Method (Wood et al, 1991; Suaysompol and Wood, 1991a & b) allows energy transfer criss-crossing the pinch while retaining an energy target to reduce the complexity associated with a strict pinch decomposition. This energy relaxation provides benefits in simplifying the network structure and the networks generated are usually simpler compared to strict pinch design. However, this method only addresses network simplification but fails to consider the trade-off between units and area. As a result, it is occasionally possible to achieve a simple network whilst sacrificing area. This may produce networks with large area and capital cost.

4.6 Case Studies

4.6.1 Case Study 1 (Table 4.1)

This example demonstrates two key points. First, network area can be reduced by considering individual ΔT-contributions. Second, changes in stream structures may affect network structures. Figure 4.6 is derived neglecting the individual ΔT-contributions. The stream Cl possessing the smallest film coefficient is assigned an identical ΔT-contribution (half of HRAT) to other streams. If C1 is matched with Hl or H3 (high film coefficients), large area penalties are incurred. Matches between Cl and Hl or H3 are inevitable as a consequence of the stream structure. An initial design for this stream structure is shown in Figure 4.10. This network was designed using the block method.

By contrast, if the differences in film coefficients are considered, then the streams are shifted based on their individual ΔT-contributions according to the diverse pinch algorithm. The stream structure for $z = 0.9$ and $\kappa = 1.052$ is presented in Figure 4.11a. This stream structure is used to demonstrate that with a fixed energy consumption corresponding to HRAT = 30 K used in Figure 4.6, how the overall area can be reduced by applying individual ΔT–contributions and the block method. The initial design based on the stream structure in Figure 4.11a is given in Figure 4.11b. Both networks (Figures 4.10 and 4.11b) are designed with the same energy consumption (corresponding to HRAT = 30 °C). Considering the individual ΔT-contributions, the area is reduced by 49 m^2 (17.7%) compared to the case of a uniform HRAT. This reduction in area is significant.



Bath Area Target (HRAT = 30 °C) = 299 m^2; Network area = 326 m^2.

Figure 4.10: Initial design at HRAT = 30°C for example 1

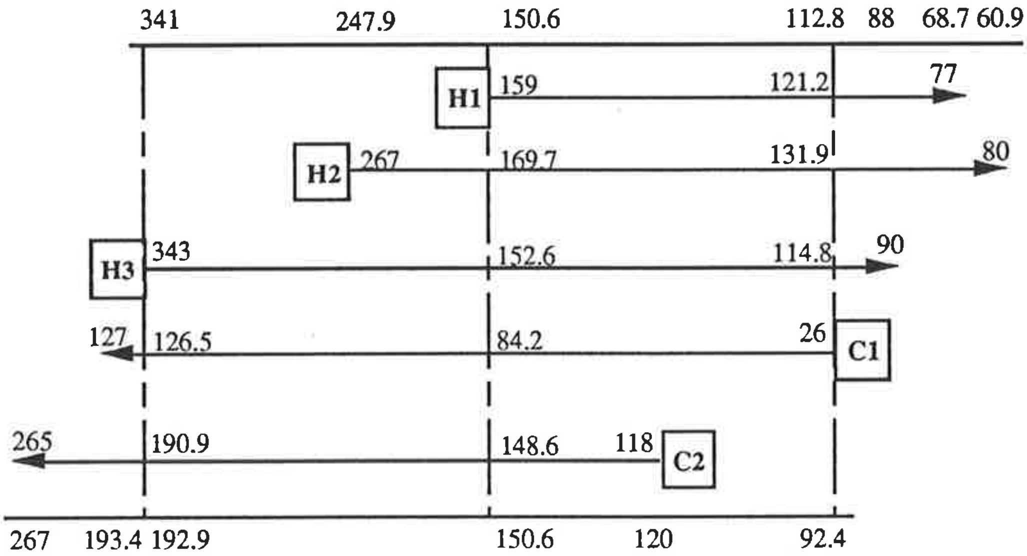
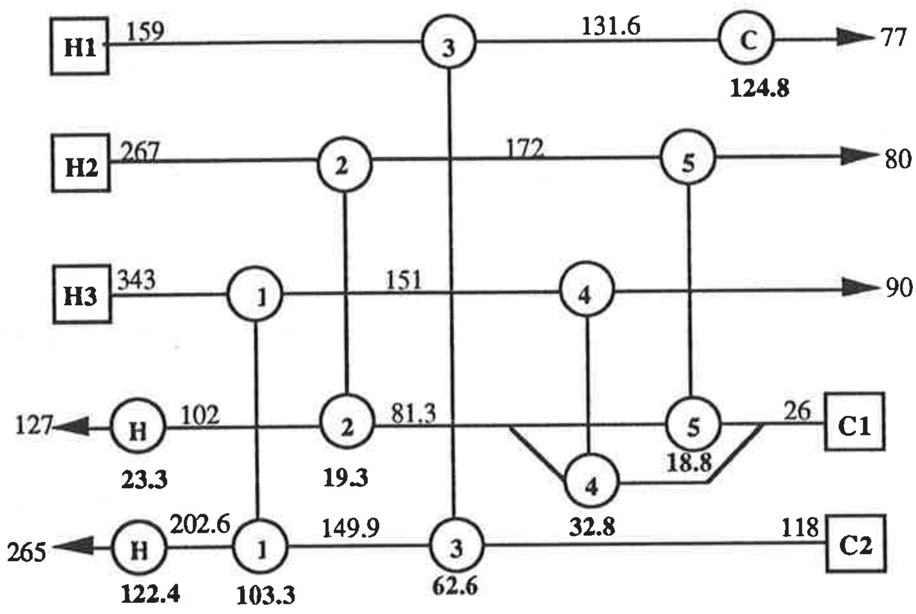


Figure 4.11a: Stream structure at κ = 1.052 and z = 0.9 for example 1

(the utility consumption corresponds to HRAT = 30 K)



Diverse Bath Area target (κ = 1.052, z = 0.9) = 275 m^2; Network area = 277 m^2

(the utility consumption corresponds to HRAT = 30 K)

Figure 4.11b: Initial design at κ = 1.052 and z = 0.9 for example 1

Next consider potential changes in the stream structure resulting from variations in z. Three optima, i.e. κ = 5.3154 and z = 0.5, κ = 1.2356 and z = 0.9, and κ = 0.36696 and z = 1.2 are selected for comparison. Based on the associated stream structures (Figures 4.5, 4.7 and 4.8), the initial networks are produced in Figures 4.12a, 4.13a and 4.14a respectively. These networks are compared in Table 4.2, for the cost data in Table 4.1. (The exchanger cost equation is similar to that in Ahmad et al (1990) but was modified so that for the size of exchangers used here the constant exchanger cost is about 20–25% of the total cost of an average exchanger). The first design (Figure 4.12a) is based on three blocks, and as expected is more complex (10 units) than the other two designs with two blocks (8 units). In addition, the stream structure (Figure 4.8) for κ = 0.36696 and z = 1.2 is optimal (as previously discussed) and its initial design (Figure 4.14a) has the lowest area requirement and the simplest structure.

Although the stream structures (Figures 4.7 and 4.8) seem quite similar, the corresponding designs (Figures 4.13a and 4.14a) are substantially different. This follows because the location of cold stream 2 in block 2 is a key difference between the two structures. In Figure 4.7, cold stream 2 is located in the middle of the block 2 and the very small driving force between hot stream 3 and cold stream 2 impedes the possible match between these two streams (of highest film coefficients). Thus, the match between hot stream 1 and cold stream 2 was selected as a result of the block area calculations (Chapter 3; Zhu et al, 1993a). By contrast, in the stream structure for κ^{*} = 0.36696 and z = 1.2 (Figure 4.8), cold stream 2 is shifted towards to the boundary of the block 2 and this shift enlarges the driving force for the heat transfer between hot stream 3 and cold stream 2. The match between these two streams stands out with a low area requirement as this match is achieved with both streams having high heat transfer film coefficients.

These initial networks were optimized and the resulting networks presented as Figures 4.12b, 4.13b, and 4.14b and 4.14c. Figure 4.14c is an alternative network produced by including a 'dummy' cooler on stream H2 in the initial network (Figure 4.14a) when undertaking cost minimization. Network comparison is shown in Table 4.3. All networks possess a simple structure and low cost. Design 3a (Figure 4.14b) achieves the units target with a total cost lower than the target. Design 3b (Figure 4.14c) incurs the second lowest cost. It eliminates the stream split and each stream (except C1) includes a utility exchanger. This should provide advantages in terms of operability and flexibility. These designs (Figures 4.14b & 4.14c) are derived from the best stream structure (Figure 4.8).

It should be noted, for this example, that neither energy nor capital cost is very dominant as the proportion of the annual costs, due to capital charges, vary from 46%

to 62%. By comparing Tables 4.2 and 4.3, it is evident that the utility costs are sometimes increased substantially by the optimization process. It seems that although designs are produced at the 'optimal' conditions with estimated best trade-off between energy and capital, this is subsequently modified when the NLP process is using the actual exchanger sizes. These trade-offs seem to be network dependent as the optimized designs have different proportions of capital cost.

Table 4.2: Results for different values of z for Example 1 (Initial Designs)

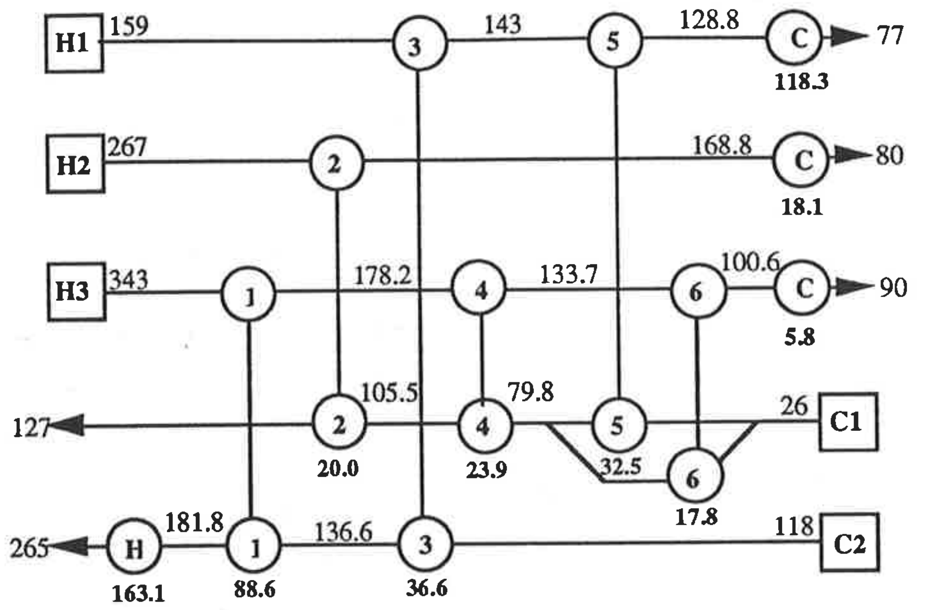
	Hot utility kW	Cold utility kW	Area m^2	Units	Total Cost $ yr^{-1}
Design 1 (Fig. 4.12a) (κ = 5.3154, z = 0.5)	163.1	142.2	248	10	51838
Design 2 (Fig. 4.13a) (κ = 1.2356, z = 0.9)	151.1	130.2	254	8	48858
Design 3 (Fig. 4.14a) (κ = 0.3670, z = 1.2)	168.3	147.4	241	8	49049

Table 4.3: Results for different values of z for Example 1 (Optimized Designs)

Cost Target (Bath area formula) = 48975 $ yr^{-1}

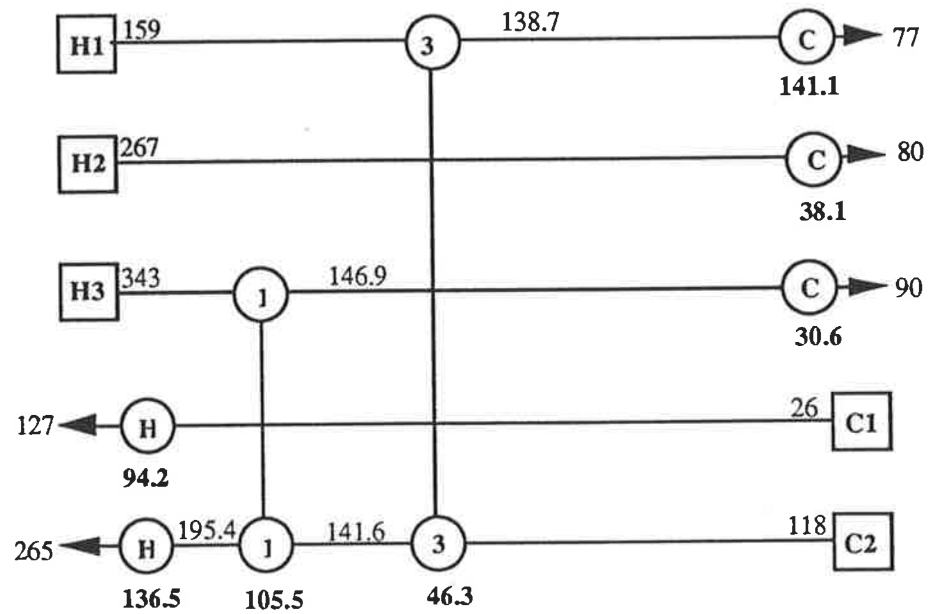
Cost Target (Diverse Bath area formula) = 48393 $ yr^{-1}

	Hot utility kW	Cold utility kW	Area m^2	Units	Total Cost $ yr^{-1}
Design 1 (Fig. 4.12b) (κ = 5.3154, z = 0.5)	230.7	209.8	183	7	50969
Design 2 (Fig. 4.13b) (κ = 1.23555, z = 0.9)	157.1	136.2	268	7	48804
Design 3a (Fig. 4.14b) (κ = 0.36696, z = 1.2)	169.2	148.3	242	6	46551
Design 3b (Fig. 4.14c) (κ = 0.36696, z = 1.2)	169.2	148.3	237	7	47060



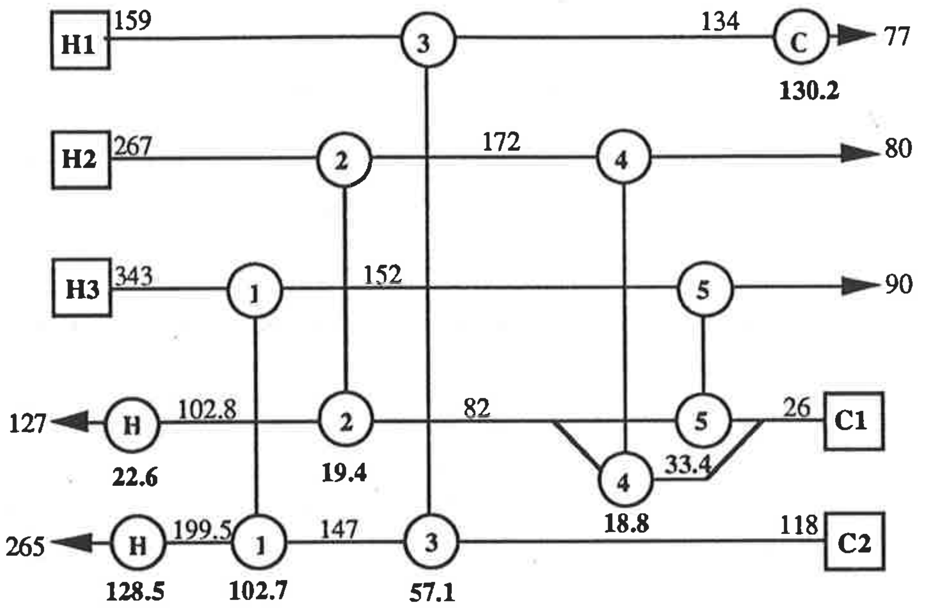
QH = 163.1 kW; Network area = 248 m^2; Total cost = 51838 \$/yr.

Figure 4.12a: Initial design at $\kappa = 5.3154$ and $z = 0.5$ for example 1



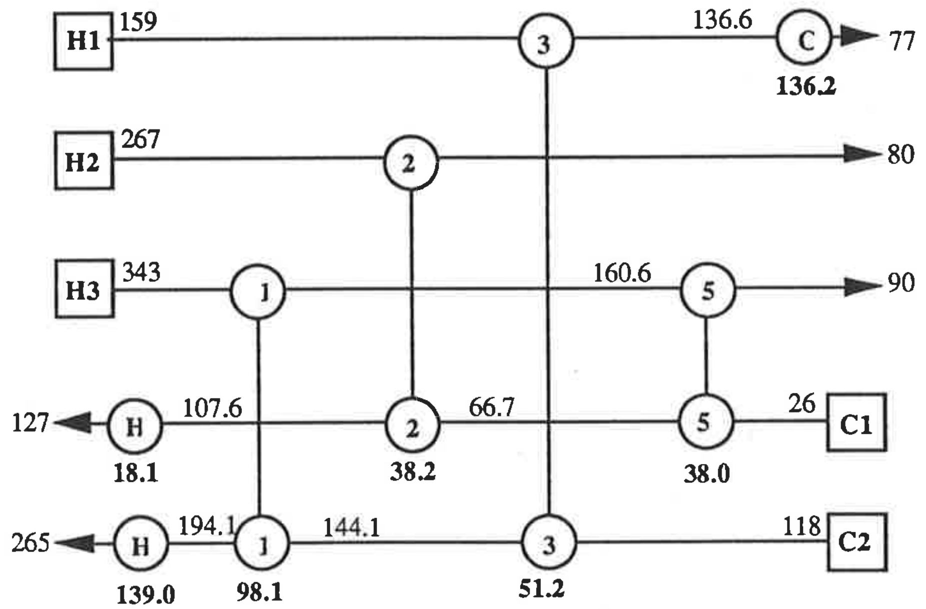
QH = 230.7 kW; Network area = 183 m^2; Total cost = 50969 \$/yr.

Figure 4.12b: Optimized design at $\kappa = 5.3154$ and $z = 0.5$ for example 1



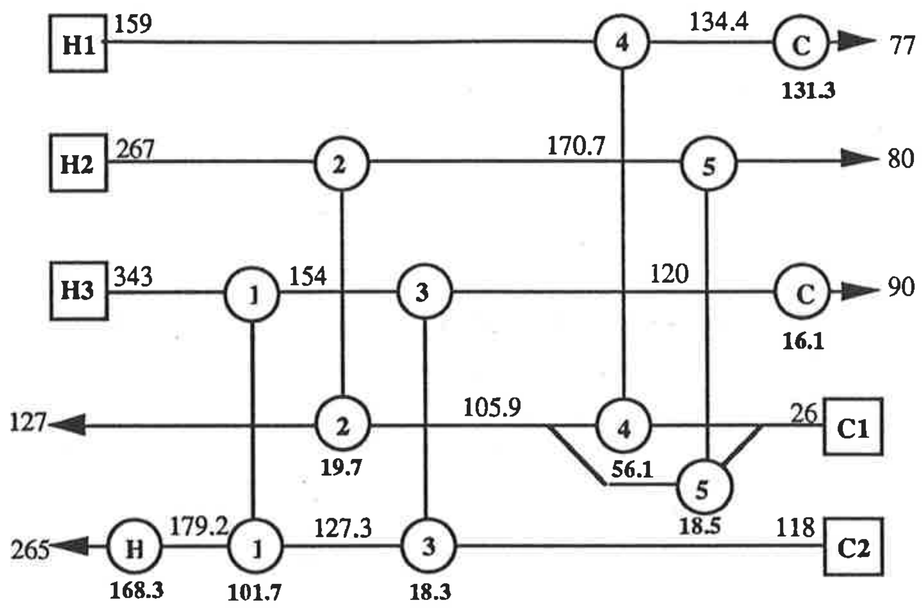
Q_H = 151.1 kW; Network area = 254 m^2; Total cost = 48858 \$/yr.

Figure 4.13a: Initial design at $\kappa = 1.2356$ and $z = 0.9$ for example 1



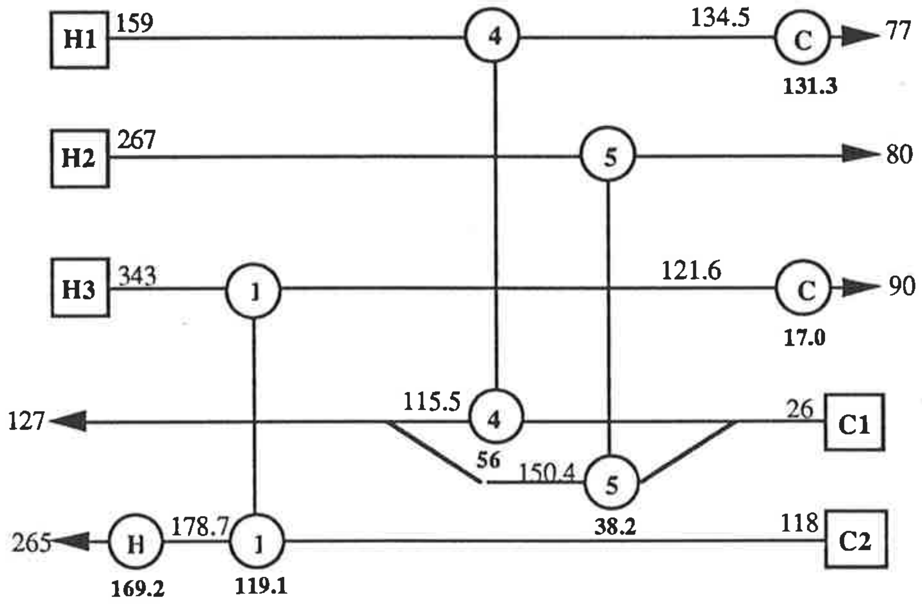
Q_H = 157.1 kW; Network area = 268 m^2; Total cost = 48804 \$/yr.

Figure 4.13b: Optimized design at $\kappa = 1.2356$ and $z = 0.9$ for example 1



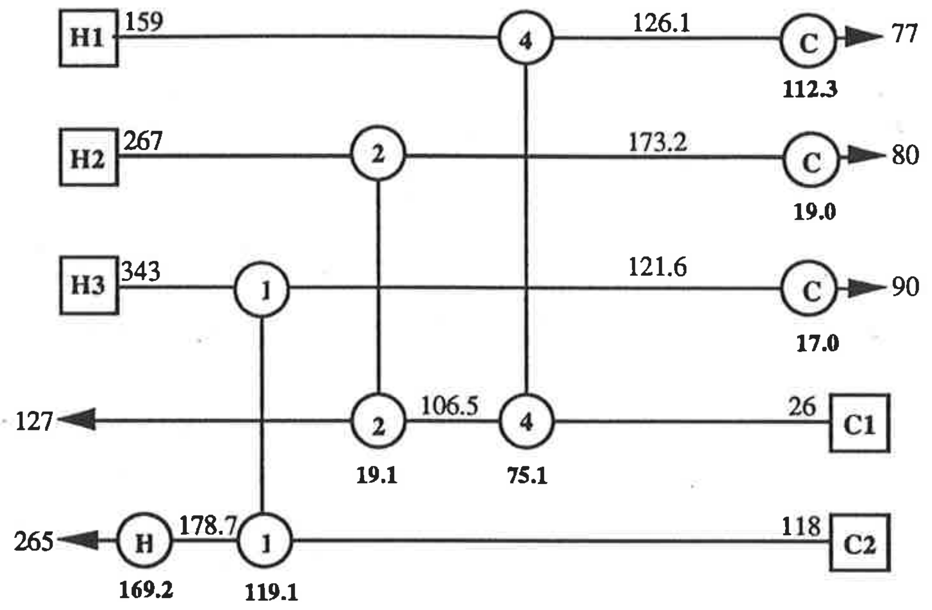
Q_H = 168.3 kW; Network area = 241 m^2; Total cost = 49049 \$/yr.

Figure 4.14a: Initial design at κ = 0.36696 and z = 1.2 for example 1



Q_H = 169.2 kW; Network area = 242 m^2; Total cost = 46551 \$/yr.

Figure 4.14b: Optimized design 1 at κ = 0.36696 and z = 1.2 for example 1



Q_H = 169.2 kW; Network area = 237 m^2; Total cost = 47060 \$/yr.

Figure 4.14c: Optimized design 2 at $\kappa = 0.36696$ and $z = 1.2$ for example 1

4.6.2 Case Study 2 (Table 4.4)

Topology traps inherent in the pinch decomposition were explained by Gundersen and Grossmann (1990). They concluded that such traps can be avoided using systematic criss-crossing at the pinch which violates the original pinch rules. This effect was demonstrated using the example presented by Gundersen and Grossmann (Table 4.4). The pinch method yields the design in Figure 4.15 with 27.5% excess area and 20% excess cost compared to the network shown in Figure 4.16. This was obtained by permitting the criss-cross of energy through the pinch point. As a result, energy is balanced and no extra utility is required.

Table 4.4: Stream data for example 2

Stream	T_s °C	T_t °C	CP kW K^{-1}	h W $m^{-2}K^{-1}$
H_1	300	200	10	100
H_2	200	190	100	1000
H_3	190	170	50	1000
C_1	160	180	50	100
C_2	180	190	100	1000
C_3	190	230	25	1000
Steam	350	350		4000
CW	30	50		2000

Exchanger cost model: $\$ = 10{,}000 + 1000A^{0.8}$

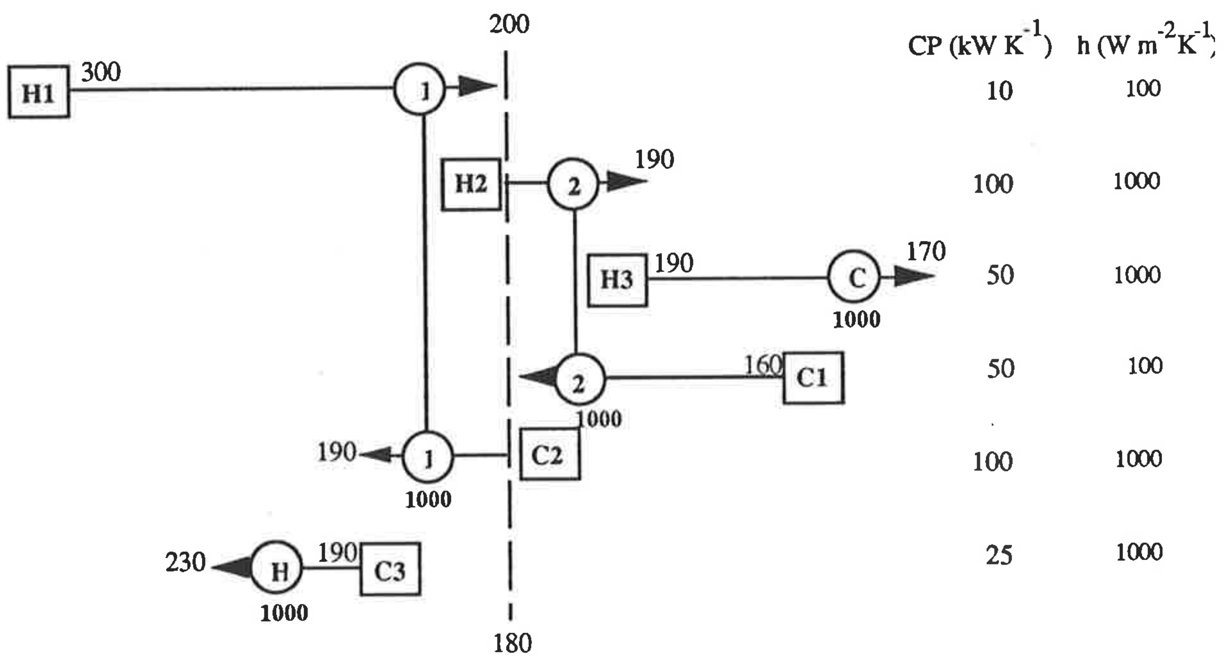


Figure 4.15: Pinch design for example 2 with universe pinch concept at HRAT = 20°C (Gundersen and Grossmann, 1990)

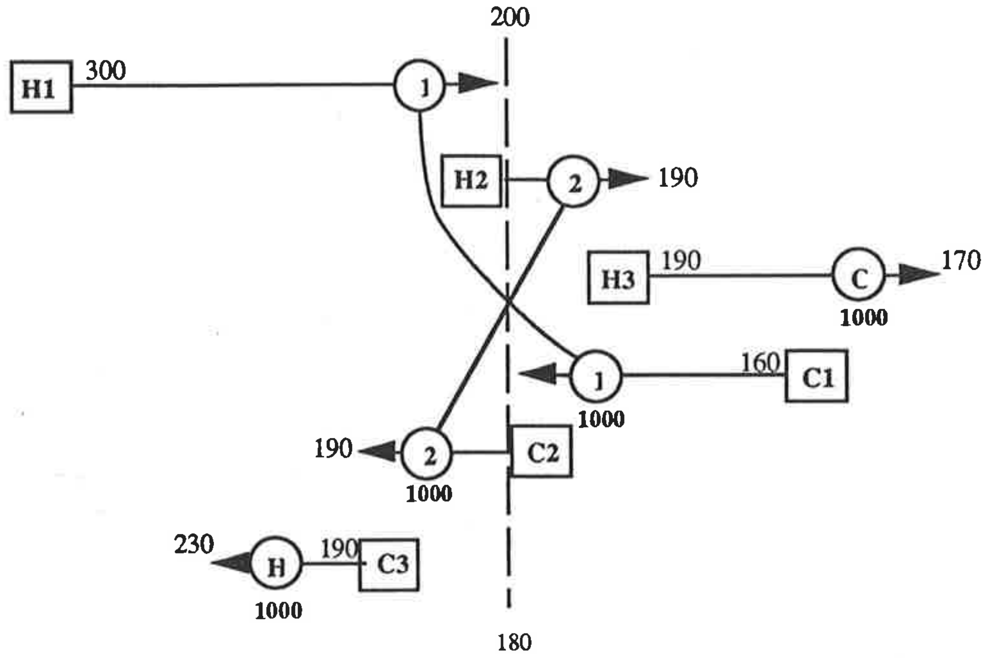


Figure 4.16: Criss-cross design for example 2 with universe pinch concept at HRAT = 20°C (Gundersen and Grossmann, 1990)

However, Rev and Fonyo (1991) noted that this systematic violation becomes very complicated in more complex cases. A simpler alternative is provided by the block method. Streams can be temperature shifted and stream structures adjusted using different combinations of κ and z to yield good starting stream structures. Design is performed simply using the block method. In this manner, the topology traps are effectively avoided.

Considering Figure 4.15, matches between Hl and Cl, and H2 and C2 are not permitted as Hl and C2 are located at above the pinch and H2 and Cl appear below the pinch. For this reason, the network (Figure 4.15) may not be evolved to the optimal network (Figure 4.16).

By way of comparison, consider the stream structure (Figure 4.17) with the decomposition into two blocks for κ = 3.26 and z = 1.0. (Again, for z = 1.0, a κ value of 3.26 kW/m^2 is equivalent to the minimum heat flux of 1630 W/m^2). Stream Cl is moved partly above the pinch due to its low film coefficient. It is assigned a large ΔT-contribution. Stream C2 is shifted below the pinch as a result of its large film coefficient (small ΔT-contribution). Matches between Hl and Cl, and H2 and C2 become attractive and a new initial network (Figure 4.18) results. This network is easily evolved to the optimal network in Figure 4.16.

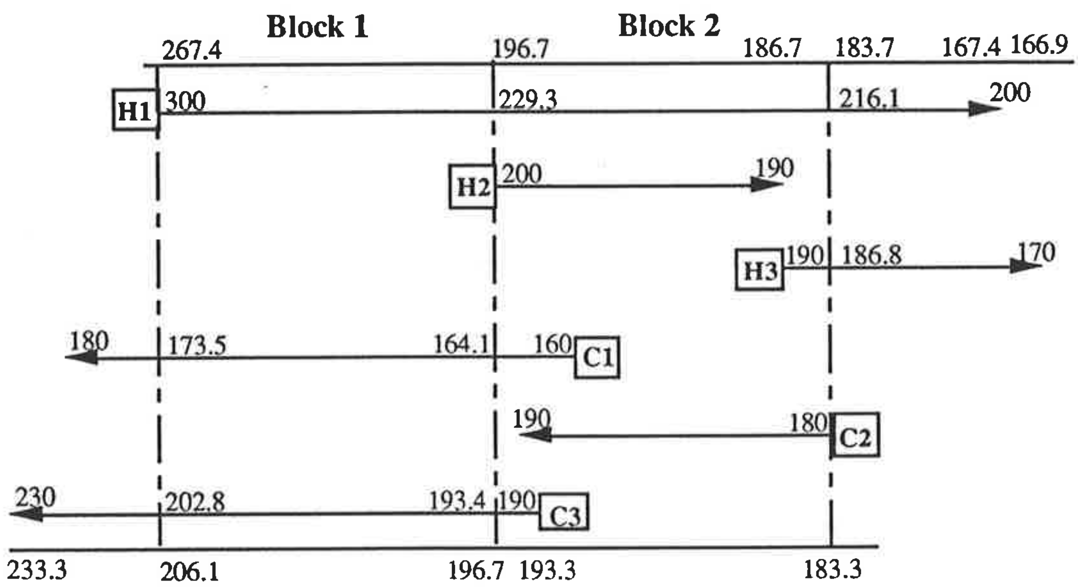


Figure 4.17: Stream structure at κ = 3.26, z = 1 for example 2

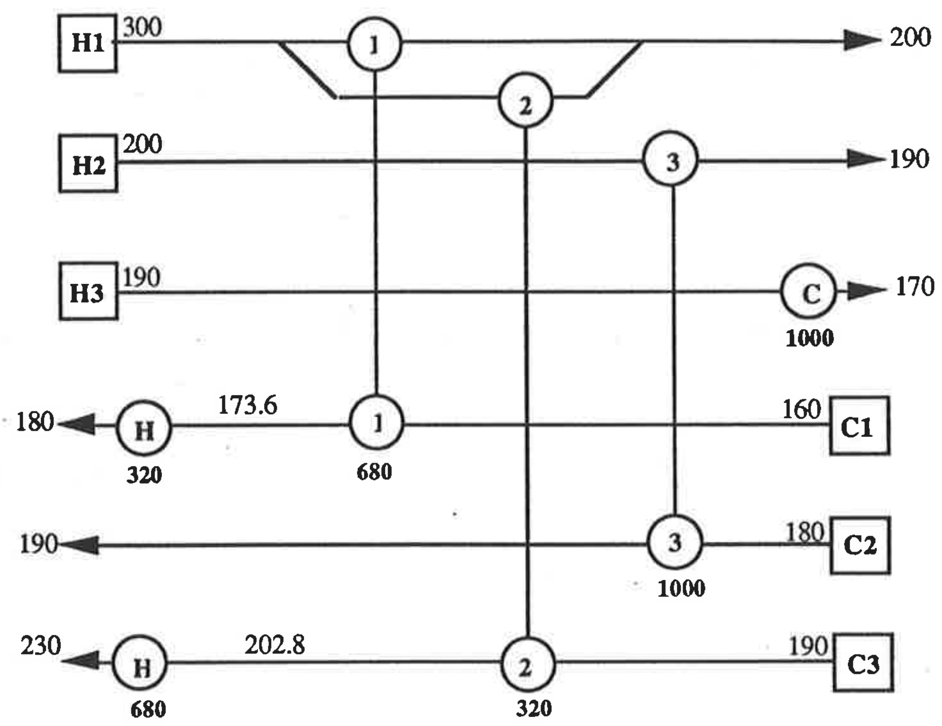


Figure 4.18: Initial design at $\kappa = 3.26$, $z = 1$ for example 2

It should be noted that despite individual ΔT-contributions to avoid the topology traps, significant differences in solutions are generated by using different design methods. Thus following determination of ΔT adjustments, the initial network produced using the diverse pinch method by Rev and Fonyo (1991) is shown in Figure 4.19. This network is more complicated than the network (Figure 4.18) devised using the block method. The evolution of the network in Figure 4.18 to the optimal network (Figure 4.16) is straightforward. However, the evolution of the network in Figure 4.19 to the network in Figure 4.16 is complex.

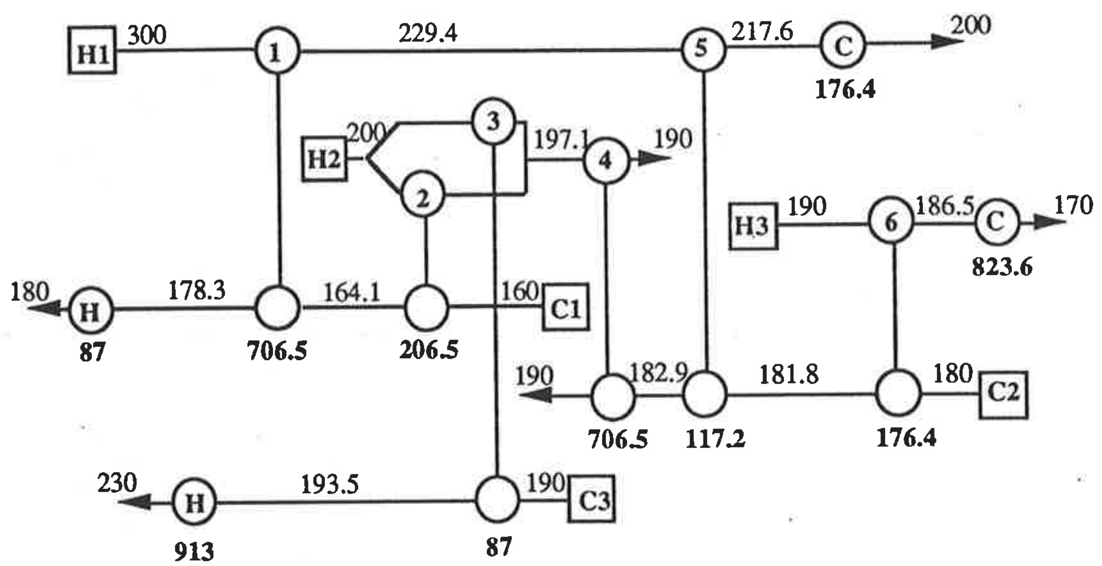


Figure 4.19: First candidate Pinch design for example 2 with diverse pinch concept of Rev and Fonyo (1991)

4.7 Conclusions

In the conventional pinch design method, an uniform minimum driving force is assigned to each stream independent of its film heat transfer coefficient. It is possible to match streams with widely differing heat transfer coefficients thereby incurring an area penalty. This deficiency is overcome by the diverse pinch concept introduced by Rev and Fonyo (1991). In this study this concept is coupled with the newly proposed block method for the synthesis of heat exchanger networks.

The objective of this methodology is to derive an initial network which simultaneously features a low overall area requirement and a small number of units for problems involving streams with widely-differing film coefficients. In contrast to the supertargeting approach of Linnhoff and Ahmad (1986a & b) which optimizes ΔT_{min} (HRAT) prior to design, the new method optimizes two parameters κ and z and thereby assigns the individual stream ΔT's to best exploit the differences in film coefficients. The new approach allows different stream structures to be compared prior to design and attractive structures may be derived for further network synthesis.

CHAPTER 5

BLOCK DECOMPOSITION AND MATHEMATICAL PROGRAMMING

SUMMARY

Previously, the 'block' concept has been applied successfully to HEN design problems. The methodology is to produce initial designs by employing certain heuristic rules and then optimize the initial designs using NLP techniques. In this chapter, an extension of the block concept to mathematical programming is discussed with superstructures allowing variable topologies. Results demonstrate that this application of mathematical programming has a number of advantages over current methods. The main two advantages are a reduction in the size of a NLP problem and the good quality of initial solutions.

5.1 Introduction

Although much progress is being made in the application of mathematical programming to heat exchanger network synthesis, two serious problems plague most mathematical algorithms. First, the mathematical formulation is often based on a large number of small intervals (either temperature intervals (TI's) or enthalpy intervals (EI's)) defined by the kinks in the composite curves. Even for moderately-sized problems, the number of intervals may become prohibitively large. This causes the corresponding non-linear optimization problem (NLP) to grow to an unmanageable size. Yee et al (1990) proposed the 'stage' concept to overcome this problem and the problem size can be usually reduced by applying this concept. However, a stage has no physical definition and therefore it does not provide an initial solution which is associated with an actual network structure. The second problem is that a good starting point for a design problem is not available in most current mathematical programming methods. Now, conventional general purpose NLP solvers rely on a good starting point to initiate the search for an optimal solution and if a poor initial guess is provided, the problem may fail to converge or converge to an inferior solution.

A new strategy is proposed to overcome these deficiencies. The block concept introduced provides a physical insight into mathematical programming for HEN synthesis. It defines reasonable regions, viz blocks, by which the minimum area can be approached for designs having a small number of units. A significant reduction in problem size and complexity is achieved as a block normally encompasses a number of intervals. In each block, a superstructure is used to represent the possible matches between streams. The composite curves corresponding to the 'optimal' HRAT is obtained by applying the supertargeting approach (Linnhoff and Ahmad, 1986 a & b; Zhu et al, 1994) and the composite curves generated are used as the starting point for building the block-based superstructures. A linear programming (LP) model for area targeting and a simple NLP for cost targeting are developed and solved to provide good initial solutions. These ensure that subsequent NLP models for area and cost targets are easily solved and that the quality of final solution is increased. The key features of this approach are the reduction in problem dimensionality even for networks with a large number of streams and that good initial solutions achieved by locating the optimal composite curves, followed by block decomposition and good initialization procedures.

5.2 Brief Review of Related Work

Prior to commencement of the detailed synthesis of a heat exchanger network, it is possible to calculate an area, a capital cost and an overall cost target. The concept of the area target was introduced independently by Hohmann (1971) and Nishida et al (1971). Hohmann observed that the minimum area could be calculated exactly using the composite curves for the case of a network composed of exchangers with equal film heat-transfer coefficients. Townsend and Linnhoff (1984) extended Hohmann's method to account for streams with different film coefficients. The computation of the area target is exact when all film coefficients are identical. As well, it provides a reasonable approximation for problems with similar film coefficients. These methods all use simple models to calculate minimum area and may give a poor estimate for the true minimum area target if a significant variation exists in the film coefficients.

To provide a more precise estimate of minimum area, researchers resorted to the application of mathematical programming techniques. Saboo et al (1986) developed a linear programming (LP) approach for predicting the area target. The formulation is based on the temperature intervals (TI's) defined by 'kinks' in the composite curves. The number of TI's is increased and a new LP is solved. This procedure is repeated until either the calculated area converges to within some preset tolerance or until the problem dimensionality becomes excessive. Unfortunately, in practical problems, the number of TI's tends to grow prohibitively large before the algorithm converges (Colberg and Morari, 1990). The method can however, provide better estimates of the area target compared with the previous algorithms.

Colberg and Morari (1990) developed an improved method using non-linear programming techniques (NLP) to calculate the area and capital-cost targets. The resulting NLP's can handle both constraints on specific matches and the situation with unequal film coefficients. These NLP models are based on temperature intervals (TI's) determined from the 'kinks' on the composite curves. The number of TI's approximately equals twice the total number of streams. Hence, the number of TI's in this method is usually fewer than the temperature intervals (TI's) used by Saboo et al (1986). However, for a large problem, the number of TI's determined by Colberg and Morari may still be large and the time required to solve such problems becomes prohibitive.

Clearly, any reduction in the number of intervals to be considered in formulation of the optimization problem means that the solution of the NLP is simpler and problems may be efficiently solved. Recently, Yee et al (1990) invented the 'stage' concept which provides the basis for mathematical formulation. Typically, the number of stages is equal to the maximum of the numbers of hot streams and cold streams. Obviously, the number of stages is greatly reduced compared with the number of TI's or EI's. However, the stage concept is created solely from the point view of mathematical programming. By definition, a stage does not have any physical meaning and does not posses any actual predetermined boundaries. Also the initialization procedures (Appendices D & E) proposed by Yee and Grossmann (1990) and Yee et al (1990) do not provide an initial solution which corresponds to an actual superstructure. There are many similarities in the mathematical formulations of the block and stage based approaches; however, the drawbacks inherent in the stage concept can be overcome by applying the block concept. As discussed in detail in Chapter 3, though the block-based superstructure is similar to that based on the stages, the block concept provides the physical insight necessary to achieve a near-minimum area design with a simple network structure. By applying this concept to mathematical programming, a significant reduction in problem dimensionality will be realized. In the meantime, the use of blocks provides reasonable estimates of the area target. The blocks form the basis of the NLP rather than the TI's or EI's and the required number of blocks are determined from the composite curves. In each block, a superstructure is constructed. Solution of a LP model for area targeting or a simple NLP for cost targeting provides a good starting point for the sophisticated optimization models (NLP1, NLP2 or NLP3) (if integer variables are required, then a corresponding MINLP model is produced) and substantially increases the likelihood of discovering the global optimum. A key advantage of this approach is that the dimensionality of the problem remains reasonable even for problems with a large stream population. The algorithm converges efficiently due to the limited number of blocks and good initial solutions.

5.3. Superstructure based on Blocks

As stated, Townsend and Linnhoff (1984) produced a simple area target method, the 'Bath formula', which is based on the composite curves. In their method, the composite curves (Figure 5.la) are divided into a number of enthalpy intervals (EI's) defined by the 'kink' points. In each enthalpy interval, a superstructure (Figure 5.lb) is constructed with the imposed constraint that all streams entering a mixing point are at same temperature. Corresponding hot streams are matched with corresponding cold streams to achieve a pattern of vertical heat transfer. The key property of the resulting

HEN structure is that the temperature profiles of all hot/cold streams follow the temperature profiles of the hot/cold composite curves. This method produces an exact calculation of the area target when the film coefficients of all streams are equal. Even if the film coefficients differ somewhat, the method still can provide a reasonable estimate of the area target.

As the number of EI's required is normally large and the heat transfer is constrained to vertical matching, the resultant HEN possesses a very complicated structure. It is called a 'spaghetti structure' by Linnhoff and his co-workers, which was also used by Yee et al (1990) for their stage-based superstructure. Imposing the constraint of strictly vertical heat transfer on a problem with significantly-different film coefficients causes the calculated area target to deviate substantially from the true area target.

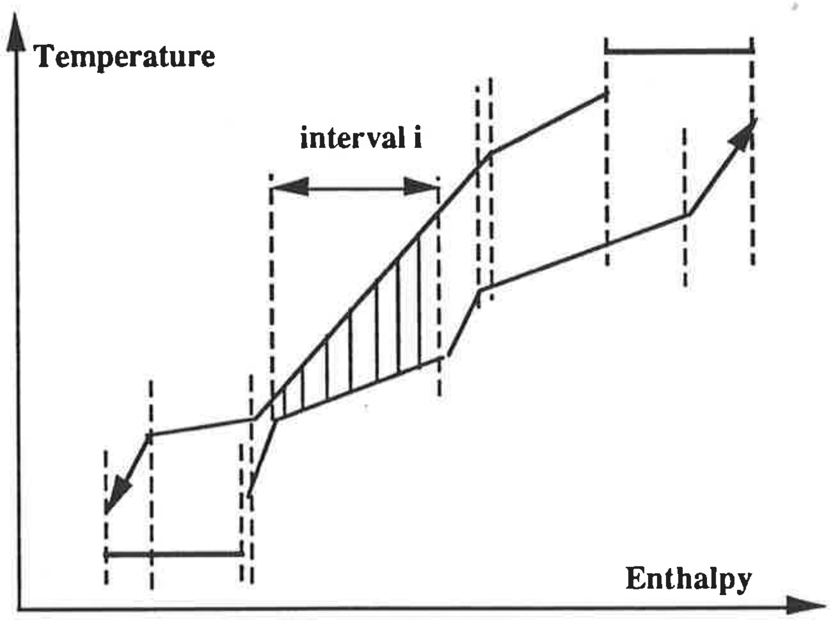


Figure 5.1a: Enthalpy interval of composite curves

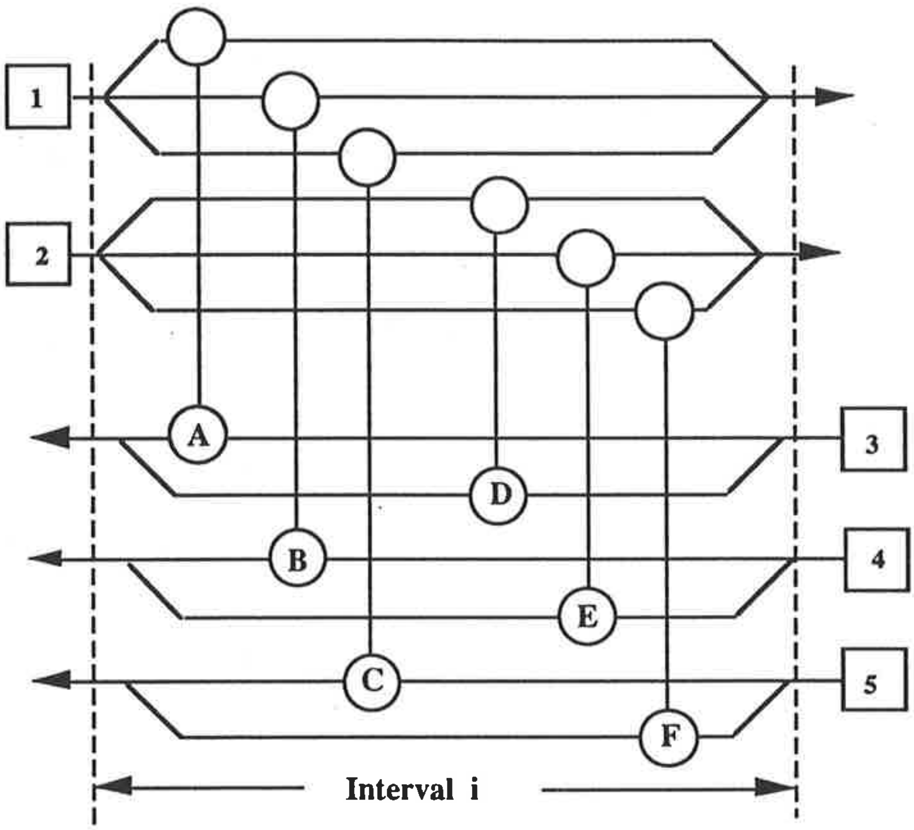


Figure 5.1b: 'Spaghetti structure' and matching scheme for vertical heat transfer in the interval

In this work, the proposed approach is also based on a superstructure similar to the 'spaghetti structure', but it overcomes the dual problems of incorrect estimation of the targets and excessive dimensionality. The network is synthesized using blocks to replace EI's when formulating an NLP. The results presented in Chapter 3 for problems with uniform or similar film coefficients confirm that the area target produced by the BATH formula can be approached closely with blocks replacing the EI's. This area-targeting method also provides a physical insight facilitating the achievement of a minimum area HEN with a small number of blocks. Since a block usually spans a number of EI's where the hot/cold temperature profiles on the composite curves are quite similar, the associated HEN structure is simpler than that based on EI's. In addition, the problem size in terms of the number of variables is reduced greatly by replacement of EI's by blocks.

The constraint of strictly vertical heat transfer in the 'spaghetti structure' introduces two problems. First, it eliminates the opportunity of exploiting 'criss-crossing' matches which may reduce area or capital cost. Second, in each EI, a number of matches with small heat loads may be required to achieve energy balance. These units complicate the HEN's structure. In this approach, such problems are reduced by defining the temperature boundaries of blocks for which there are distinct hot and cold values as variables, thereby providing opportunities for 'criss-cross' matches.

The general 'block-based' superstructure is illustrated in Figures 5.2a & b and 5.3a & b. It is still a rather complicated structure. However, for a particular problem, it is not necessary to split streams of small size in the spaghetti structure. Thus, the related block based superstructure can be less complicated. In addition, when building block–based superstructures, the stream population in each block is the same as that of the composite curves. In other words, not all streams are in each block. This can be seen from Figure 5.3a & b that cold stream C2 does not appear in block 2 and it is not necessary to consider matches involving C2 in the superstructure for block 2, which makes the superstructure less complicated.

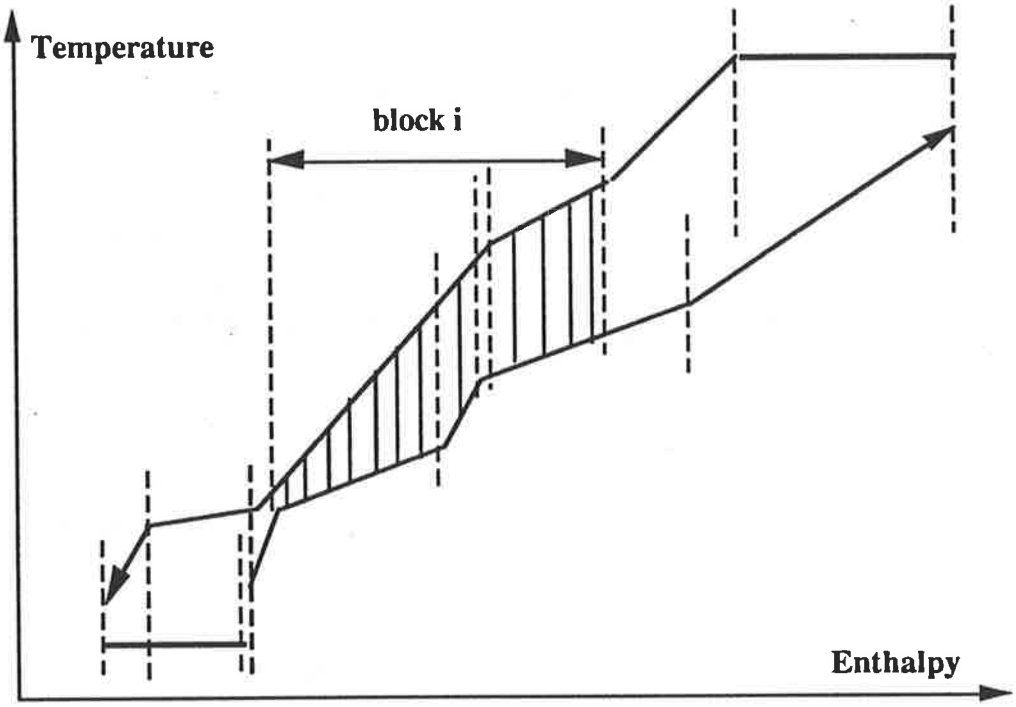


Figure 5.2a: 'Block' interval of composite curves

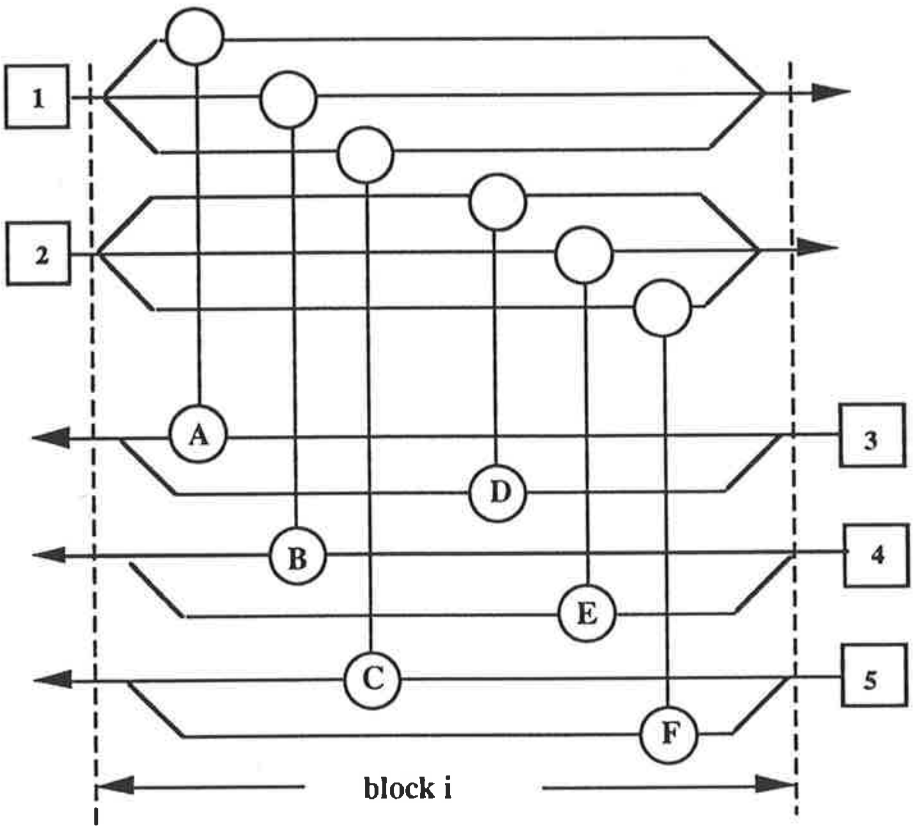


Figure 5.2b: 'Superstructure' and matching scheme for 'criss-cross' heat transfer in a block of the composite curves

In the superstructure, the outlet temperatures of an exchanger are defined as distinct variables (Figure 5.3). In other words, the isothermal mixing characteristic of the 'spaghetti structure' is not assumed. This provides an opportunity to exploit branch temperature and criss-crossing trade-offs whilst searching for the minimum of the objective function. The rigid assumption of isothermal mixing precludes such a possibility. However, a possible disadvantage of non-isothermal mixing is the introduction of additional non-linear constraints thereby increasing the degree of non-linearity in the model to some extent.

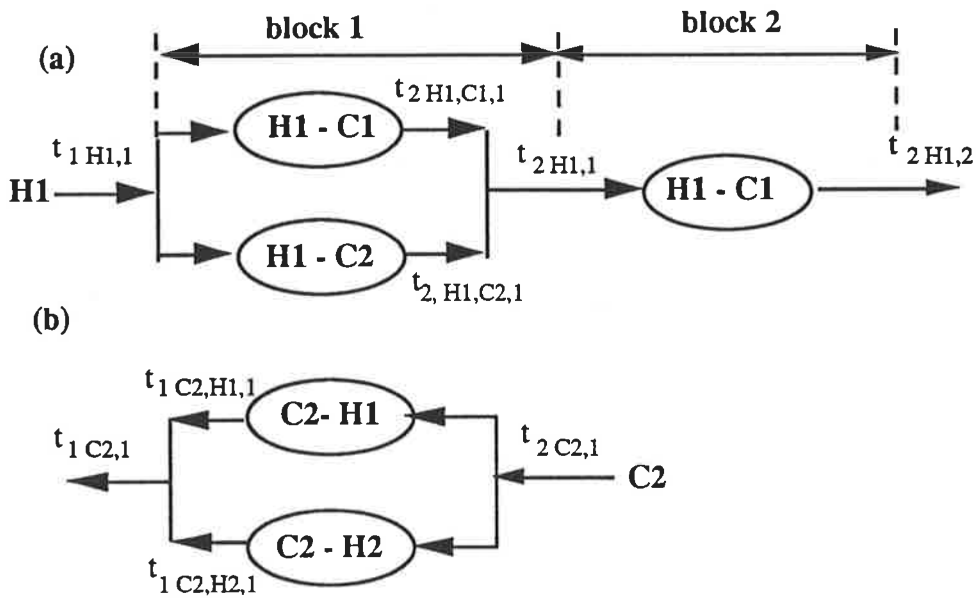


Figure 5.3: Definition of temperatures at splitting junctions and mixing points (Case Study 1)

The superstructure proposed above is similar to that by Yee et al (1990). However, two major differences exist. First, the former superstructure is block-based and the latter one is stage-based. As discussed above, the block concept was invented through physical insights into the process of heat exchanger network synthesis. This means that the number of streams in the superstructure for any block reflects the stream populations in the composite or quasi–composite curves. Thus, not only are the superstructures simplified, but usually a good initial solution can be provided by employing this concept. By contrast, the stage concept is created merely from the consideration of reduction of an NLP problem size and a good initial solution is not guaranteed. Isothermal mixing is assumed in the stage-based superstructure.

5.4 Optimization Models for Targeting and Synthesis

Since a similar superstructure to that of a stage–based superstructure (Yee et al, 1990) is adopted for the present method, the following mathematical models are similar to those proposed by Yee et al (1990). However, as stated above, the application of the block concept provides more physical insights into these models which may produce advantages in improving both solution efficiency and quality .

Prior to the formulation of the various NLP models, it is necessary to define important parameters. These definitions follow the specification from GAMS (Brooke et al, 1988) and this software for mathematical programming was used in this work. Parameters are indicated by an upper-case character whereas variables are denoted by a lower-case character.

indices and sets

$I = \{i | i$ denotes a hot process stream$\}$,

$J = \{j | j$ denotes a cold process stream$\}$,

$S = \{s | s$ denotes a hot utility$\}$,

$W = \{w | w$ denotes a cold utility$\}$,

$K = \{k | k$ represents a block in the superstructure, $k = 1 .. M\}$

parameters

T_{in} = supply temperature of a stream;

T_{out} = target temperature of a stream;

Q_{hu} = total hot utility consumption;

Q_{cu} = total cold utility consumption;

Q_{max} = maximum heat transfer between two streams;

U = overall heat transfer coefficient;

CP = heat capacity flow rate;

F = fixed cost in an exchange cost model;

B = area cost coefficient;

C = exponent for area cost;

$Area^L$ = lower bound of area for an exchanger;

$Area^U$ = upper bound of area for an exchanger;

ΔT_{min} = minimum temperature approach for an exchanger;

M = total number of blocks;

N = number of exchangers;

NS = number of splitting branches of a stream.

variables

q_{ijk} = heat exchanged between hot stream i and cold stream j in the kth block;

q_{iw} = heat exchanged between hot stream i and cold utility stream w;

q_{js} = heat exchanged between cold stream j and hot utility stream s;

t_{1ik} = temperature of hot stream i at the hot end of block k;

t_{2ik} = temperature of hot stream i at the cold end of block k;

t_{1jk} = temperature of cold stream j at the hot end of block k;

t_{2jk} = temperature of cold stream j at the cold end of block k;

t_{1ijk} = cold stream outlet temperature of an exchanger between hot stream i and cold stream j in block k;

t_{2ijk} = hot stream outlet temperature of an exchanger between hot stream i and cold stream j in block k;

cp_{hijk} = branch heat capacity flow rate of hot stream i matched with cold stream j in block k;

cp_{cijk} = branch heat capacity flow rate of cold stream j matched with hot stream i in block k;

Overall energy balance for each stream

A stream of one type (e.g. hot) may only transfer its enthalpy to streams of the other kind (i.e. cold). The remaining energy must be exchanged with a utility. These balances are summarized as:

$$(T_{in,i} - T_{out,i})CP_i = \sum_{k \in K} \sum_{j \in J} q_{ijk} + \sum_{w \in W} q_{iw} \tag{5.1a}$$

$$(T_{out,j} - T_{in,j})CP_j = \sum_{k \in K} \sum_{i \in I} q_{ijk} + \sum_{s \in S} q_{js} \tag{5.1b}$$

Energy balance at each block

As the temperatures at the block boundaries have been introduced as optimization variables, using the superstructure of Figure 5.3 the energy balances over each block are as follows:

$$\begin{aligned}
(t_{1ik} - t_{2ijk})\, cp_{h\,ijk} &= q_{ijk} \\
(t_{1ijk} - t_{2jk})\, cp_{c\,ijk} &= q_{ijk} \\
(t_{1ik} - t_{2ik})\, CP_i &= \sum_{j \in J} q_{ijk} \\
(t_{1jk} - t_{2jk})\, CP_j &= \sum_{i \in I} q_{ijk}
\end{aligned} \tag{5.2}$$

Assignment of superstructure temperatures

Supply temperatures for the hot process streams ($T_{in,i}$) are assigned as the temperatures (t_{1i1}) at the hot end of the first block and supply temperatures of the cold process streams ($T_{in,j}$) are assigned as the temperatures (t_{2jM}) at the cold end of the last block. As well, the cold end temperatures (t_{2ik}/t_{2jk}) of the current block are assigned as the hot end temperatures ($t_{1i,k+1}/t_{1j,k+1}$) of the next block. These assignments may be denoted as follows:

$$t_{1i1} = T_{in,i}; \qquad t_{2jM} = T_{in,j}$$
$$t_{2ik} = t_{1i,k+1}; \qquad t_{2jk} = t_{1j,k+1} \qquad (1 \le k \le M-1) \tag{5.3}$$

Mass balance at mixing point

Any stream may be split into a number of branches and the mass flows of such branches should be balanced at the mixing point.

$$\sum_{j \in J} cp_{h\,ijk} = CP_i$$
$$\sum_{i \in I} cp_{c\,ijk} = CP_j \tag{5.4}$$

Utility requirement

For simplicity, the utility exchangers are placed at opposite ends of the superstructure. Hence, the utilities are not involved in any blocks. Hot (cold) utility consumption for each stream is defined in terms of the temperature at a mixing point at the first (last) block and its target temperature. Multiple utilities may be available. The use of lower (higher) grade hot (cold) utilities will save operating cost but incur a penalty in capital. Hence the trade–off between them should be considered.

$$(t_{2iM} - T_{out,i})\, CP_i = \sum_{w \in W} q_{i\,w}$$
$$(T_{out,j} - t_{1j1})\, CP_j = \sum_{s \in S} q_{j\,s} \tag{5.5}$$

Temperature approaches

$$\Delta t_{1ijk} = t_{1ik} - t_{1ijk} \tag{5.6a}$$

$$\Delta t_{2ijk} = t_{2ijk} - t_{2jk} \tag{5.6b}$$

$$\Delta t_{iw} = t_{2iM} - T_{out,w} \tag{5.6c}$$

$$\Delta t_{js} = T_{out,s} - t_{1jl} \tag{5.6d}$$

Feasibility conditions

Constraints to ensure a monotonic decrease of temperature at each successive block must be specified. As well, each match must be thermodynamically feasible. Specification of a positive temperature approach ensures feasibility. These conditions may be expressed mathematically as:

$$t_{1ik} \geq t_{2ijk} \; ; \; t_{1ik} \geq t_{2ik} \; ; \; t_{1ijk} \geq t_{2jk} \; ; \; t_{1jk} \geq t_{2jk}$$
$$\Delta t_{1ijk} > 0; \; \Delta t_{2ijk} > 0; \; \Delta t_{iw} > 0; \; \Delta t_{js} > 0 \tag{5.7}$$

Objective function for area targeting (NLP1)

The appropriate objective function for such targeting minimizes the total heat transfer area for a fixed network utility consumption. The problem formulation is:

$$\min \sum_{i\in I} \sum_{j\in J} \sum_{k\in K} \left[\frac{q_{ijk}}{U_{ij}\ \mathrm{lmtd}_{ijk}}\right] + \sum_{i\in I} \sum_{w\in W} \left[\frac{q_{iw}}{U_{iw}\ \mathrm{lmtd}_{iw}}\right] + \sum_{j\in J} \sum_{s\in S} \left[\frac{q_{js}}{U_{js}\ \mathrm{lmtd}_{js}}\right] \tag{5.8a}$$

subject to (s.t.)

constraints (5.1–5.7) and

$$\sum_{i\in I} \sum_{w\in W} q_{iw} = Q_{cu} \tag{5.8b}$$

$$\sum_{j\in J} \sum_{s\in S} q_{js} = Q_{hu} \tag{5.8c}$$

Objective function for capital cost targeting (NLP2)

The capital-targeting objective function minimizes the capital cost for a fixed utility consumption:

$$\min \sum_{i\in I}\sum_{j\in J}\sum_{k\in K}\left[F_{ij} + B_{ij}\left(\frac{q_{ijk}}{U_{ij}\,lmtd_{ijk}}\right)^{C_{ij}}\right] +$$

$$\sum_{i\in I}\sum_{w\in W}\left[F_{iw} + B_{iw}\left(\frac{q_{iw}}{U_{iw}\,lmtd_{iw}}\right)^{C_{iw}}\right] + \sum_{j\in J}\sum_{s\in S}\left[F_{js} + B_{js}\left(\frac{q_{js}}{U_{js}\,lmtd_{js}}\right)^{C_{js}}\right] \quad (5.9)$$

s.t. constraints (5.1-5.7) and (5.8(b) & 5.8(c))

Objective function for total cost targeting (NLP3)

The final objective function considers the combined cost of energy and capital simultaneously. The relevant formulation is:

$$\min \sum_{i\in I}\sum_{w\in W} C_w\, q_{iw} + \sum_{j\in J}\sum_{s\in S} C_s\, q_{js} + \sum_{i\in I}\sum_{j\in J}\sum_{k\in K}\left[F_{ij} + B_{ij}\left(\frac{q_{ijk}}{U_{ij}\,lmtd_{ijk}}\right)^{C_{ij}}\right] +$$

$$\sum_{i\in I}\sum_{w\in W}\left[F_{iw} + B_{iw}\left[\frac{q_{iw}}{U_{iw}\,lmtd_{iw}}\right]^{C_{iw}}\right] + \sum_{j\in J}\sum_{s\in S}\left[F_{js} + B_{js}\left(\frac{q_{js}}{U_{js}\,lmtd_{js}}\right)^{C_{js}}\right] \quad (5.10)$$

s.t. constraints (5.1-5.7).

$lmtd_{ijk}$ is the logarithmic-mean temperature difference of a match between hot stream i and cold stream j in kth block. This is given as:

$$lmtd_{ijk} = \frac{\Delta t_{1ijk} - \Delta t_{2ijk}}{\ln\left[\dfrac{\Delta t_{1ijk}}{\Delta t_{2ijk}}\right]} \quad (5.11)$$

To avoid the singularity inherent in the above logarithmic function when approach temperatures of both sides of the exchanger are identical, the following approximation for the lmtd term (Paterson, 1984) is employed:

$$\text{lmtd}_{ijk} = \frac{2}{3}\sqrt{\Delta t_{1ijk} \times \Delta t_{2ijk}} + \frac{1}{3}\left[\frac{\Delta t_{1ijk} + \Delta t_{2ijk}}{2}\right] \tag{5.12}$$

Similar expressions may be written for lmtd_{iw} and lmtd_{js}.

5.5 Constraints

The previous specification of the three optimization problems, i.e. NLP 1, NLP2 and NLP3 involves no imposed constraints. In practice, such constraints are often present and hence must be considered in targeting and synthesis. Such restrictions on a network are readily incorporated into the problem specification. Adding new constraints to the problems is a relatively simple task.

Some constraints are expressed by the introduction of binary variables. Three types of binary variables exist: viz. x_{ijk} denoting a match between the ith hot stream and the jth cold stream within the kth block, x_{iw} indicating a match between hot stream i and cold utility w and finally x_{js} associated with a match between cold stream j and hot utility s. If a match is made then the corresponding binary variable is assigned the value 1, otherwise it is assigned zero.

Heat load constraints

When binary variables are employed in a model, the following inequalities are required:

$$q_{ijk} \le x_{ijk}\, Q_{max,ij} \tag{5.13a}$$

$$q_{iw} \le x_{iw}\, Q_{max,iw} \tag{5.13b}$$

$$q_{js} \le x_{js}\, Q_{max,js} \tag{5.13c}$$

where $Q_{max,ij}$ = the maximum heat transfer between hot stream i and cold stream j;

$Q_{max,iw}$ = the maximum heat transfer between hot stream i and cold utility w;

$Q_{max,js}$ = the maximum heat transfer between cold stream j and hot utility s.

Additional restrictions for the synthesis of the constrained heat exchanger network can then be deduced. Possible constraints include:

Area bounds on required matches

$$\text{Area}_{ij}^{L} \leq \frac{q_{ijk}}{U_{ij}\ \text{lmtd}_{ijk}} \leq \text{Area}_{ij}^{U} \tag{5.14a}$$

$$\text{Area}_{iw}^{L} \leq \frac{q_{iw}}{U_{iw}\ \text{lmtd}_{iw}} \leq \text{Area}_{iw}^{U} \tag{5.14b}$$

$$\text{Area}_{js}^{L} \leq \frac{q_{js}}{U_{js}\ \text{lmtd}_{js}} \leq \text{Area}_{js}^{U} \tag{5.14c}$$

Constrained matches

Based on safety and economic considerations, matches between certain pairs of streams may be forbidden or imposed. Assume that a match between hot stream i and cold stream j is prohibited. This prohibition can be guaranteed by the following constraint:

$$\sum_{k \in K} x_{ijk} = 0 \tag{5.15a}$$

Likewise, the constraint enforcing an imposed match between hot stream i and cold stream j is:

$$\sum_{k \in K} x_{ijk} \geq 1 \tag{5.15b}$$

Specified number of matches

The total number of matches in a HEN may be specified and the corresponding area target or cost targets may be calculated. The constraint fixing the total number of matches is:

$$\sum_{i\in I}\sum_{j\in J}\sum_{k\in K} x_{ijk} + \sum_{i\in I}\sum_{w\in W} x_{iw} + \sum_{j\in J}\sum_{s\in S} x_{js} = N_t \tag{5.16a}$$

Suppose we only specify the number of process-process matches, then the associated constraint is:

$$\sum_{i\in I}\sum_{j\in J}\sum_{k\in K} x_{ijk} = N_p \tag{5.16b}$$

If the maximum number of process-process matches is specified for a hot stream or cold stream, then the constraints to ensure these limits are:

$$\sum_{k\in K}\sum_{j\in J} x_{ijk} \le N_i \tag{5.16c}$$

and

$$\sum_{k\in K}\sum_{i\in I} x_{ijk} \le N_j \tag{5.16d}$$

Prohibition of stream splits

Usually, a network not featuring stream splits possesses advantages in terms of operability and controllability. However, it may incur an investment cost penalty compared to a network featuring stream splits. A designer may accept this penalty and require a network design without stream splitting; appropriate constraints are:

$$\sum_{j\in J} x_{ijk} \le 1, \quad \sum_{i\in I} x_{ijk} \le 1, \quad \sum_{w\in W} x_{iw} \le 1, \quad \sum_{s\in S} x_{js} \le 1 \tag{5.17}$$

The constraints for avoiding stream splitting are usually used for process streams as normally utility matches involve splitting. Thus each process stream will have its own utility. Situation in which cooling water from one cooler is used in another cooler, rarely occurs. In such a situation, the cooling water flowrate will be very high which is not practical. Hence, the above constraints are not supposed to be used for utilities.

Maximum number of splitting branches allowed for a stream

For many problems, attainment of the requirement of a low area or low cost coupled with a simple network structure is only achievable with stream splitting. However, in practice, the specification of a large number of split streams may incur additional piping and valve costs and introduce unwanted controllability problems. The designer may wish to limit the maximum number of split branches on any stream in a block. This constraint may be expressed as:

$$\sum_{j \in J} x_{ijk} = NS_i \qquad \text{(for a hot stream)} \qquad (5.18a)$$

$$\sum_{i \in I} x_{ijk} = NS_j \qquad \text{(for a cold stream)} \qquad (5.18b)$$

Minimum temperature approaches

Streams involved in matches may have a distinctive minimum temperature approach which can be defined as:

$$\Delta t_{1ijk} \geq \Delta T_{min\ ij}, \quad \Delta t_{2ijk} \geq \Delta T_{min\ ij} \qquad (5.19a)$$

$$\Delta t_{iw} \geq \Delta T_{min\ iw}, \quad \Delta t_{js} \geq \Delta T_{min\ js} \qquad (5.19b)$$

These imposed constraints are sufficient but not necessary. The presence of a large number of constraints significantly increases the difficulty of solution. Imposed constraints should be applied with caution and only when the solver generates an optimal solution which violates a desirable constraint.

5.6 Determination of the Blocks

The number of blocks required for a specific problem is readily determined from the composite curves (Chapter 3). Those EI's with similar temperature profiles are combined to form a block. These blocks provide the basis for formulating the LP model and the simple NLP model used to generate an initial solution and the various sophisticated NLP models for targeting. In initial set up of superstructures, utility exchangers are placed at both ends of the superstructures. Only, those sections of composite curves not including the utilities are considered when determining the number of blocks. Since any block boundaries are defined as variables, the trade-off between energy and capital can be done in the optimization process. In other words, the optimization for the superstructures includes utility and process exchangers. It should be noted that in the superstructure proposed, the issue of proper use of multiple utilities has not yet been considered as utility exchangers are placed at the both ends of the superstructures in the present method as stated above. The work can be improved by considering this practical issue: when using multiple utilities, some utility exchangers should be placed at intermediate levels according to their temperatures.

If one desires a more accurate area or cost targets, more blocks can be added. Usually, the addition of one or two blocks ensures that the area calculated from the NLP model converges to the correct area target within a small tolerance.

5.7 LP (Area) or Simple NLP (Cost) Model Providing an Initial Solution

Non-linear optimization problems traditionally require a good initial solution.

Commencing the search from such a guess improves the quality of solution and increases the likelihood of convergence to the global optimum. In the excellent study of Colberg and Morari (1990), an initial starting point for minimizing area is obtained by solving a utility-targeting LP. However, the solution from utility-targeting LP provides a minimum utility design which may be at variance with the NLP model for area minimization. Yee and Grossmann (1990) and Yee at al (1990) proposed two procedures for initialization, one for NLP models and the other for MINLP models. In the first procedure (Yee et al, 1990), all temperature variables of hot (cold) streams are initialized with the supply temperatures of hot (cold) streams and a heat load for an exchanger is initialized to a value which spreads out the heat transfer amongst the number of stages (see Appendix D for detail). In the second initialization procedure by Yee and Grossmann (1990), the average driving forces are calculated by a weighting method and the driving forces are fixed in the MINLP model at the average driving forces calculated. This reduces the MINLP model to a MILP. Following this step, initialization for all heat loads is completed by solving the MILP model (see Appendix E). The common property of above two procedures is that solutions from these two initializations do not produce physically realizable superstructures. Such an initial solution without a physical existence may not provide a good starting for the subsequent NLP or MINLP models.

In this study, a LP (for area target) model or a simple NLP (for cost targets) is solved to provide an initial solution. First, the optimal HRAT is determined based on the targeting approaches (Linnhoff and Ahmad, 1986a & b; Zhu et al, 1994). Then the number of blocks is determined based on the composite curves corresponding to the optimal HRAT determined. The temperatures at the block boundaries are fixed equal to the values on the composite curves. The heat loads are then optimized using either the LP model (Eq. 5.20) or the simple NLP model (Eq. 5.22).

Fixing the temperature boundaries means that the heat transfer pattern is vertical. As discussed previously, the area calculation assuming vertical heat transfer provides a reasonable estimate of the real area target in problems with streams possessing film coefficients which are not significantly different. In addition, the vertical pattern of heat transfer simplifies the mathematical formulation. The next stage of the optimization permitting energy 'criss-crossing' between blocks is solved using a sophisticated NLP model (NLP1 for area, NLP2 for capital cost and NLP3 for total cost targeting). In some cases, some integer variables are required to account for match restrictions, then the MINLP model is generated by associating these constraints involving integer variables with the corresponding NLP model.

The initial LP model providing an initial solution for NLP1 is:

$$\min \quad \sum_{i\in I} \sum_{j\in J} \sum_{k\in K} \frac{q_{ijk}}{U_{ij}\, LMTD_{ijk}} \tag{5.20}$$

s.t.

$$(T_{1ik} - T_{2ik})CP_i = \sum_{j\in J} q_{ijk} \tag{5.21a}$$

$$(T_{1jk} - T_{2jk})CP_j = \sum_{i\in I} q_{ijk} \tag{5.21b}$$

The simple NLP model providing the heat loads for an initial network for NLP 2 or NLP 3 is:

$$\min \quad \sum_{i\in I} \sum_{j\in J} \sum_{k\in K} \left[F_{ij} + B_{ij} \left(\frac{q_{ijk}}{U_{ij}\, LMTD_{ijk}} \right)^{C_{ij}} \right] \tag{5.22}$$

s.t. constraints (21(a) & 21(b))

where CP_i, CP_j, q_{ijk}, U_{ij}, F_{ij}, B_{ij} and C_{ij} are defined previously.

$LMTD_{ijk}$ = the log mean temperature difference between hot stream i and cold stream j in block k. This is constant as the blocks are determined prior to the solution of the LP or the NLP.

$T_{1ik}, T_{2ik}, T_{1jk}, T_{2jk}$ = temperatures on both hot (cold) ends of block k in the composite curves. These temperatures are constant.

Since the block boundaries are fixed for the previous two models, the utility consumption and utility exchanger areas are known prior to this stage of optimization. Hence, these fixed items need not be included in Eqs. (5.20) and (5.22).

For situations involving a large variation of the film coefficients, the area calculation from the LP model (Eq. 5.20) based on the composite curves with a uniform HRAT may deviate significantly from the true area target. The reason is that the uniform HRAT does not account for the difference in the film coefficients (see Chapter 4 for details). As a consequence, the quality of the starting point may be not as good as that obtained by applying the diverse pinch concept (Rev and Fonyo, 1991).

For such situations, the composite curves may be modified using the individual ΔT-contributions as suggested by Rev and Fonyo (1991). These may be used to shift streams according to their film coefficients and so generate the shifted composite curves. Blocks are then determined using the shifted composite curves and the LP model or the simple NLP model is formulated and solved. This technique results in an improved initial solution. An algorithm incorporating the method for individual ΔT-contributions (Rev and Fonyo, 1991) as outlined in Chapter 4 has been completed.

It should be noted that when it is required to place stream matching constraints in terms of prohibited matches or imposed matches, these constraints will only be associated with the NLP1, NLP2 or NLP3 and they are not linked with the LP (Eq 5.20) or the simple NLP model (Eq. 5.22). Otherwise, it may not be possible to obtain a feasible solution from the LP or the simple NLP model. As stated above, these two simple models only involve vertical heat transfer. With such matching constraints imposed, energy balance in each block for these two models may be unachievable by the vertical heat transfer.

5.8 The Procedure for Targeting and Synthesis

The models (NLP3) for total cost incorporate the trade–off between capital and energy costs. First, it is to generate a good initial solution. The composite curves used to generate a starting point may be determined by using simple pre-optimization schema. If film coefficients are similar, a single approach temperature difference, namely HRAT or ΔT_{min}, may be employed and the supertargeting approach suggested by Linnhoff and Ahmad (1986a & b) applied. Otherwise, the difference in film coefficients are considered using the individual ΔT contributions (Rev and Fonyo, 1991) and the pre–optimization scheme discussed in Chapter 4 or the paper by Zhu et al (1994) employed. Using the composite curves deduced as above, the number of blocks and block boundaries can be determined and a simple NLP model (Eq. 5.22) formulated and solved to provide an appropriate initial solution. Then NLP3 model is applied to deduce a final solution. In some cases, some constraints associated with integer variables are required and then a corresponding MINLP model is created. During the optimization process, the level of energy consumption is not fixed and the optimal energy consumption is determined through overall trade-off between energy and capital costs.

When targeting the area or the capital cost, the utility consumption is fixed at a desired level. The corresponding composite curves are used to determine the blocks and an initial solution is provided by solving either the LP model (for area targeting) or the simple NLP model for capital (Eq. 5.22). Then, either the NLP1 (for area) or NLP2 model (for capital) is employed to compute the corresponding target.

5.9 Case Studies

5.9.1. Case Study 1

This example was provided by Colberg and Morari (1990). The relevant stream data is summarized in Table 5.1. The appropriate composite curves are presented in Figure 5.4. For comparison purposes, the area is calculated with HRAT fixed at 10 K. This implies the minimum hot and cold utility requirements of 620 and 230 kW, respectively.

Table 5.1: Stream data for Case Study 1

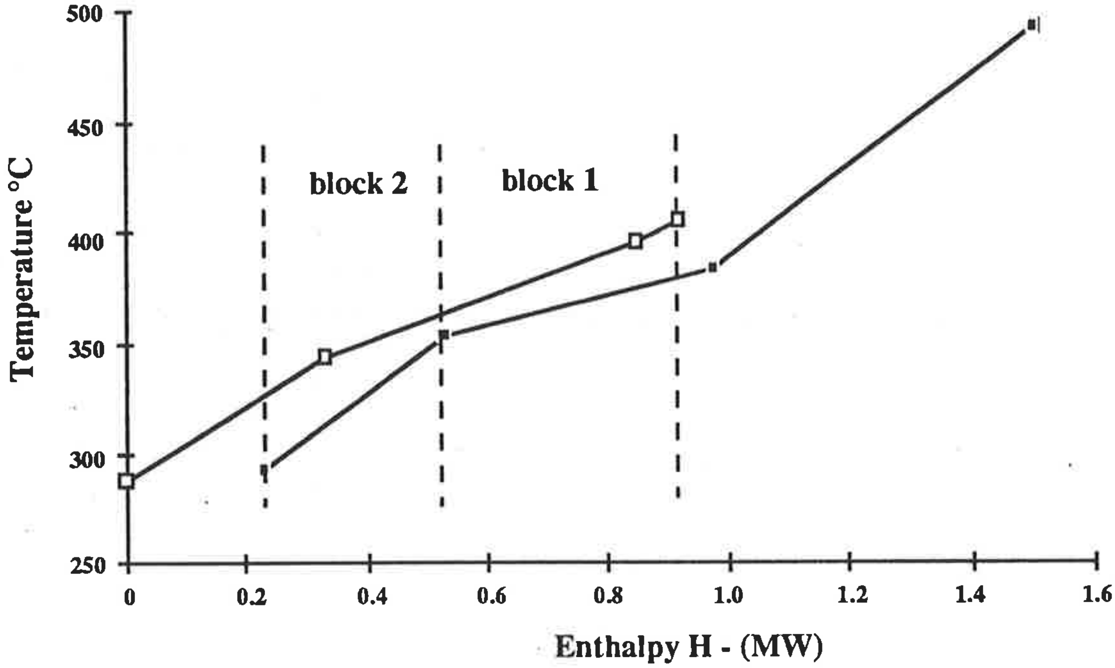
Stream	Supply temperature K	Target temperature K	Heat capacity flowrate kW K^{-1}	Film heat transfer coefficient W $m^{-2}K^{-1}$
H1	395	343	4	2000
H2	405	288	6	200
C1	293	493	5	2000
C2	353	383	10	200
Steam	520	520		2000
Water	278	288		2000

ΔT_m = 10K (for utility targeting)

Cost data: Steam = 80 \$ kW^{-1} yr^{-1}; Water = 20 \$ kW^{-1} yr^{--1}

Exchanger cost (annual basis) = \$ 350 $\left[A\ (m^2)\right]$

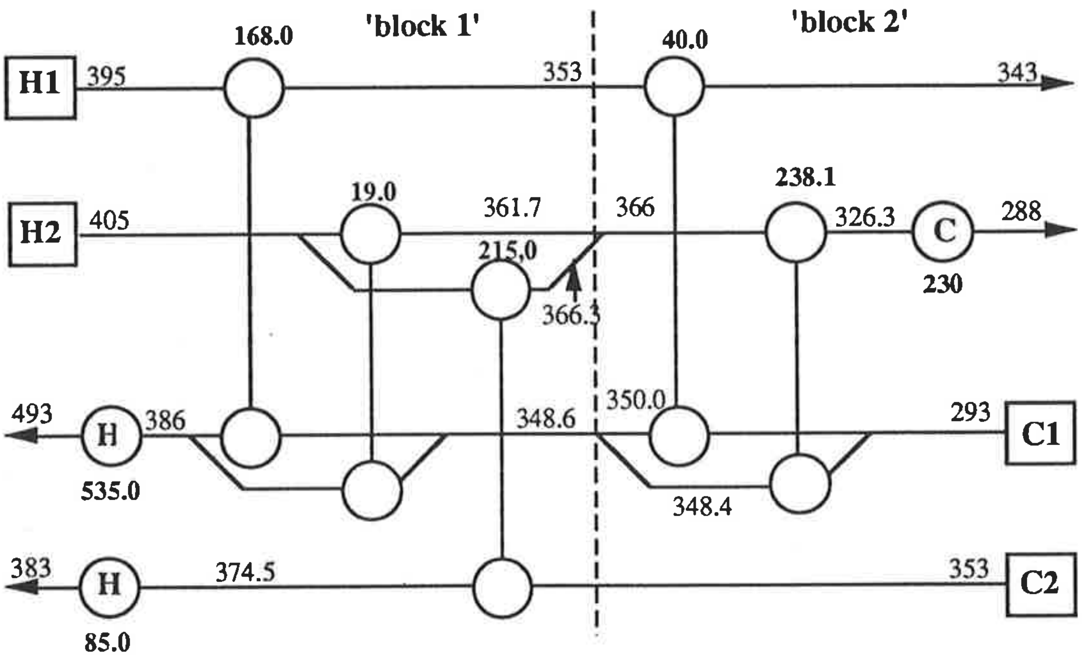
Those sections of the composite curves involving utility requirements are not considered in determining the number of blocks. Two sections exist where the hot/cold composite curves are distinctively different (Figure 5.4). Hence, the number of blocks is fixed at two. A two-block NLP1 model is formulated. The temperatures on the boundaries of two blocks can be deduced from the composite curves. These temperatures and associated stream data provide the basis for discovering an initial solution based on the LP model. The initial network requires 290.6 m^2 of exchanger area and the initial heat loads for all exchangers are obtained by solving the LP model. Using this initial solution, the solution to the NLP1 model has an minimum area of 262.9 m^2. The associated network (Figure 5.5) achieving this area target has eight exchangers.



Targets (Supertargeting; HRAT = 10 K): Q_H = 620 kW; Bath area target = 295.7 m^2;

cost target = 1.28 x 10^5 \$/yr

Figure 5.4: Composite curves for Case Study 1



Q_H = 620 kW; area = 262.9 m^2; Bath area target = 295.7 m^2

Figure 5.5: The network obtained using NLP1 model based on two blocks (Case Study 1)

Determination of the number of blocks using simple heuristics normally provides an adequate solution for targeting purposes. Increasing the number of blocks includes more structures and provides increased opportunities for re-matching streams thereby employing more exchangers. The solution quality (in area terms) may be improved but usually not significantly. However, an increase in the number of blocks is accompanied by substantial increases in problem size. The resultant networks generated in area targeting are also more complex.

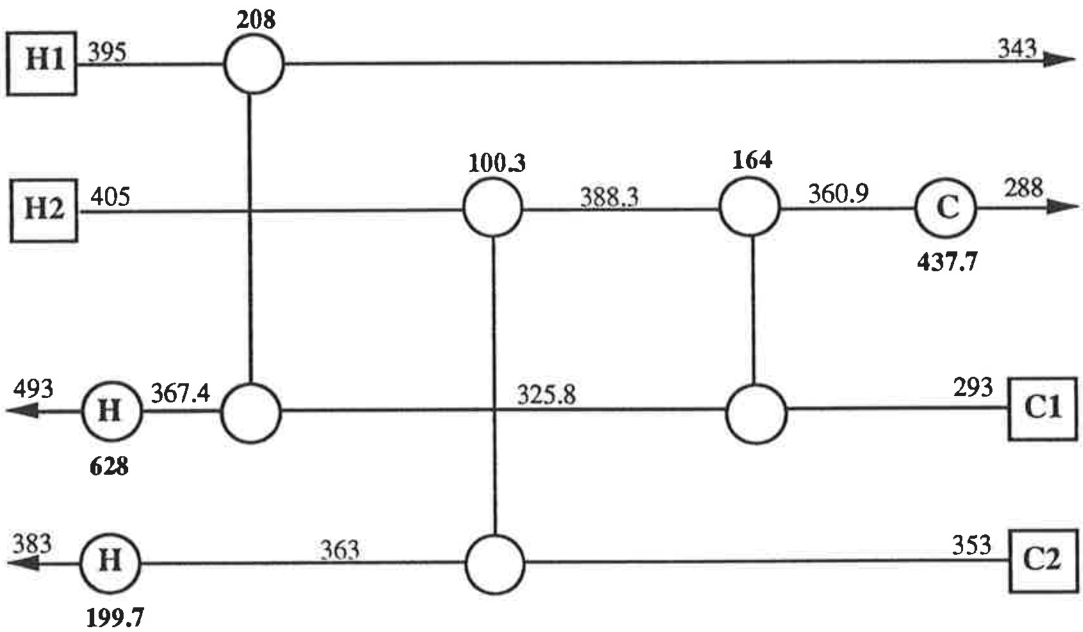
To illustrate the effect of increasing the blocks, consider a three block formulation. The solution generates an area of 258.6 m^2 with nine exchangers. The improvement in area is marginal (4.3 m^2 or 1.7%) and an additional exchanger is required. Clearly, for this problem, the two-block approximation is adequate.

The two solutions obtained compared favorably with the target derived using the NLP transshipment model of Colberg and Morari (1990). Their NLP model is based on TI's. Hence, seven TI's are required for the NLP model providing an area target of 258.8 m^2. However, using the proposed superstructure and a good initial solution, the new method using a formulation based on two blocks requires 262.9 m^2 of area whilst the use of three blocks results in an area target of 258.6 m^2. Both solutions are adequate as the area target. The area calculated using the simple equation of Townsend and Linnhoff (1984) is 295.7 m^2. This is 14.3% higher than the solution provided by the proposed method.

Another interesting comparison is between the superstructure proposed here and that deduced based on the superstructure with isothermal mixing. The two block solution requires 263.6 m^2 vs 262.9 m^2 and the use of three blocks 259.1 m^2 vs 258.6 m^2. This suggest no significant difference between the two superstructures. However, changing the film coefficients of H2 and C2 from 200 W $m^{-2}K^{-1}$ to 20 W

$m^{-2}K^{-1}$ produces an interesting outcome. In this case, the solutions using the model based on the two-block and three-block proposed superstructure require 2104.8 and 2056.3 m^2 in contrast to 2597.7 m^2 (23.4% higher) and 2463.2 m^2 (19.8% higher) obtained from the superstructure with isothermal mixing, respectively. Clearly, for situations involving large variations in the film coefficients, the superstructure with non-isothermal mixing provides an opportunity to trade-off branch temperatures thereby improving solution quality.

Design constraints are readily incorporated into the model. For example, if an unsplit solution is required, using the cost data and exchanger cost model provided, the solution achieving a minimum total cost using the MINLP model (NLP3 coupled with Eq. 5.17 as the 'split' constraint) in a two-block superstructure produces a network with six exchangers and total cost of $\$1.25 x 10^5$ (Figure 5.6). The network achieves this total cost (lower than the cost target of 1.28 x 10^5 \$/yr from the supertargeting) with a simple structure.



Total cost = 1.25 x10^5 \$/yr; Cost target (Supertargeting) = 1.28 x 10^5 \$/yr
Figure 5.6: The network obtained using NLP3 model based on two blocks with the constraint of no stream splits for Case Study 1

5.9.2 Case Study 2

This example (Table 5.2) is also taken from Colberg and Morari (1990). It includes four hot streams and one cold stream.

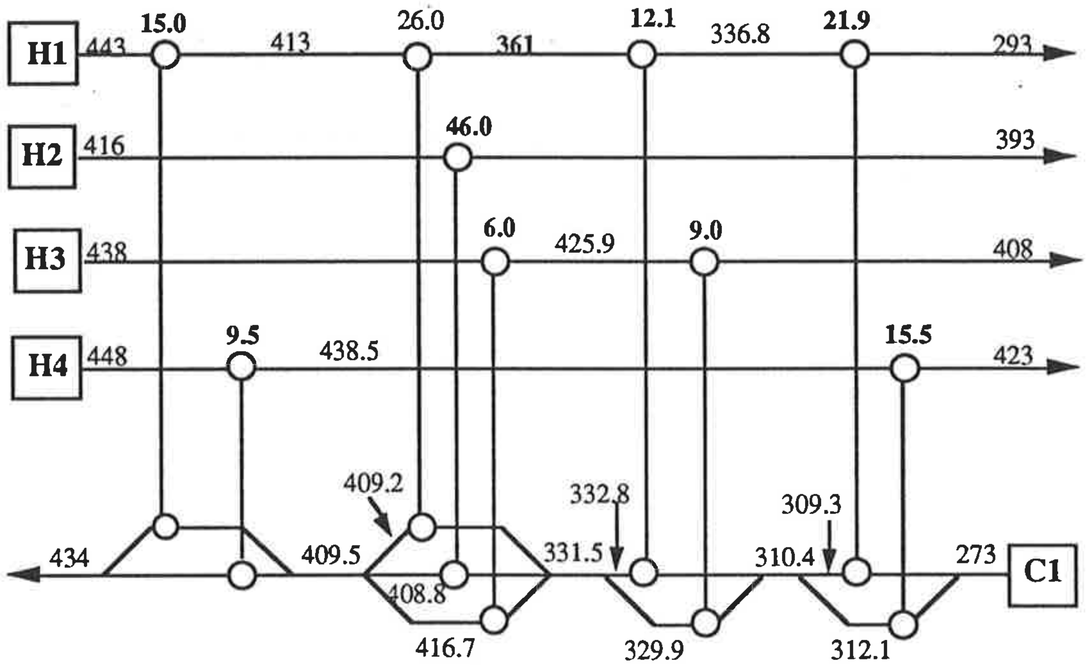
Table 5.2 Stream data for Case Study 2

Stream	Supply temperature K	Target temperature K	Heat capacity flowrate kW K^{-1}	Film heat transfer coefficient W $m^{-2}K^{-1}$
H1	443	293	0.5	2000
H2	416	393	2.0	285.7
H3	438	408	0.5	64.5
H4	448	423	1.0	40.8
C1	273	434	1.0	2000
Steam	None			
Water	None			

$\Delta T_m \leq 15K$ (for utility targeting)

Based on the data provided in Table 5.2, the problem has a large variation in film coefficients ranging over two orders of magnitude. For a HRAT less than 15 K, utility heating and cooling requirements are not required. Considering individual ΔT contributions (see Chapter 4 for detail), the associated composite curves may be obtained and four blocks determined as a reasonable compromise. The initial solution by LP model produces 43.2 m^2. This is 4.5 m^2 (about 10%) less than 47.7 m^2 of area calculated by the method (Townsend and Linnhoff, 1984). The model (NLP1) yields 31 m^2 of exchanger area and the associated network is given in Figure 5.7. This area is very close to the true area target of 29.84 m^2, calculated by using Nishimura's method (1980). The network structure derived by Nishimura is illustrated in Figure 5.8. Clearly, the structure in Figure 5.7 is significantly simpler than that in Figure 5.8. It incurs an area penalty of 1.16 m^2 but employs 11 fewer units. Colberg and

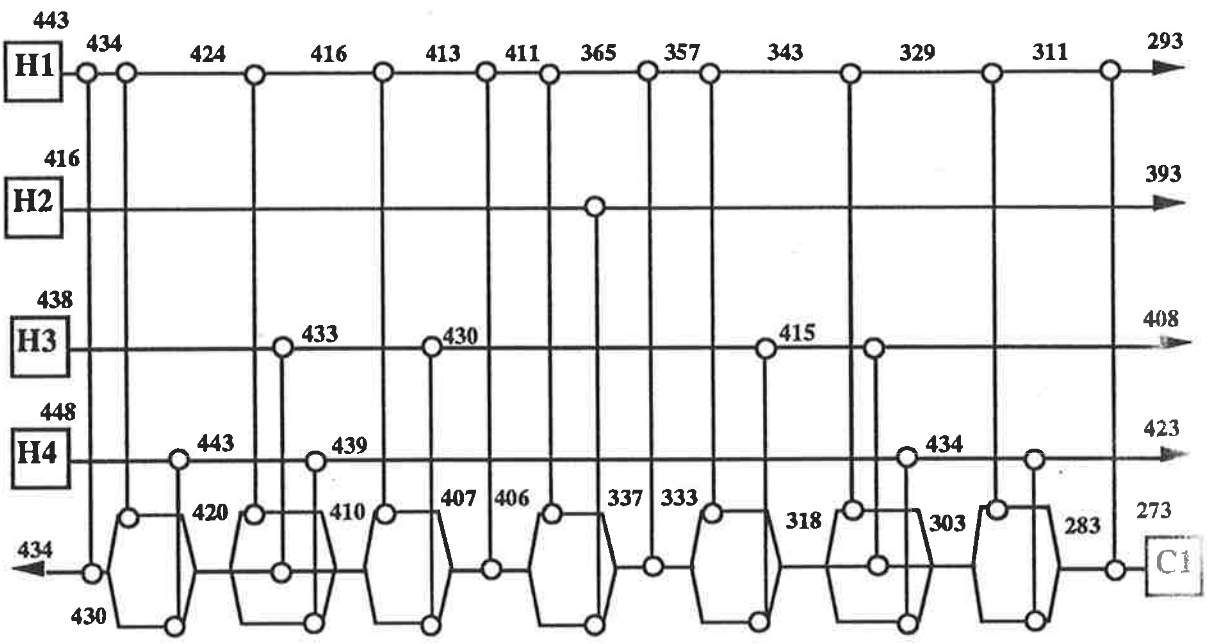
Morari (1990) studied this problem and their NLP solution shown in Figure 5.9 achieved the minimum area of 29.84 m^2 with 11 units which are 9 units less than the Nishimura's solution and 2 more units than the solution presented in Figure 5.7.



Area = 31 m^2; Bath area target = 47.7 m^2; units = 9

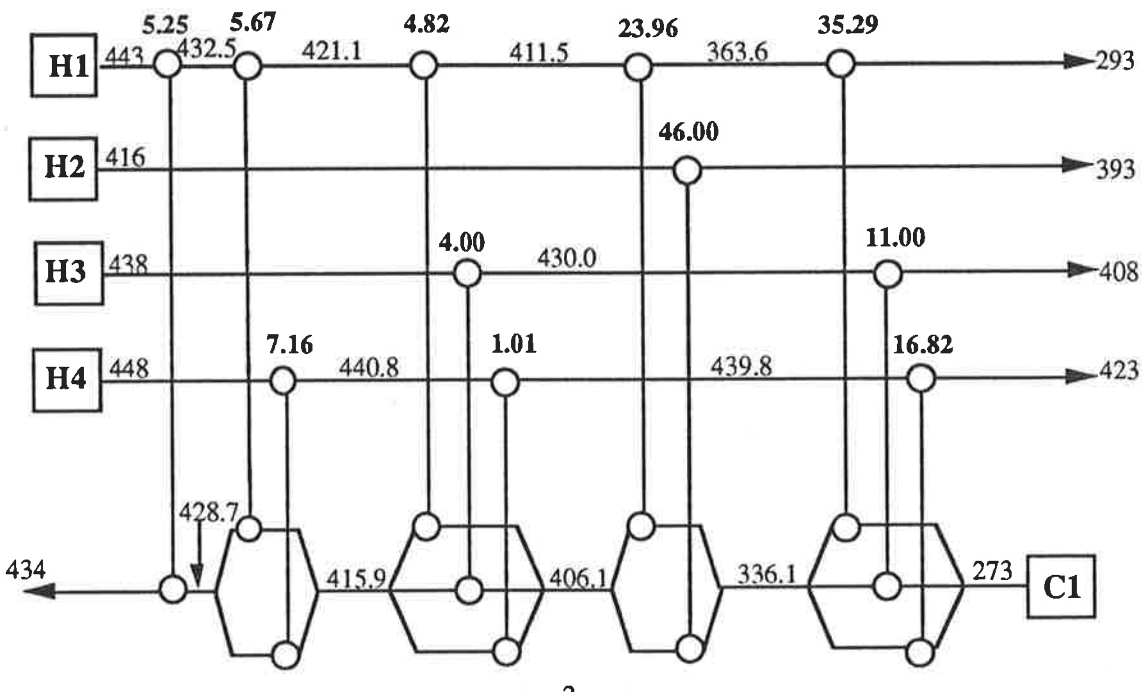
Figure 5.7: The resulting network using NLP1 model based on four blocks

(Case Study 2)



Area = 29.84 m^2; units = 20

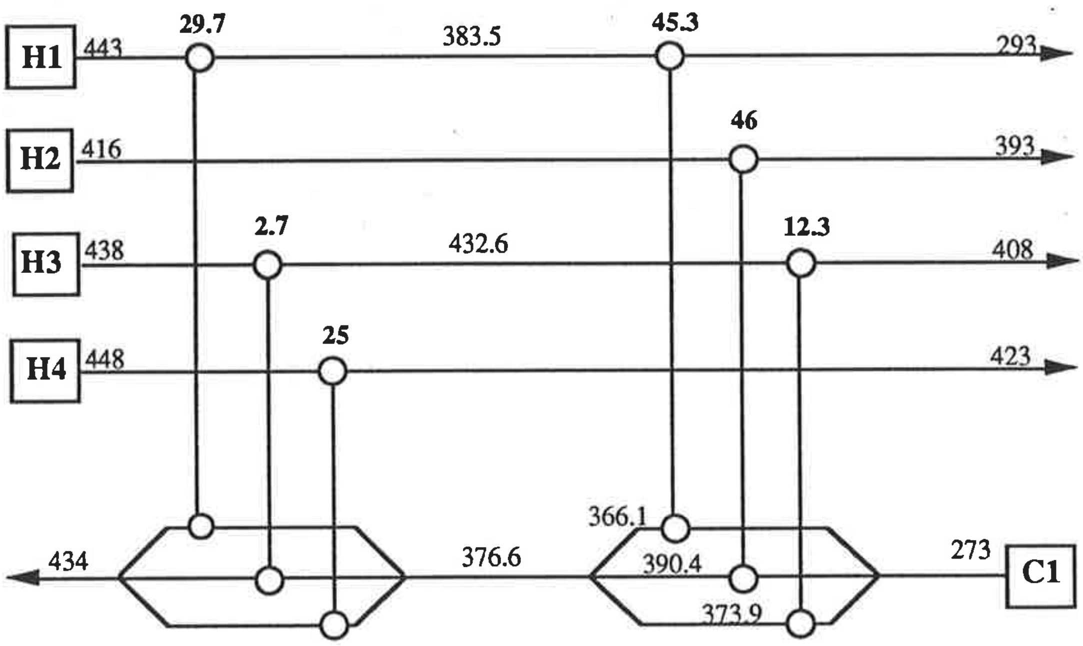
Figure 5.8: HEN structure deduced by Nishimura's method which achieves the real area target (Case Study 2)



Area = 29.84 m^2; units = 11

Figure 5.9: HEN structure deduced using the NLP model (Colberg & Morari, 1990) which achieves the area target (Case Study 2)

This example is also calculated based on two blocks. The area calculated is 36.58 m^2 and the network (Figure 5.10) has 6 units. This result shows that with the number of blocks reduced by two, the network structure is simplified by eliminating three exchangers (compared with the four block model) but with the penalty in area increase of 5.58 m^2 or 19.9%.



Area = 36.58 m^2; units = 6

Figure 5.10: The resulting network using NLP1 formulation based on two blocks (Case Study 2)

5.9.3 Case Study 3

This example demonstrates the targeting of the overall cost for network synthesis. The test problem was first proposed by Linnhoff et. al. (1982). It contains two hot and two cold streams. The stream data and appropriate cost data are summarized in Table 5.3. Prior to formulation of the mathematical programming model, pre-optimization is completed to deduce the appropriate composite curves. These form the basis for determination of the blocks on which the formulation will be based. An initial point at which to commence the solution of NLP 3 is next discovered by solving the simple NLP model presented as Eq. 5.22.

Table 5.3: Stream data for Case Study 3

Stream	Supply temperature K	Target temperature K	Heat capacity flowrate kW K^{-1}	Cost \$ kW^{-1} y^{-1}
H1	443	333	30	-
H2	423	303	15	-
C1	293	408	20	-
C2	353	413	40	-
Steam	450	450	-	80
Water	293	313	-	20

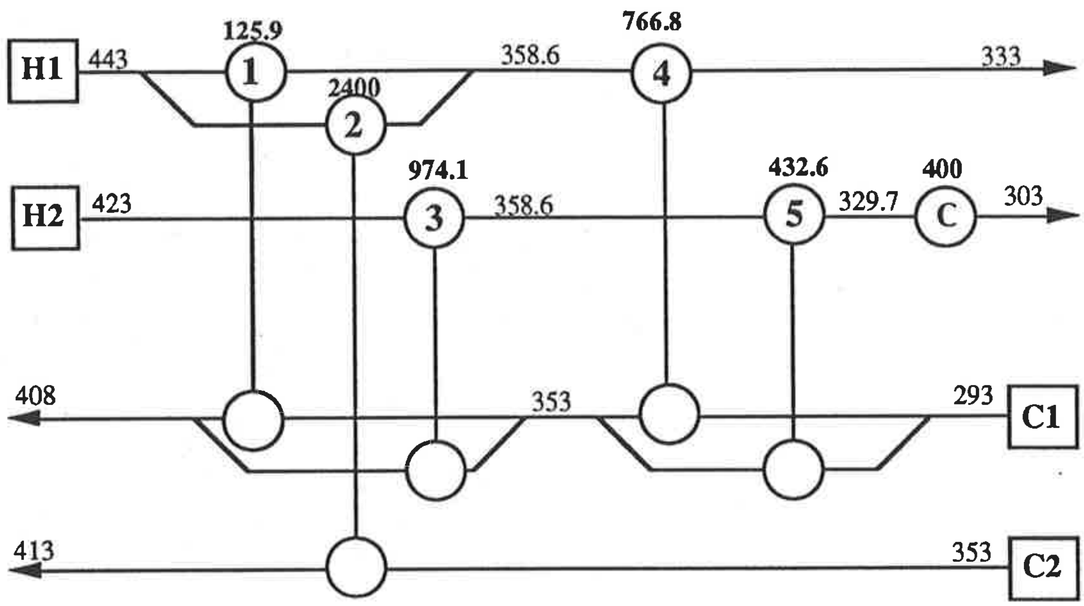
Coefficients:

U = 800 W $m^{-2}K^{-1}$ for all matches except involving steam
U = 1200 W $m^{-2}K^{-1}$ for all matches involving steam

Cost data:

Exchanger cost (annual basis) = \$ 1000 x $\left[A\ (m^2)\right]^{0.6}$ for all exchangers except heaters
Exchanger cost (annual basis) = \$ 1200 x $\left[A\ (m^2)\right]^{0.6}$ for heaters

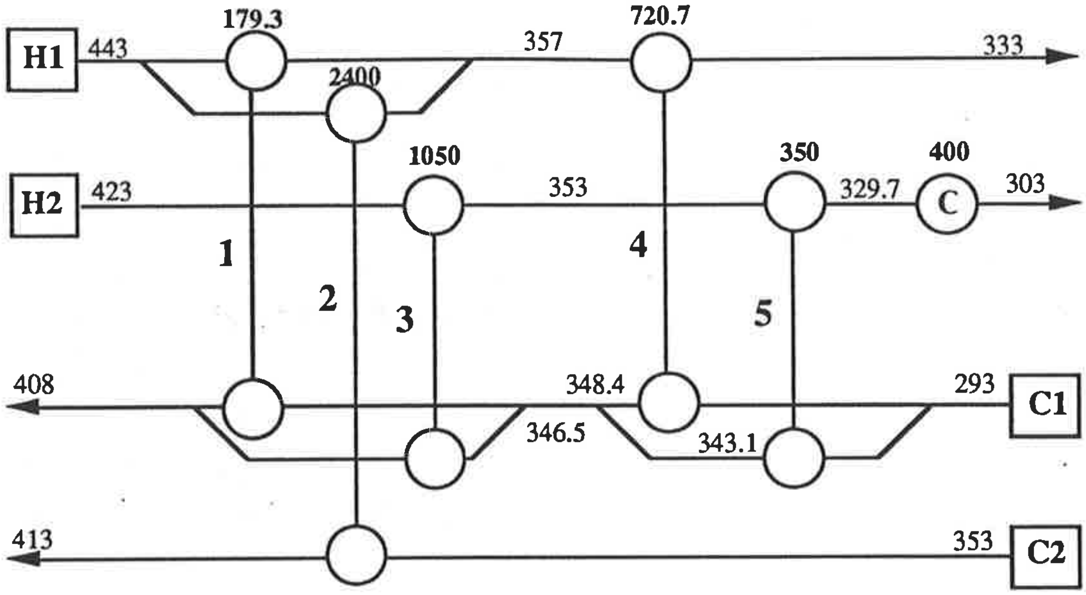
This pre-optimization stage using the supertargeting approach (Linnhoff and Ahmad, 1986a & b) yields a cost target of \$77,017 $annum^{-1}$ (corresponding to HRAT = 5 K) using the supertargeting approach. Only two blocks are needed based on the corresponding composite curves and no hot utility is required. Using these blocks and solving the simple NLP (Eq. 5.22) yields an initial network (Figure 5.11) with total cost of \$83,195 $annum^{-1}$.



Total cost = 83,195 $/yr

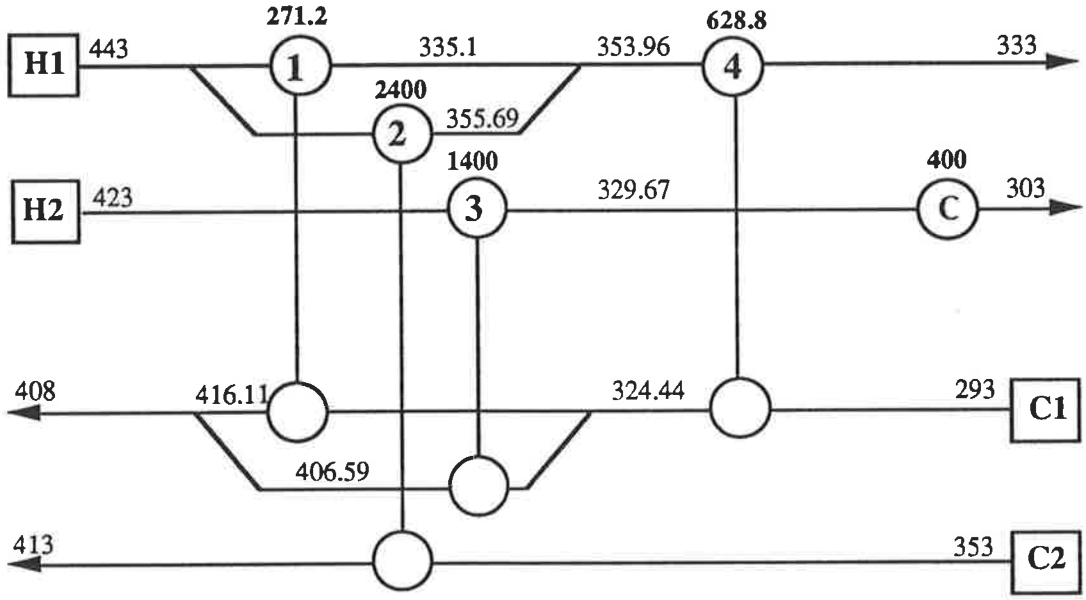
Figure 5.11: The initial solution to the simple NLP model (Eq. 5.22) (Case Study 3)

Based on this initial solution, the optimized solution to the NLP3 model gives the design shown in Figure 5.12. The NLP cost target is \$81,769 annum^{-1} and the network has an identical topology to the initial topology. Although the heat loads and temperatures differ somewhat, it can be seen that the initial solution of Figure 5.11 provides an excellent starting point for subsequent optimization to give Figure 5.12. This network is further optimized using the optimization procedure discussed in Chapter 3. The final optimal network is shown in Figure 5.13 with the total annual cost of \$80,274. This network minimizes the utility consumption to just \$8,000 annum^{-1} needing only cooling water. Obviously, the cost data favor the trade-off of requiring more area to minimize the utility requirement. The level of energy recovery corresponds to that of a threshold problem since only cooling water is needed. However, an internal pinch exists according to the composite curves at 358.56-353 K. A noteworthy feature of this network is that it includes three exchangers (1, 2, 3) which span the pinch . As well, exchanger 2 has a minimum approach temperature (EMAT) of 2.69 K.



Total cost = 81,769 $/yr; Cost target (Supertargeting) = 77,017 $/yr

Figure 5.12: The solution to the NLP3 model for Case Study 3

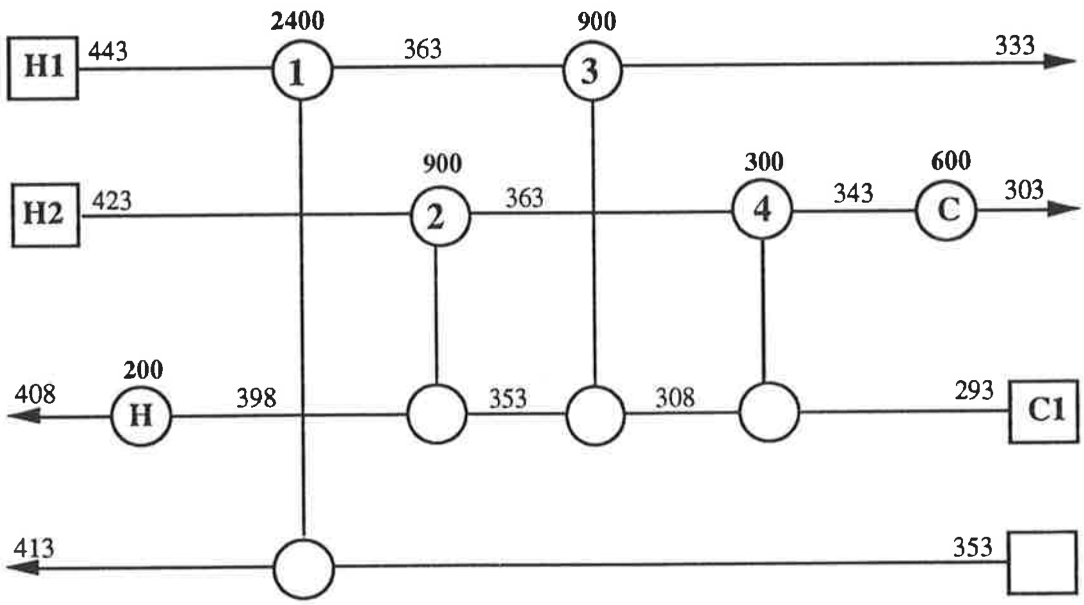


Total cost = 80,274 $/yr

Figure 5.13: The final optimized network based on the NLP3 solution

(Case Study 3)

Yee and Grossmann (1990) solved this problem and also obtained the solution in Figure 5.13. The procedure used was to solve an MINLP model first so as to produce the network with isothermal mixing splits and then a sub-optimization was performed to optimize split ratios and temperatures for the matches involving split streams. According to Yee and Grossmann (1990), the problem was also solved with an earlier procedure used in the program MAGNETS with a fixed HRAT = 10 K. The solution obtained (Figure 5.14), which is the same as the one reported by Linnhoff et al (1982), has an annual cost of \$89,832 annum^{-1} (10% higher than Figure 5.12 and 11% higher than Figure 5.13). Yee and Grossmann commented on the MAGNETS solution which has the drawback that utility consumption or the level of energy recovery (HRAT) was fixed throughout the optimization procedure. Also, since in MAGNETS, the problem was decomposed into two independent subnetworks at the pinch, the number of units may be larger than that without strict pinch decomposition. For this problem, six units were required as compared to five by the proposed method and that of the stage method of Yee and Grossmann (1990).



Total cost = 89,832 \$/yr

Figure 5.14: The MAGNETS solution for Case Study 3 (HRAT fixed at 10 K)

Another interesting feature of this example is the cost target (\$77,017 annum^{-1}) derived from the supertargeting approach is 6.2% lower than the cost target (\$81,769 annum^{-1}) of NLP 3. It should be noted that there are several reasons to which the lower cost from the supertargeting approach may be attributed. First, this problem has uniform film coefficients and thus the BATH area target gives the true minimum area target. Second, the optimal HRAT corresponds to a threshold problem (hot utility is not required) and thus $U_{min} = 4$ was used for targeting the capital cost. If the internal pinch associated with the threshold problem is considered, $U_{min} = 6$ may be used. If this unit target ($U_{min} = 6$) would be used, the corresponding cost target from the supertargeting approach would be higher. More importantly, though the uniform area distribution assumed in the supertargeting approach (Linnhoff and Ahmad, 1986 a & b) usually gives a higher cost estimate than the non–uniform area distribution, in some instances this penalty can be compensated by this simplified assumption that does not consider the physical reality of such a cost target. By contrast, the solution of the NLP 3 model simultaneously determines a feasible network and the cost target. Hence, it is not surprising to discover that, in some instances, the supertargeting approach may yield a lower cost target than the non-linear optimizer.

5.9.4 Case Study 4: Aromatics Plant Problem

This example is the well known aromatics plant problem. The modified version of the problem was studied by Linnhoff and Ahmad (1990). It contains four hot and five cold streams. The stream data and appropriate cost data are summarized in Table 5.4.

Prior to formulation of the mathematical programming model, pre-optimization is completed to deduce the appropriate composite curves. These form the basis for determination of the blocks on which the formulation will be based. This pre-optimization stage yields a cost target of \$2.91 x 10^6 annum^{-1} and the BATH area target (Townsend and Linnhoff, 1984) of 16984 m^2 which corresponds to HRAT = 26 K, using the supertargeting approach (Linnhoff and Ahmad, 1986a & b).

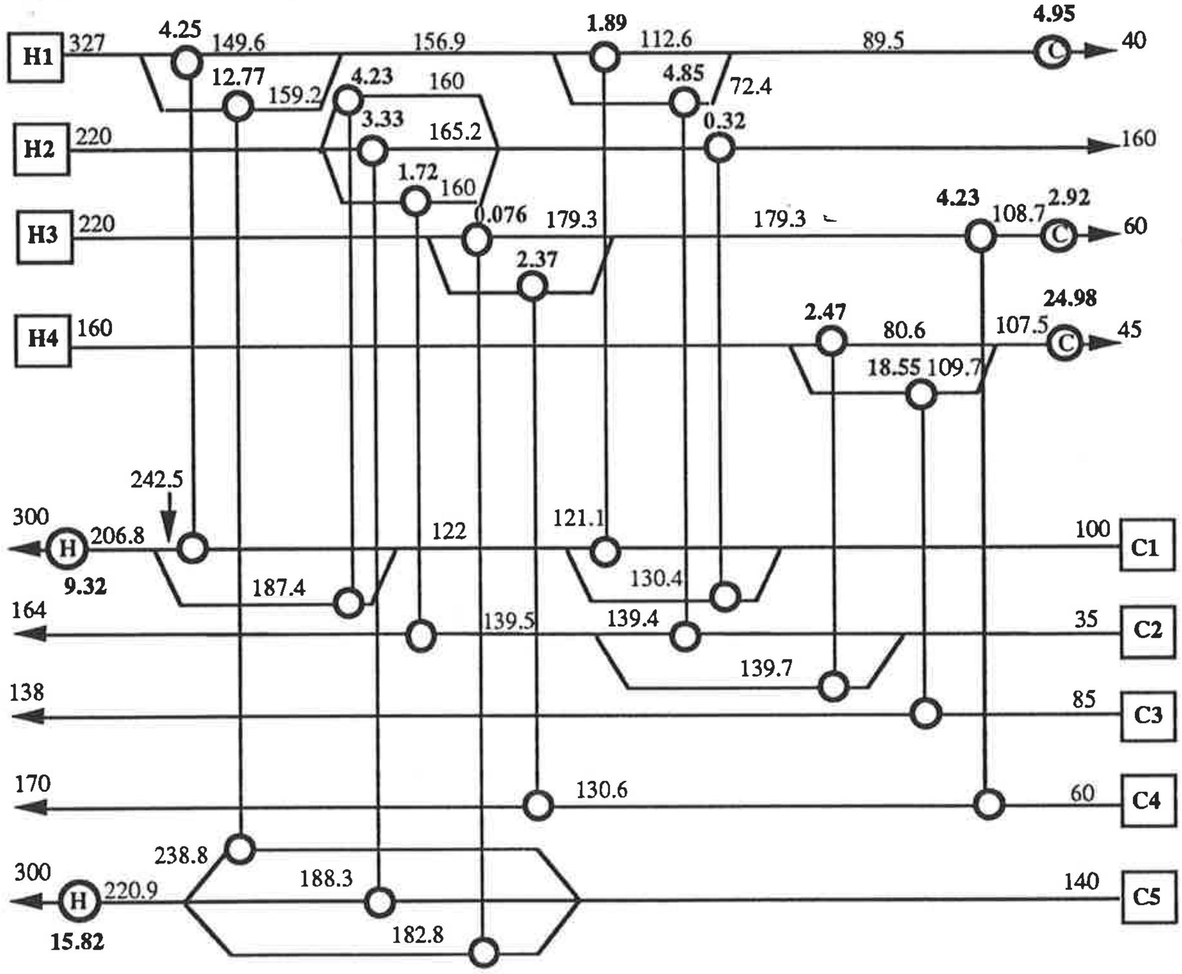
Table 5.4: Stream data for Case Study 4

Stream	Supply temperature K	Target temperature K	Heat capacity flowrate kW K^{-1}	Film coefficient kW m^{-2} K^{-1}
H1	327	40	100	0.50
H2	220	160	160	0.40
H3	220	60	60	0.14
H4	160	45	400	0.30
C1	100	300	100	0.35
C2	35	164	70	0.70
C3	85	138	350	0.50
C4	60	170	60	0.14
C5	140	300	200	0.60
Hot oil	330	250		0.50
Water	15	30		0.50

Cost data:

Exchanger cost (\$) = 10,000 + 350 x Area (m^2)
Plant lifetime = 5 (yr); Rate of interest = 0 (%)
Cost of hot oil = 60 (\$ kW yr^{-1}); Cost of cooling water = 6 (\$ kW yr^{-1})

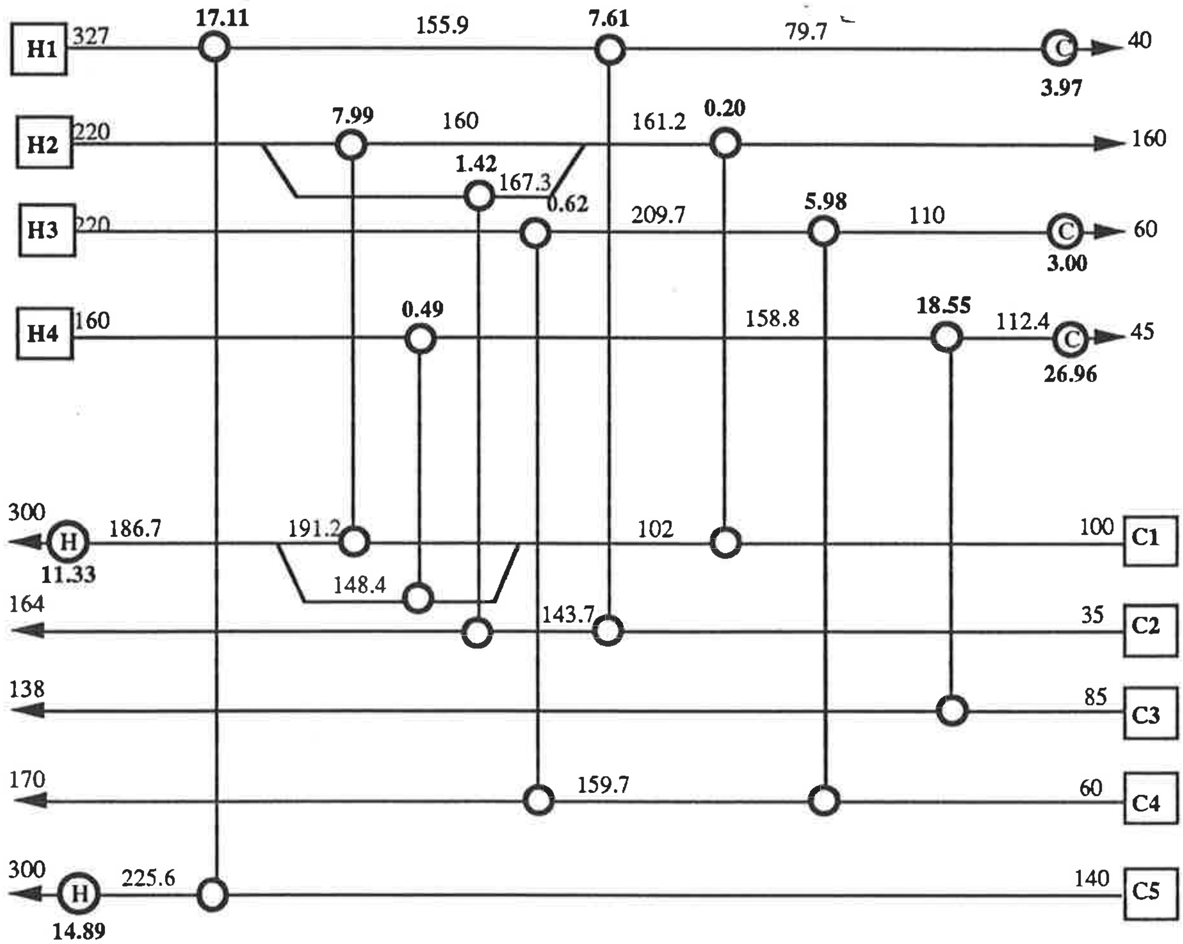
The minimum area is calculated using NLP1 based on two-block and four-block formulations respectively. From the composite curves at HRAT = 26 K, there are two regions with distinct profiles of composite curves and thus two-block formulation is applied initially. The solution (Figure 5.15) to the NLP1 has minimum area of 17225.5 m^2 with 18 units at HRAT = 26K. The four block formulation is also used to find out the potential in area reduction by increasing the number of blocks. The related solution from NLP1 gives the minimum area of 17083.9 m^2 obtained with 24 units. This only has achieved 141.6 m^2 (0.82%) reduction in area but needs 6 more units compared with the solution from the two-block formulation. With two blocks, the number of variables required by GAMS is 337, but the four block formulation has almost twice this number (653 variables). Obviously, this makes a NLP problem much more complex. Again, it is shown that the NLP1 model based on the blocks determined according to the profiles of the composite curves gives a good estimate of the minimum area.



Total Area = 17225 m^2 (HRAT = 26 K)

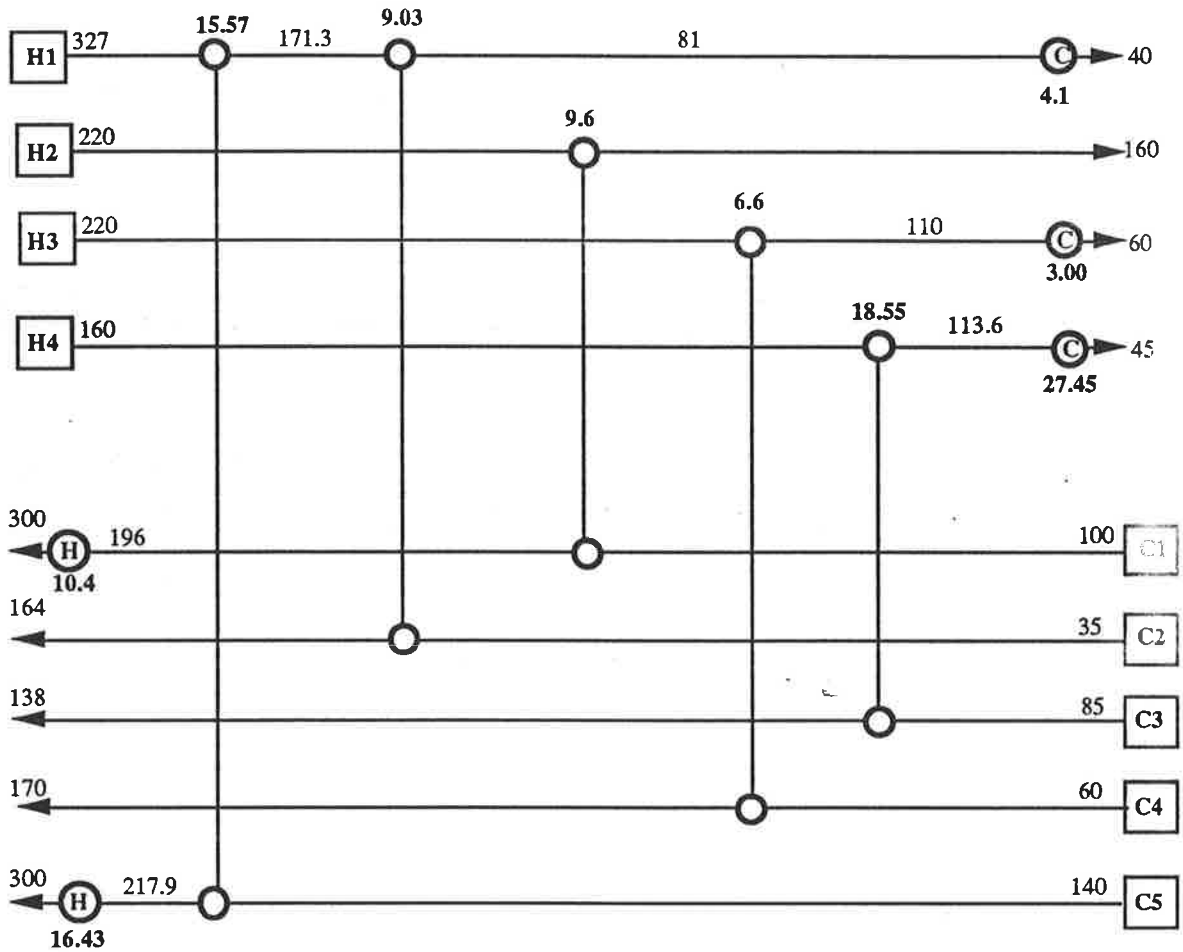
Figure 5.15: The solution to the NLP1 model for Case Study 4.

Two blocks are also used to calculate the minimum cost network using NLP3 based on the cost data provided. An initial solution at which to commence the NLP3 optimization is provided by solving the simple NLP model presented as Eq 5.22. The cost optimal network (Figure 5.16) requires 26.22 MW of hot utility, 16627 m^2 area and has the minimum total cost of \$2.97 x 10^6 per annum with a relatively simple structure (although 4 in excess of the unit target). This network can be optimized further on using the cost optimization method (see Chapter 3). This network was constrained to be a U_{min} design. The final optimized network (Figure 5.17) achieves the unit target (10 units) and has the total cost of \$2.98 x 10^6 $annum^{-1}$.



Q_H = 26.22 MW; Total area = 16,627 m^2; Units = 14; Total Cost = \$2.97x10^6 $annum^{-1}$

Figure 5.16: The solution to the NLP3 model for Case Study 4

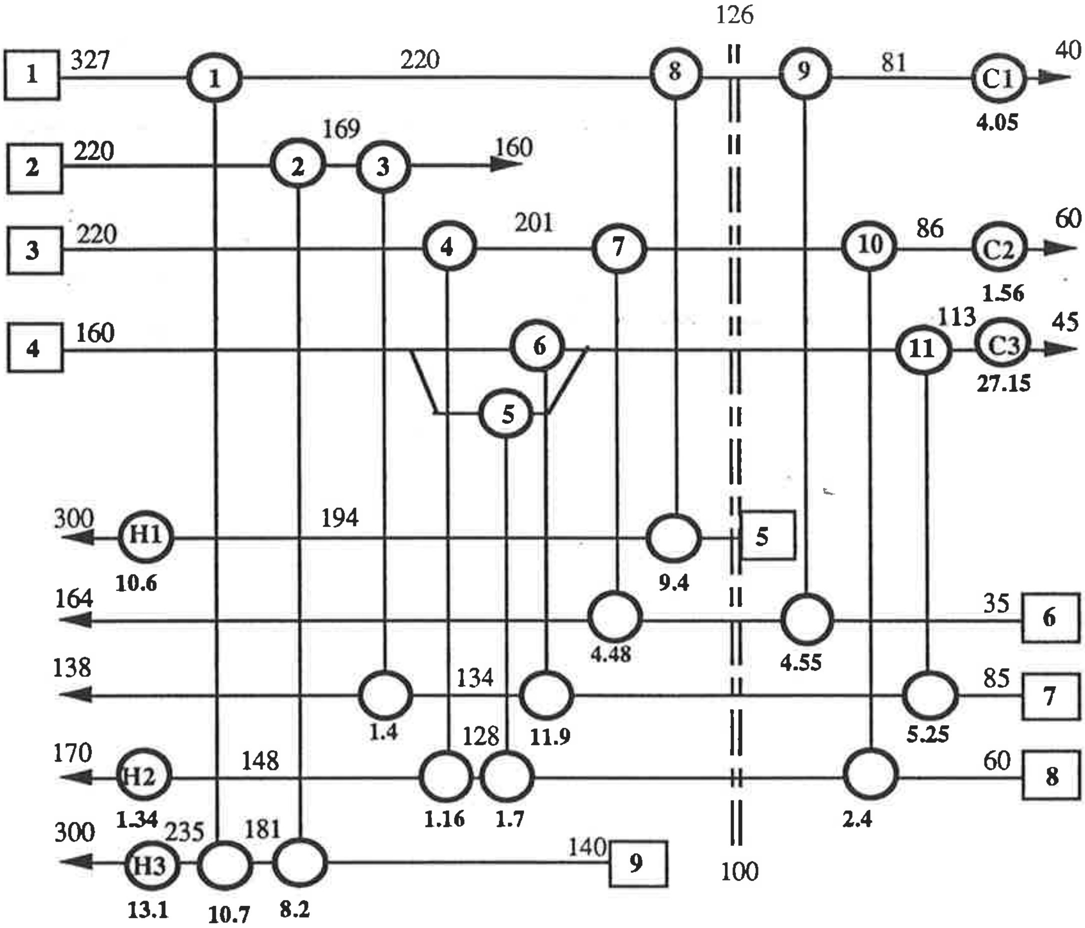


Q_H = 26.83 MW; Total area = 16,381 m^2; Units = 10;

Total Cost = $\$2.98 \times 10^6$ annum^{-1}

Figure 5.17: Optimized network based on the solution to NLP3 for Case Study 4

These two solutions (Figures 5.16 & 5.17) compare well with the two designs produced by Linnhoff and Ahmad (1990), an initial design (Figure 5.18) and an optimized network (Figure 5.19). Detailed comparison of the designs is summarized in Table 5.5.

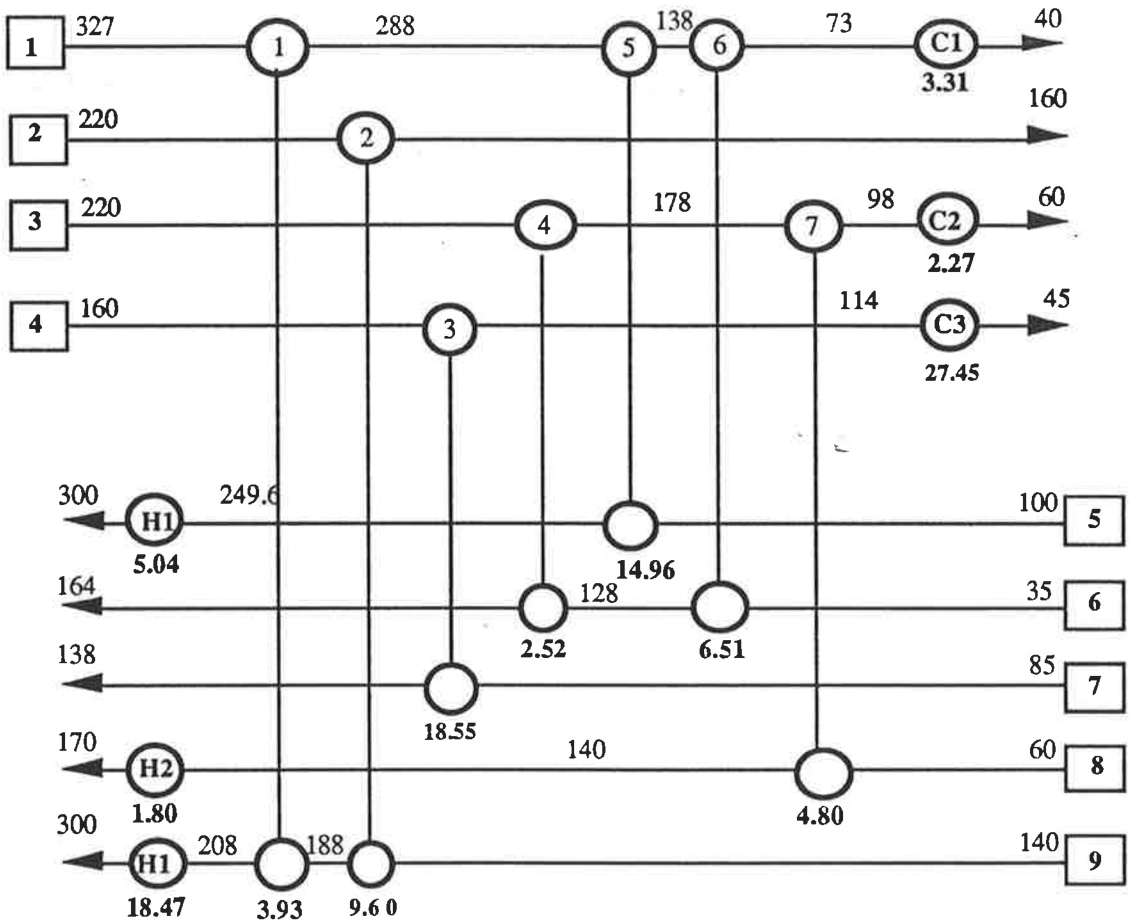


Q_H = 25.04 MW; Total area = 17,716 m^2; Units = 17;

Total Cost = $\$2.97 \times 10^6$ annum^{-1}.

Figure 5.18: Initial design applying the PDM for Case Study 4

(Linnhoff & Ahmad, 1990)



Q_H = 25.31 MW; Total area = 17,398 m^2; Units = 13;

Total Cost = $\$2.96 \times 10^6$ annum^{-1}.

Figure 5.19: Optimized Pinch Design for aromatics plant - Case study 4

(Linnhoff & Ahmad, 1990)

Table 5.5: Targets and Designs for Case Study 4

	Hot Utility (MW)	Cold Utility (MW)	Area (m^2)	Units	Total Cost $ $annum^{-1}$
Targets HRAT = 26 K (from supertargeting)	25.04	32.76	16984	10	2.91×10^6
Initial design Fig 5.18* Linnhoff & Ahmad	25.04	32.76	17716	17	2.97×10^6
Final design Fig 5.19* Linnhoff & Ahmad	25.31	33.03	17398	13	2.96×10^6
NLP3 solution (Fig.5.16)	26.22	33.94	16627	14	2.97×10^6
Final design # (Fig. 5.17) from NLP3	26.83	34.55	16381	10	2.98×10^6

---

* Linnhoff and Ahmad (1990) presented the total costs as M$ 2.93 yr^{-1} and M$ 2.89 yr-1 for the initial Pinch design in Figure 5.18 and the final Pinch design (Figure 5.19) respectively. The author was unable to reconcile this value with their calculations. The values for the areas and total costs used for these two designs were provided by a reviewer for the paper of Zhu et al (1993a). The calculations provided by the reviewer required that the hot utility be split for two of the heats with third in series following the split. This arrangement is not suggested in the paper of Linnhoff and Ahmad (1990). The arrangement is important as it avoids the low driving forces on some heaters.

\# The NLP3 solution (Figure 5.16) was further optimized with the constraint of a U_{min} design.

The cost model used above is linear and thus a minimum cost network tends to be a minimum area design. Clearly, the initial Pinch design (Figure 5.18) by Linnhoff and Ahmad (1990) has same total cost as the NLP3 solution (Figure 5.16). However, the latter design does posses some advantages related to its simpler network structure (14 units vs 17 units). As well, the final design (figure 5.17) based on the NLP3 solution has fewer three units with a marginal cost difference (2.98 M$ vs 2.96 M$) compared to the final Pinch design of Linnhoff and Ahmad (Figure 5.19). This difference would be amplified in favour of the proposed lower unit solution (Figure 5.17) if a typical non-linear cost model was used.

5.10 Conclusions

A mathematical algorithm employing block-based superstructures has been developed. The block concept provides the physical insight of how to achieve a minimum area HEN with a simple network structure and it has been successfully applied as the basis of the mathematical formulation. The number of blocks can be readily determined according to the composite curves. As a result of using blocks rather than TI's, the problem size is reduced greatly and good quality solutions are still maintained. In Case Study 1 of this Chapter, two blocks are used compared to seven TI's defined by 'kinks', a good area target is also achieved. With three-block superstructures, the area is only reduced by 1.7% but with the expense of one more exchanger. It has been shown that the small number of blocks as derived from the composite curves is usually adequate for targeting purposes.

Another physical insight is provided to mathematical programming through the application of the supertargeting approach (Linnhoff and Ahmad, 1986 a & b). With several simplifying assumptions, this approach can still give a good estimate of an 'optimal' HRAT through 'optimal' trade-off between energy and capital prior to design. This 'optimal' HRAT can be used as a good starting point for mathematical formulation. Therefore, together with a good starting point and simplified overall superstructures based on the block decomposition, the solution efficiency and quality can usually be improved.

The non-linearities in the model may lead to more than one local optimal solution due to their non-convexities. In addition, in a case with a bad initial solution, a nonlinear model may fail to find a feasible solution though such a solution exists. In order to overcome these problems and improve the quality of NLP solutions, a LP model for area targeting and a simple NLP model for cost targeting for an initial solution are also presented. These two models are formulated based on the block-superstructure with fixed block boundary temperatures. As the simple models provide excellent initial solutions (e.g. compare Figures 5.11 and 5.12), good solutions from NLP models can be found with ease and the likelihood of obtaining the global optimum is increased.

Some specific comments should be made on both the block method using the heuristic rules as outlined in Chapter 3 and the mathematical programming based on the block–based superstructure as discussed in this Chapter. It can be seen from Chapter 3, with the block decomposition and guideline by the heuristic rules, good initial solutions can usually be generated readily from the block method and the large search space for an original problem is reduced dramatically and quickly to a small spaced as defined by the initial solution. Thus, the cost optimization for the initial solution is mainly concerned with the optimization of parameters, e.g. temperatures and heat loads in the network although some exchangers may be removed when the corresponding heat loads are set to zero after optimization. Usually, an optimal or near optimal solution can be obtained by this strategy.

By contrast, although the block decomposition is also applied in mathematical programming, an initial solution is generated based on the superstructures. Clearly, this initial solution is complicated compared to an initial solution from the block method using heuristic rules. In other words, such a complicated initial solution has a much larger search space. Theoretically speaking, a large search space has a better chance of including an optimal solution with good quality (near the global optimum). Due to the power and speed of digital computers and the sophistication that modern optimization techniques have, mathematical programming may be able to find optimal solutions with good quality or give alternative solutions compared to the block method. For example, the mathematical programming based on the block concept gives the alternative optimal design (Figure 5.17) to the two optimal designs (Figures 3.23 & 3.24) from the block method using the heuristic rules. So, it is suggested that it may be worth using these two methods together to generate more designs from which a best one can be selected after investigating safety, operability, controllability and economic performance. However, it is important to realize the limitations in mathematical programming methods. Though the problem size is already reduced greatly by applying some methods, e.g. the block concept or the stage concept, it is still not an easy task for a mathematical programming method to handle large industrial problems due to the limitations of optimization techniques and computers.

CHAPTER 6

KIRCHHOFF'S LAW AND LOOP-BREAKING *

SUMMARY

Traditional evolutionary methods for the synthesis of heat exchanger networks normally produce an initial network containing excess units when compared to the minimum units target. Subsequently, this network is simplified by energy relaxation. However, current methods fail to guarantee that the evolution follows a pathway ensuring that the minimum energy penalty is incurred.

A new method to guide this evolution is presented (Zhu et al, 1993c). It is based on the application of Kirchhoff's Law to the network. This enables easy prediction of the actual energy penalties incurred by instituting different loop-breaking strategies. The minimum energy penalty may be discovered and the units to be removed while yielding an optimal solution readily identified. The precedence order for loop breaking in networks containing multiple loops can also be determined according to their respective energy penalties. The proposed algorithm enables the designer to undertake the loop-breaking phase of network design with confidence. The minimum energy path may be followed until a final network is discovered.

---

* This work was carried out prior to the development of the block method. The major focus of this work was how to achieve the U_{min} design by allowing energy relaxation while applying ΔT_{min} (HRAT) as global minimum temperature approach. However, in the block method, the network simplification is carried out in the process of non linear optimization for total cost.

6.1 Introduction

The majority of heuristic design methods proposed for synthesis of heat exchanger networks are based on the pinch decomposition/evolutionary strategy and the resulting initial network features maximum energy recovery (Gundersen and Naess, 1988). This network usually contains a larger number of units than the theoretical minimum. Such a network is complex and incurs a capital cost penalty. The extra units indicate the presence of loops and the number of independent loops equals:

$$L = U_{initial} - U_{min} \tag{6.1}$$

where $U_{initial}$ is the number of units in a network and U_{min} the target for the minimum number of units.

A simpler network with lower capital cost may be achieved by reducing the number of units using loop breaking and additional energy is usually required to restore approach temperatures to ΔT_{min}. Therefore, loop breaking results in an energy penalty and different sequences of loop breaking usually incur different energy penalties. The objective of loop breaking is to remove loops and incur a minimum energy penalty in restoring ΔT_{min}.

Various methods have been proposed to guide loop breaking (Su 1979, Linnhoff *et al.*, 1982, Trivedi *et al.*, 1990). Unfortunately, these methods rely heavily on heuristics which often produce suboptimal energy designs. A simple and efficient method is proposed based on the application of Kirchhoff's law to heat exchanger networks. The method normally provides the minimum energy penalty solution for the loop-breaking problem.

6.2 Motivating Example

A common practice is to eliminate the smallest unit in a loop (Linnhoff *et al.*, 1982). However, this heuristic cannot guarantee the minimum energy penalty for breaking a loop (Trivedi et al, 1990). Consider the network shown in Figure 6.1 using ΔT_{min} = 20 K as an example. A loop exists containing units 1 and 2. Following the principle that the smallest unit should be removed, the unit 1 is removed and its 3.0 kW load is shifted to unit 2. After energy relaxation, the energy penalty incurred is 6.0 kW.

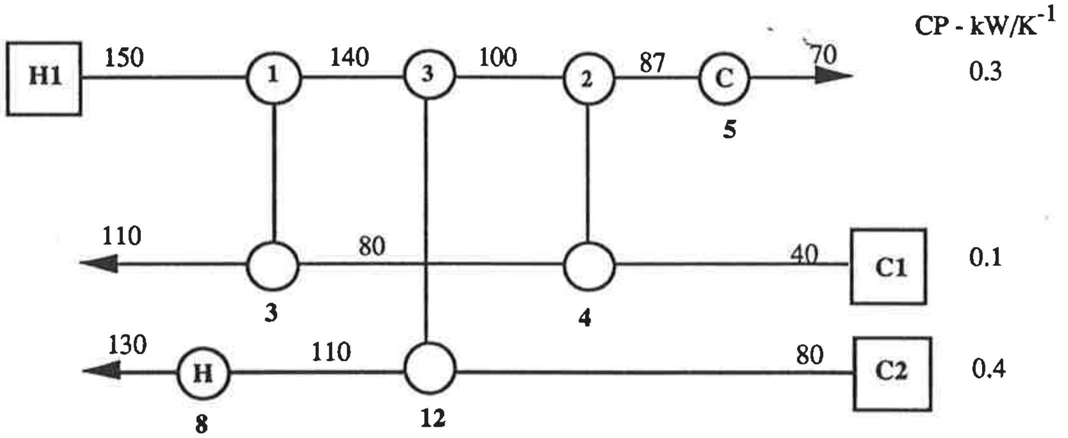


Figure 6.1: Initial MER network for motivating example

Alternatively, removing unit 2 results in an energy penalty of only 4.0 kW. This illustrates that the application of the heuristic favouring removal of the smallest load cannot guarantee the minimum energy penalty. The maximum energy penalty or net energy transfer across the pinch resulting from loop breaking does not necessarily equate to the load shifted. Clearly, a problem with loop breaking is prediction of the energy penalty incurred in breaking a loop and identification of which unit in a loop is to be removed in order to guarantee the minimum energy penalty.

The following sections will discuss the application of Kirchhoff's Law in electrical networks to heat exchanger networks and how the problem of energy relaxation with minimum energy penalty can be solved with the proposed procedure.

6.3 Kirchhoff's Law

Kirchhoff's law for electrical networks may be applied to heat exchanger networks using temperature differences as the driving forces.

For example, consider the network illustrated in Figure 6.1 involving streams H1 and C1. Unit 1 and unit 2 form a loop as shown in Figure 6.2(a). Arbitrarily defining the positive direction of the temperature difference as indicated by the arrow and summing clockwise around the mesh:

$$\frac{Q_1}{CP_{H1}} + \frac{Q_2}{CP_{H1}} + \frac{Q_3}{CP_{H1}} + \Delta T_2 - \frac{Q_2}{CP_{C_1}} - \frac{Q_1}{CP_{C1}} - \Delta T_1 = 0 \qquad (6.2)$$

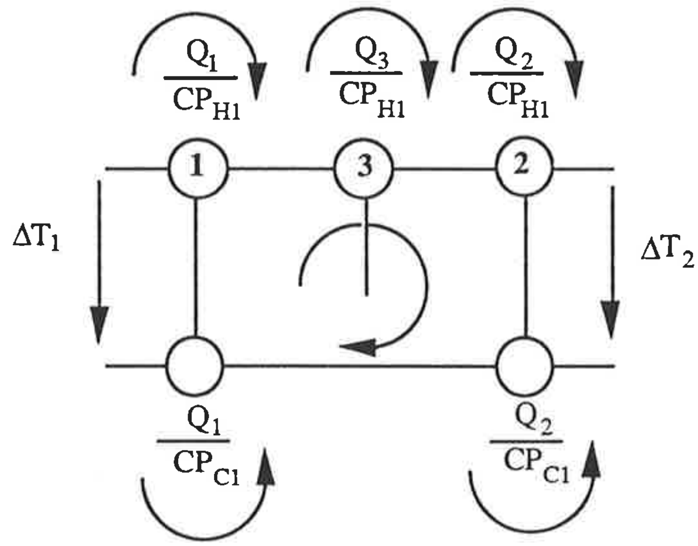


Figure 6.2(a): Example 1 for illustrating Kirchhoff's Law

This equation relates the temperature differences over the network and may easily be checked using the data in Figure 6.1 associated with the matches 1,2 and 3. Alternatively, if one selects unit 2 and the cooler for consideration, the corresponding situation is summarized in Figure 6.2(b). The following equation can be deduced:

$$\frac{Q_2}{CP_{H1}} + \frac{Q_C}{CP_{H1}} + \Delta T_4 - \frac{Q_2}{CP_{C1}} - \Delta T_3 = 0 \qquad (6.3)$$

Application of Kirchhoff's law to a heat exchanger network facilitates the calculations of temperatures and heat loads as the network is evolved.

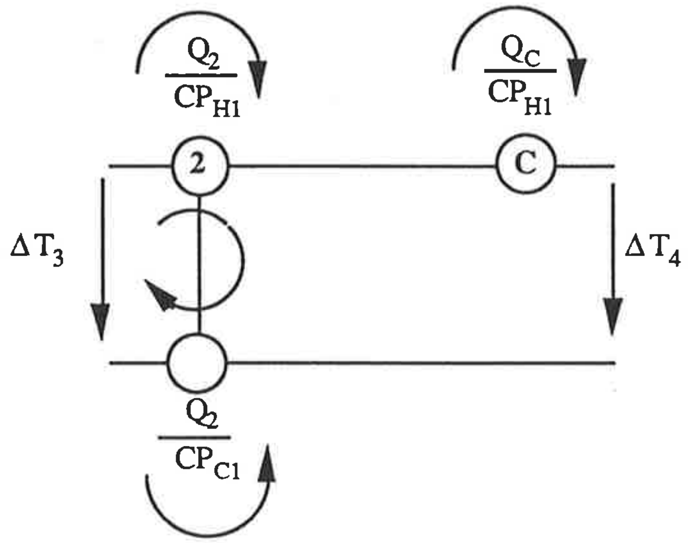


Figure 6.2(b): Example 2 for illustrating Kirchhoff's Law

6.4 Introduction of The Method for Loop Breaking

Let us reconsider the previous example [Figure 6.3(a)] in general terms to explain the method. The network in Figure 6.3(a) possesses a loop including units 1 and 2 with loads of X_1 and X_2 kW, respectively. Two ways for breaking the loop are possible and the energy penalty incurred upon loop-breaking may be derived as follows.

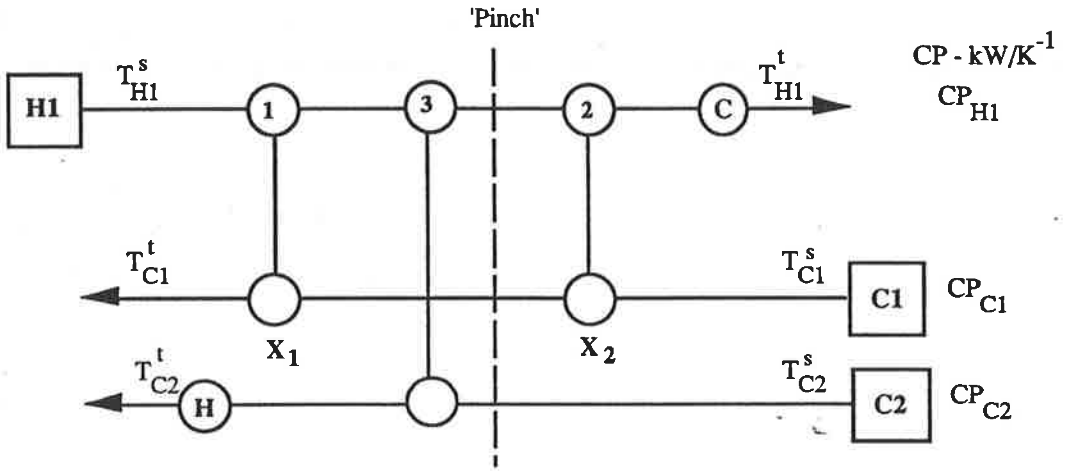


Figure 6.3(a): Network featuring a single loop (motivating example)

6.4.1 Removal of unit 1

The temperature differences around unit 2 prior to loop breaking are illustrated in Figure 6.3(b). Summing these differences clockwise yields:

$$\frac{X_2}{CP_{H1}} + \Delta T_2 - \frac{X_2}{CP_{C1}} - \Delta T_{min} = 0 \tag{6.4}$$

Upon removal of unit 1, a ΔT_{min} violation may occur at the hot end of unit 2. Assume that an energy penalty of Y_1 kW is incurred to restore ΔT_{min} to the hot end of unit 2. Applying Kirchhoff Law to the temperature differences of the unit as shown in Figure 6.3(c) yields

$$\frac{X_1+X_2}{CP_{H1}} + \frac{Y_1}{CP_{H1}} + \Delta T_2 - \frac{X_1+X_2}{CP_{C1}} - \Delta T_{min} = 0 \tag{6.5}$$

Subtracting equation (6.4) from (6.5), the energy penalty for removing unit 1 can be predicted as:

$$Y_1 = \left[\frac{CP_{H1}}{CP_{C1}} - 1\right] X_1 \tag{6.6}$$

If the match 2 has been designed correctly according to the Pinch Design Method, (Linnhoff *et al.*, 1982), i.e. $CP_{H1} > CP_{C1}$, then $Y_1 > 0$.

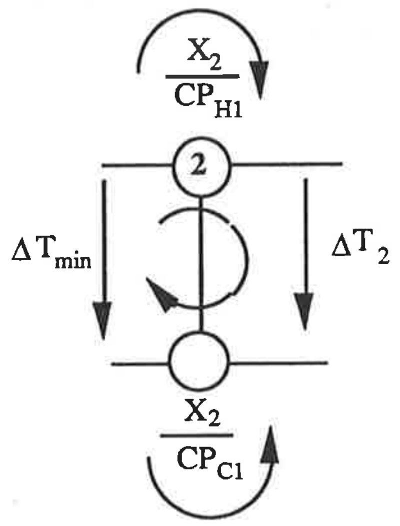


Figure 6.3(b)

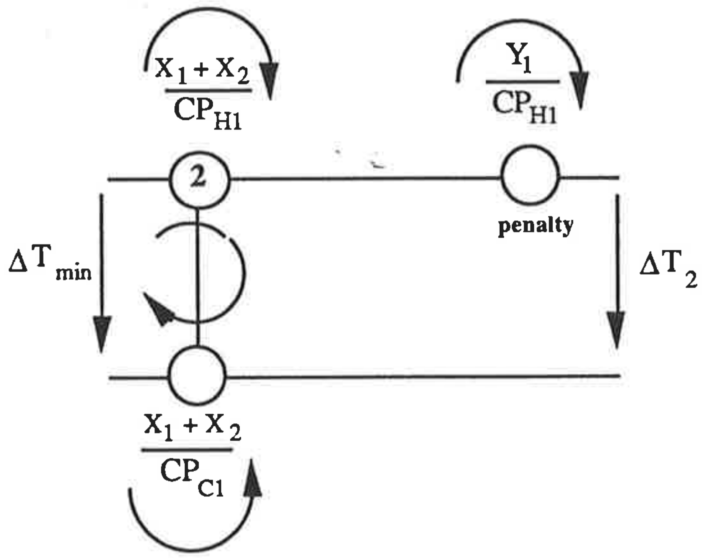


Figure 6.3(c)

6.4.2 Removal of unit 2

Although unit 3 is not included in this loop, the ΔT_{min} violation may occur at the cold end of unit 3, because this unit is located at the pinch. Figure 6.3(d) summarizes the situation prior to loop breaking. Applying Kirchhoff's law yields:

$$\frac{X_1}{CP_{H1}} + \frac{X_3}{CP_{H1}} + \Delta T_{min} - \frac{X_3}{CP_{C2}} - \Delta T_1 = 0 \tag{6.7}$$

After loop breaking, an energy penalty of Y_2 kW is incurred to restore ΔT_{min} and the new situation is summarized as Figure 6.3(e). Thus

$$\frac{X_1+X_2}{CP_{H1}} + \frac{X_3 - Y_2}{CP_{H1}} + \Delta T_{min} - \frac{X_3 - Y_2}{CP_{C2}} - \frac{Y_2}{CP_{C2}} - \Delta T_1 = 0 \qquad (6.8)$$

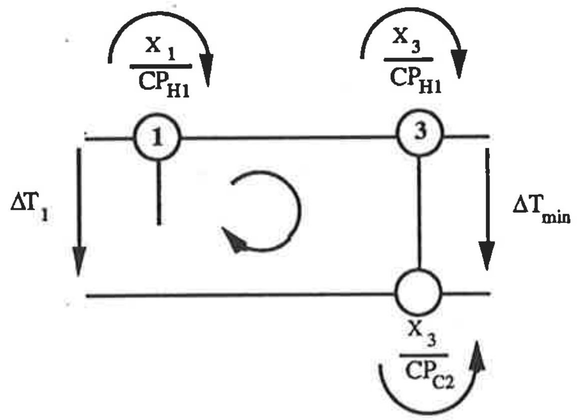


Figure 6.3(d)

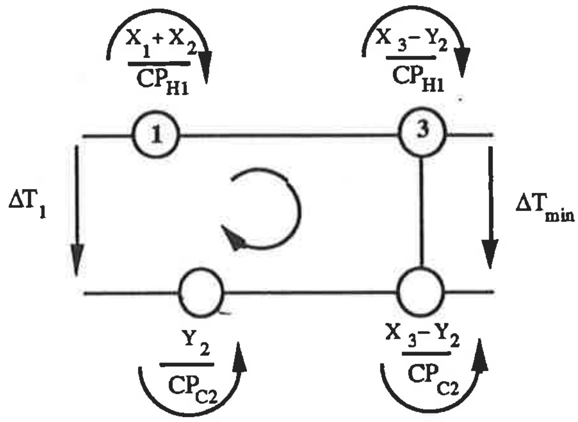


Figure 6.3(e)

Subtracting (6.7) from (6.8), the energy penalty incurred is:

$$Y_2 = X_2 \qquad (6.9)$$

Hence, the minimum energy penalty for breaking the loop in Figure 6.3(a) equals:

$$P_{min} = \mathit{min}\,(Y_1, Y_2) \qquad (6.10)$$

and the unit to be removed to achieve this minimum energy penalty is identified.

Let $CP_{H1} = 0.3$ kW K^{-1}, $CP_{C1} = 0.1$ kW K^{-1}, $X_1 = 3.0$ kW and $X_2 = 4.0$ kW, then $Y_1 = 6.0$ kW and $Y_2 = 4.0$ kW are calculated using equation (6.6) and (6.9). The minimum energy penalty for breaking this loop equals 4.0 kW and the optimal solution is removal of unit 2 with a load of 4.0 kW rather than unit 1 with a smaller load of 3.0 kW.

6.4.3 Summary of Loop-Breaking Procedure

The general procedure for breaking a loop can be summarized as:

1. Determine the candidates for removal and select for analysis the units at which the violation of ΔT_{min} may occur.
2. Apply Kirchhoff's law to the terminal temperature differences around such units and calculate the associated energy penalties.
3. Determine the minimum energy penalty incurred from the set of energy penalties and identify the unit which is to be removed to obtain an optimal solution.

For a network containing more units than the U_{min} target, many alternative routes exist for determining the candidates for loop breaking (Appendix F). Normally, it is impractical to consider all the possible alternatives. To reduce complexity and maintain a high probability of finding an optimal solution, the following heuristic is suggested. In loop-breaking, *first consider process-process loops with the smallest number of units (the lower-level loops) and those with the smallest heat loads.*

For loops selected in this manner, the order of loop breaking is determined by minimizing the energy penalty. The minimum energy penalty for each loop must be calculated. The loop incurring the global minimum energy penalty is broken and the unit with the minimum energy penalty is identified. The network is evolved by breaking this loop. The procedure is then repeated until a desired final network is discovered. As a result, the final network will contain the minimum number of process-process units whilst incurring minimum energy penalty.

Two types of loops may be identified in heat exchanger networks, namely: process-process loops and process-utility loops. If we select the latter for initial loop breaking, we may seriously affect plant operability. Process-process loops are considered first. Loop breaking may cause a violation of thermodynamic constraints on some individual exchangers. These exchangers are usually located at terminals of streams and loops including such exchangers were called "locked loops" by Trivedi et al (1990). The infeasibilities associated with breaking a locked loop may be overcome by introducing additional utility exchangers.

6.5 Case Studies

6.5.1 Case Study 1

This example was introduced by Floudas et al (1986). Trivedi et al (1990) produced a MER design (Figure 6.4) for the problem which was evolved to a U_{min} design (Figure 6.5) using an energy relaxation method based on the insights into the interaction between loops and the network. For comparison, the MER design will be evolved using the newly proposed method.

The initial network (Figure 6.4) contains ten process-process exchangers and three utility exchangers (total thirteen units). A U_{min} design would feature eight units (six for process-process units and other two for utility exchangers). Hence, five loops (13 – 8) must exist and it is possible to eliminate at least four process-process units (ten process-process exchangers in Figure 6.4 minus six which is the minimum number of process-process exchangers). The four lower-level loops are: (3, 9); (4, 11); (2, 7, 8, 5) and (2, 3, 10, 6). To establish the precedence order for loop breaking, the energy penalty to break each loop is calculated as detailed earlier and the minimum is determined. The respective energy penalties and unit removed for each loop are:

(110.5 kW, 9); (1.85 kW, 11); (402 kW, 8) and (161 kW, 2). Clearly, the second loop is broken removing unit 11. The resulting network is presented in Figure 6.6.

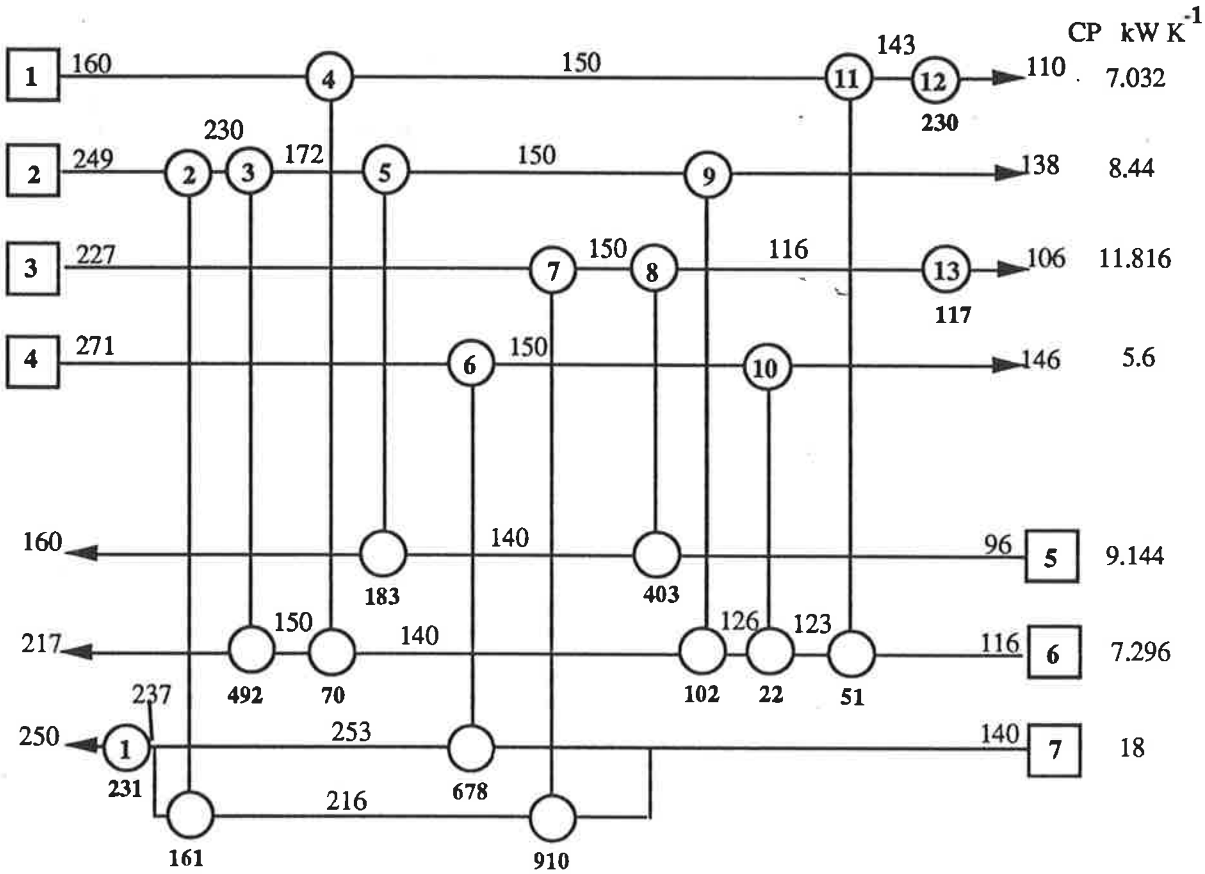
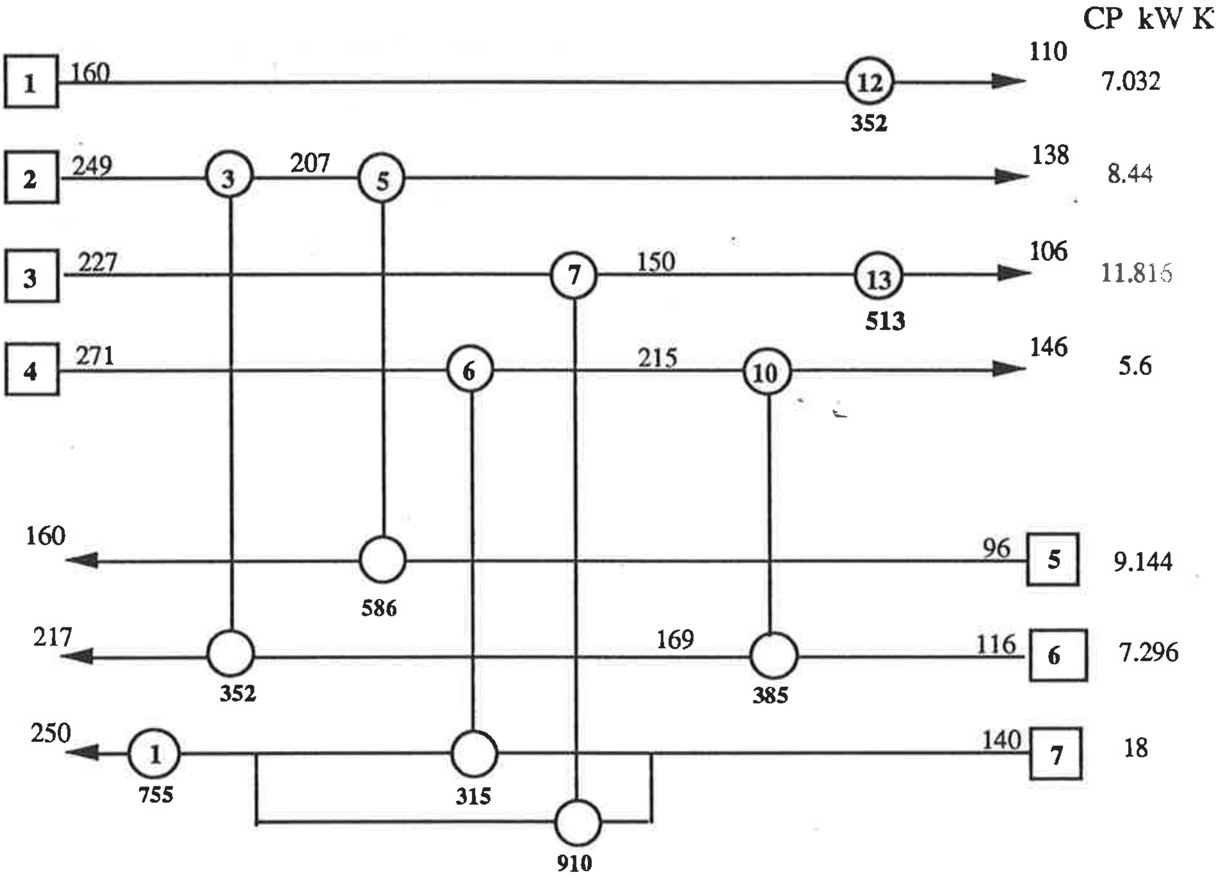
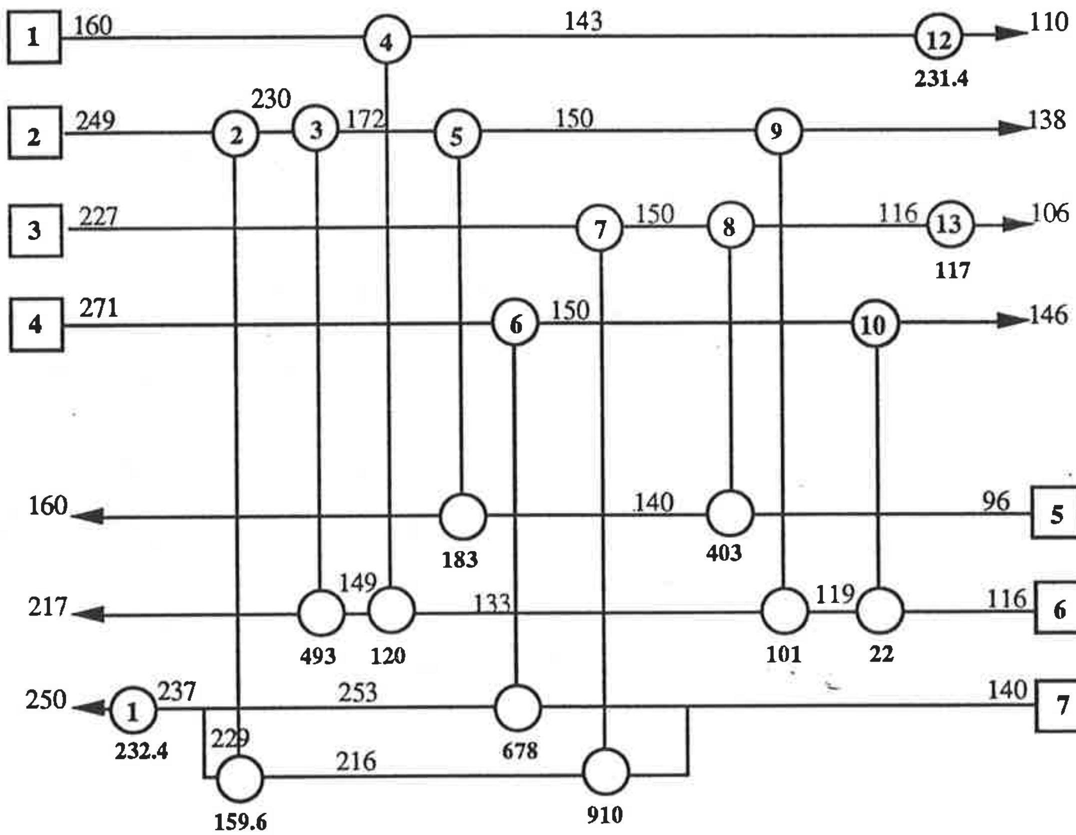


Figure 6.4: MER design at for Case Study 1 (ΔT_{min} = 10 K) (Trivedi et al., 1990)



Overall energy Penalty = 524 kW.

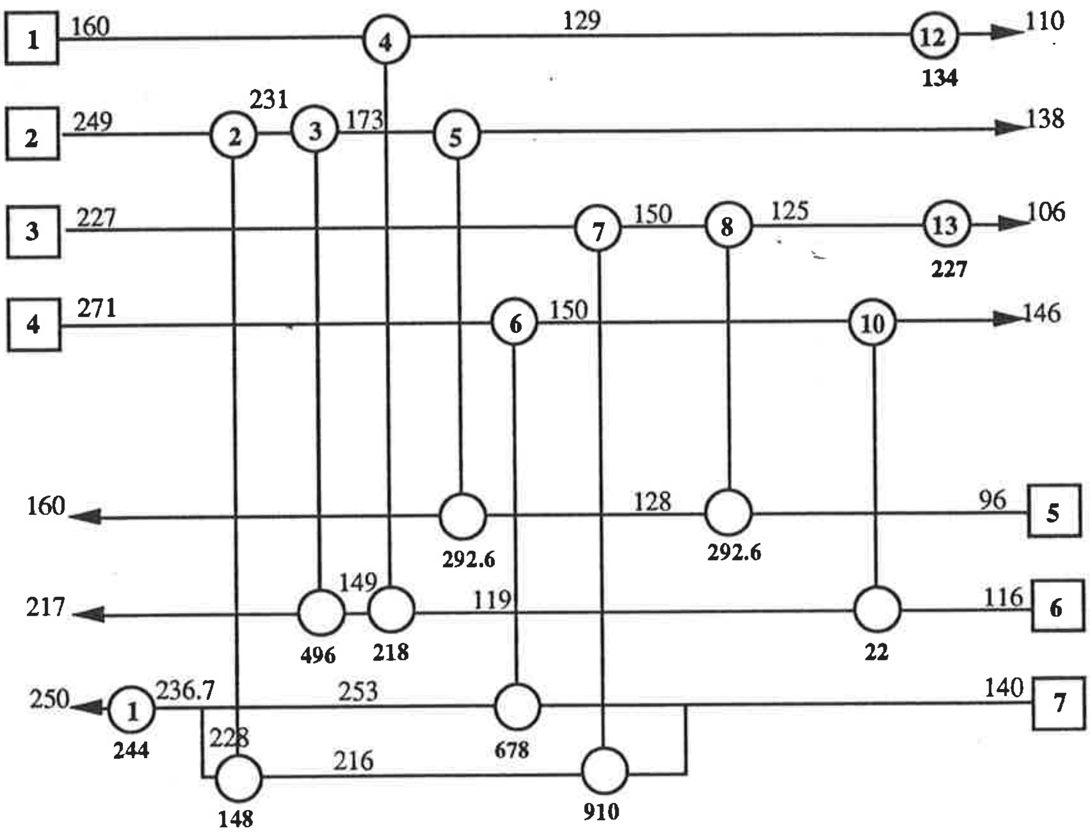
Figure 6.5: U_{min} design for Case Study 1 (Trivedi et al., 1990)



Energy penalty = 1.85 kW, Units = 12

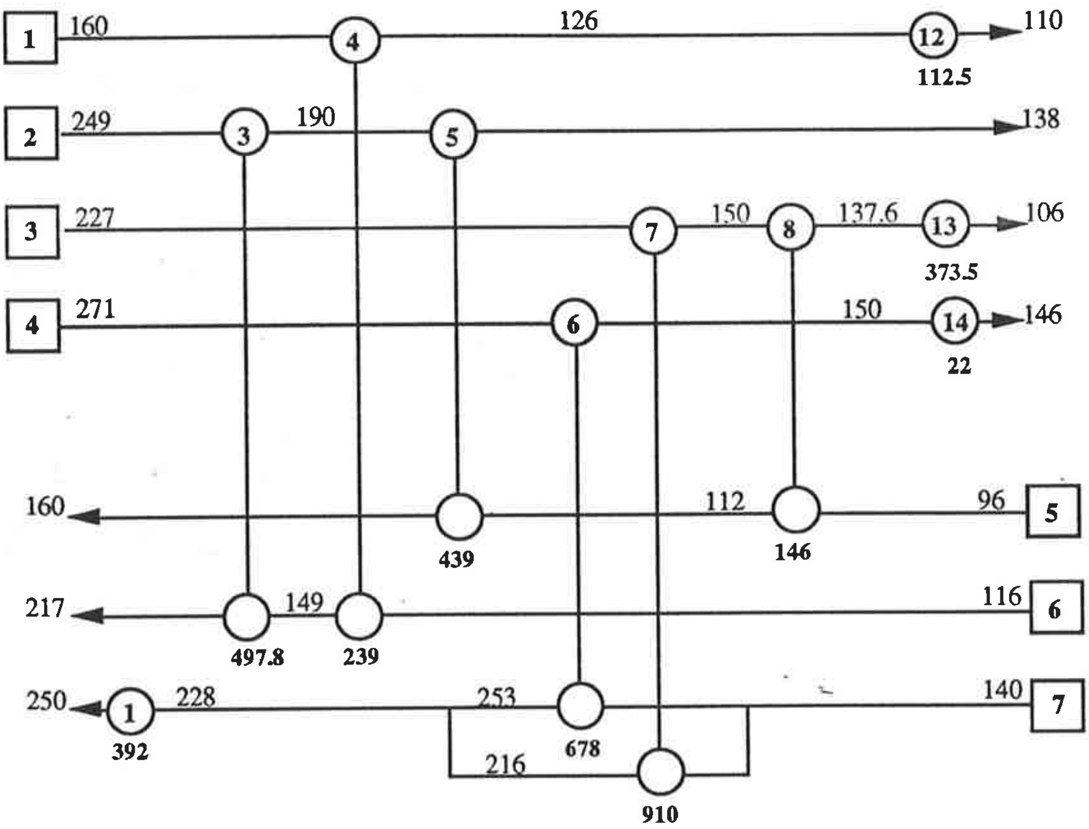
Figure 6.6: Evolution of network - first network (Case Study 1)

The remaining three loops are now considered. The associated penalties are (11.6 kW, 9); (157 kW, 5) and (159.6 kW, 2) and unit 9 is recommended for removal (Figure 6.7). After a similar analysis of the new network, unit 2 is next removed (energy penalty 126 kW). The last remaining higher-level process-process loop (3, 5, 8, 7, 6, 10) is removed by deleting unit 10. The minimum energy penalty associated with this is 22 kW. However, removal of unit 10 requires a cooler to be added to stream 4 to avoid violation of the ΔT_{min} constraint on unit 6. The evolved network is presented in Figure 6.8. The network includes six process-process units (the minimum if we consider only the process streams) but includes two additional utility units. These extra utility units cannot be removed without violating the minimum temperature constraint. Summarizing, the overall energy penalty to remove the four identified units (2, 9, 10 & 11) and add one cooler (14) is 161 kW.



(Cumulative energy penalty = 13.4 kW, Units = 11)

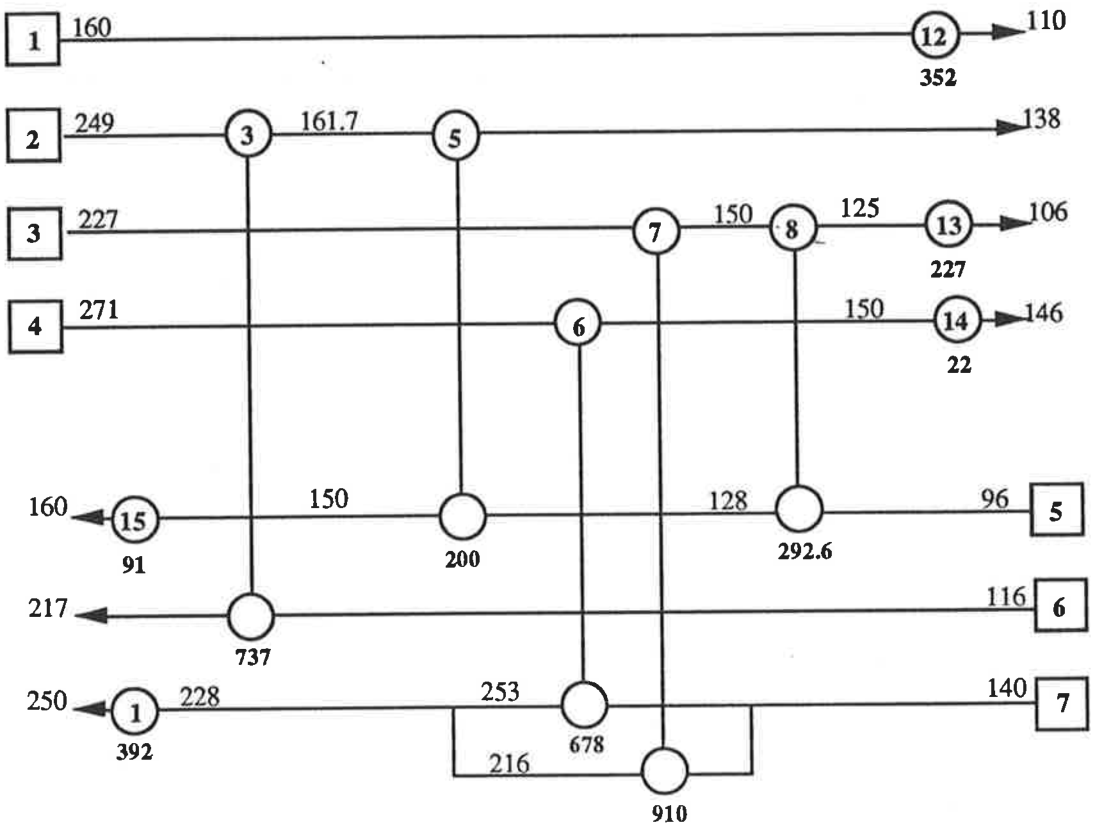
Figure 6.7: Evolved network 2 (Case Study 1)



(Cumulative energy penalty = 161 kW, Units = 10)

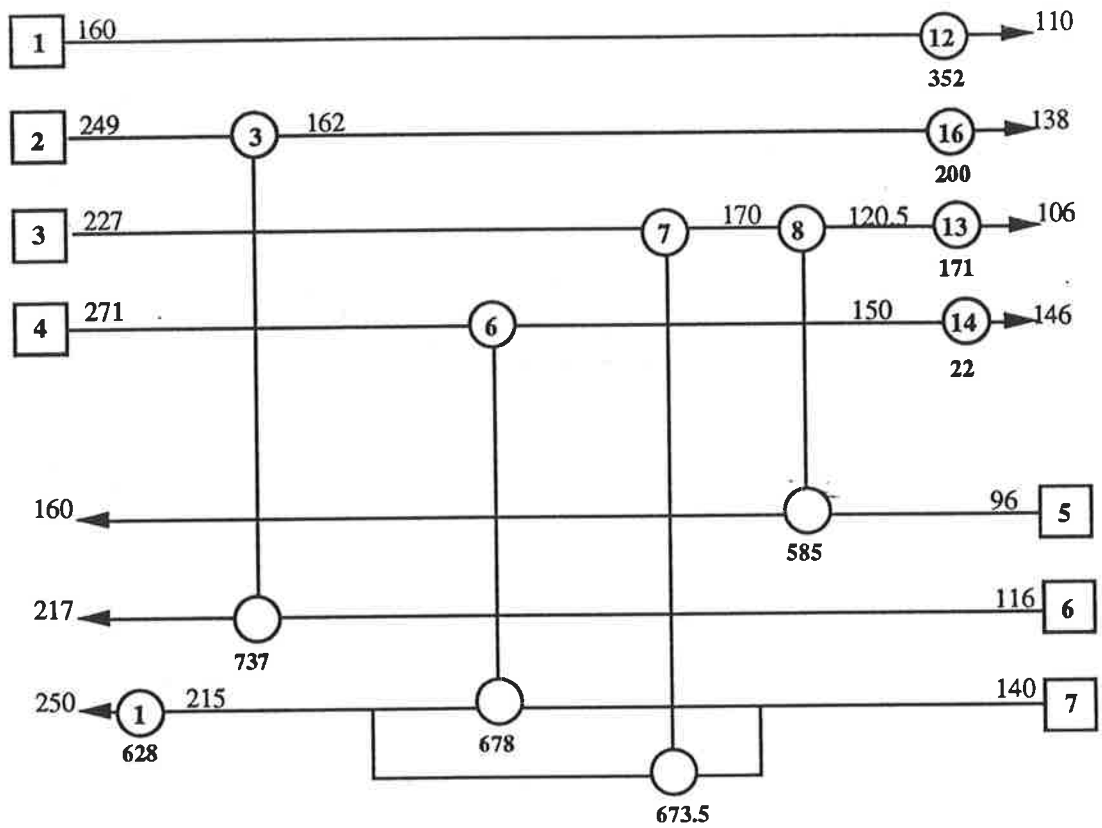
Figure 6.8: Evolved Network 3 (Case Study 1)

Next, consider the process-utility loops, two such loops remain (namely 4, 3, 5, 8, 13, 12 and 6, 7, 13, 14). Removing unit 4 produces the minimum penalty of 91 kW but an additional heater must be supplied to restore ΔT_{min} to unit 5. The resulting network is Figure 6.9. It may be further simplified by breaking the loop (5, 8, 7, 1, 15) and the final network is presented in Figure 6.10. The total penalty is 397 kW. The final network includes four process-process unit (two fewer than the minimum) and five utility exchangers (three more than the minimum). Hence, the final design exceeds the U_{min} target by one. This design may be further simplified if a small ΔT_{min} violation is permitted on unit 6. The cooler may be removed and the unit target is achieved (Figure 6.11) with an energy penalty of 375 kW. This network possesses three disconnected subnetworks and should therefore enjoy an advantage in terms of operability.



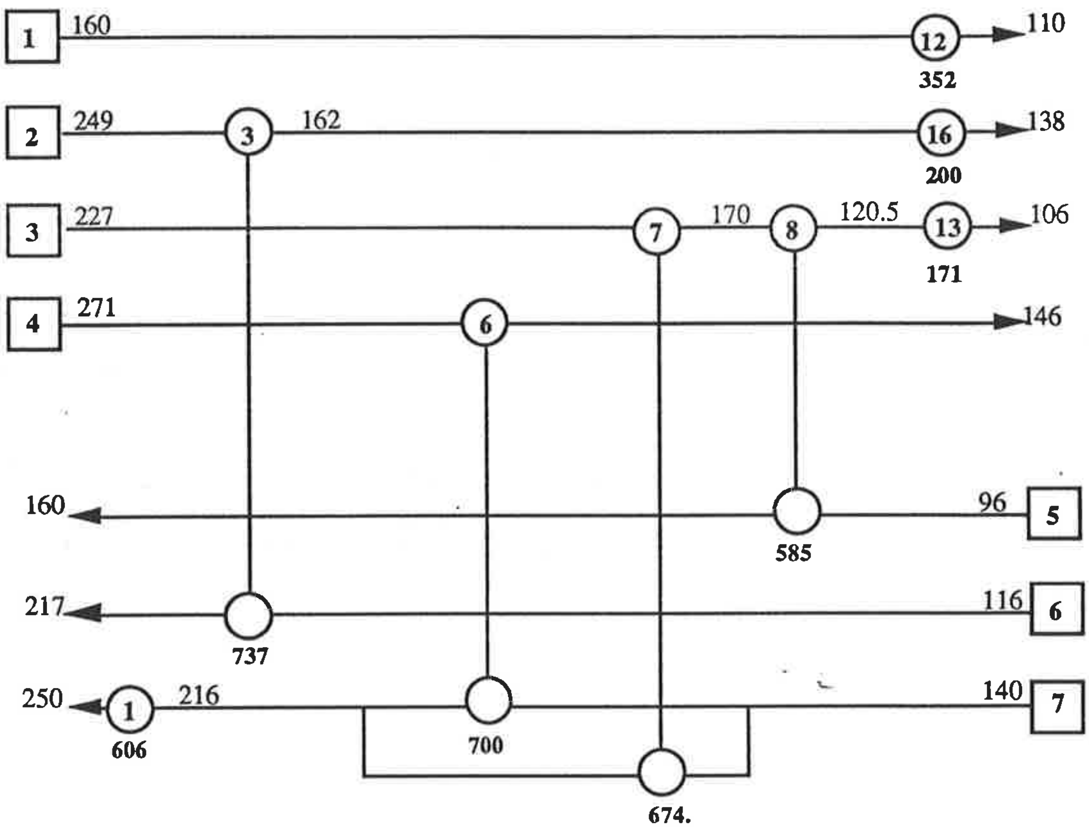
Cumulative energy Penalty = 252 kW, Units = 10.

Figure 6.9: Evolved network 4 for Case Study 1



(Cumulative energy Penalty = 397 kW, Units = 9)

Figure 6.10: Evolved network 5 (Case Study 1)



(Overall energy Penalty = 375 kW, Units = 8)

Figure 6.11: Evolved network 6 with small violation of ΔT_{min} on unit 6 (Case Study 1)

For this problem, Trivedi et al (1990) also noticed the possible removal of unit 10 with ΔT_{min} violation at an early stage to achieve a smaller energy penalty. By allowing the relaxation on ΔT_{min}, the same design as Figure 6.11 also can be achieved by using LONITA (Trivedi et al, 1990) although Trivedi et al did not produce this design in their paper. As can be seen from Table 6.1, using different methods for energy relaxation (LONITA, the present method), the search for an optimal solution may be carried out along different paths. However, the LONITA approach is not very straightforward for search of an optimal solution. By contrast, the approach by applying Kirchhoff's Law is more deterministic and straightforward in that units to be removed are determined based on the detail calculations for a minimum energy penalty. Furthermore, addition of heaters or coolers is allowed to restore ΔT_{min} in the present approach. In some instances, additional heaters and coolers (above the minimum of two) may be required but a benefit of these utility units is improved operability and flexibility.

Table 6.1: Summary of evolved designs

	LONITA (Trivedi et al, 1990)	Present Approach (Applying Kirchhoff's Law)
Units	Cumulative Energy Penalty (kW)	Cumulative Energy Penalty (kW)
13	0.0	0.0
12	1.4	1.8
11	21.9	13.4
10	161	161–252
9	231	397
8	375*	375
	524**	

*: The same solution as Figure 6.11 with a small ΔT_{min} violation can be achieved by using LONITA although Trivedi et al did not produce this solution in their paper.

**: This solution was produced by Trivedi et al (1990) without ΔT_{min} violation.

6.5.2 Case Study 2

The purpose of this case study is to show that in some cases, it may require a too large energy penalty to achieve a U_{min} design which may not therefore be cost effective. Thus, in such cases, it may not be wise to over-emphasize U_{min} designs.

This network (Figure 6.12) was introduced and synthesized by Pethe *et al.* (1989) using the Pinch Method. It achieves the energy target at $\Delta T_{min} = 20$ K. Three loops occur in the network - (3, 1) (loop 1), (6, 5, 2, 1) (loop 2) and (7, 5, 2, 4) (loop 3). First, we calculate the *minimum* energy penalty for each loop and establish the precedence order in which the loops are to be broken. Zero energy penalty occurs when breaking loop 1 by removing unit 3. The energy penalty for breaking loop 2 equals that for breaking loop 3 when unit 5 is removed in each case. This penalty is 31.3 kW. Hence, the units 3 and 5 are selected for removal and the evolved network is presented in Figure 6.13. Notice that with unit 5 removed, if the heat load of unit 5 is transferred to unit 6, the driving force of unit 1 will be less than ΔT_{min} of 20 K. To restore the ΔT_{min} for unit 1, a heater is added for stream 4 as shown in Figure 6.13.

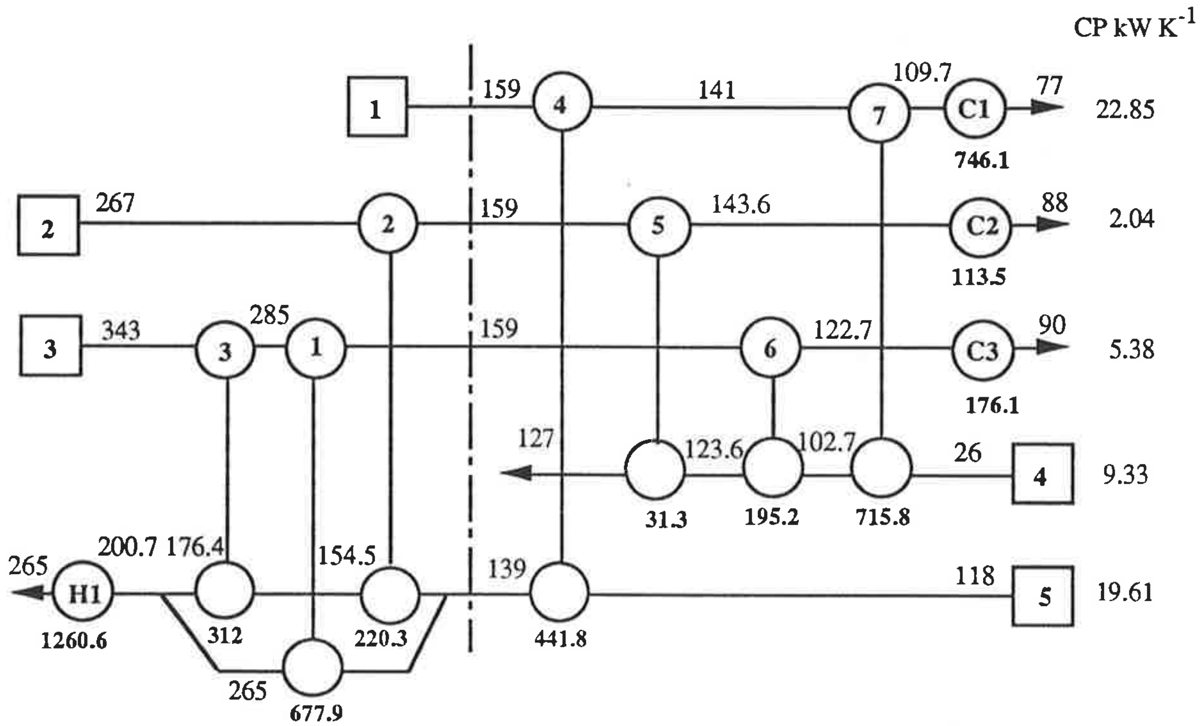
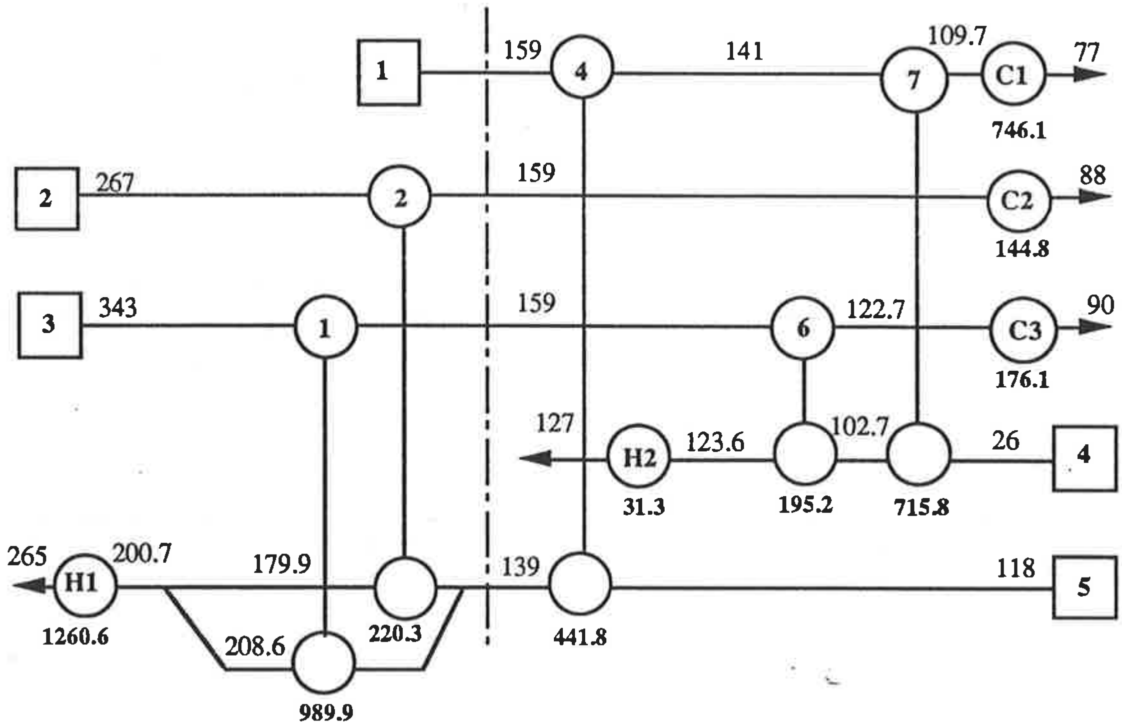


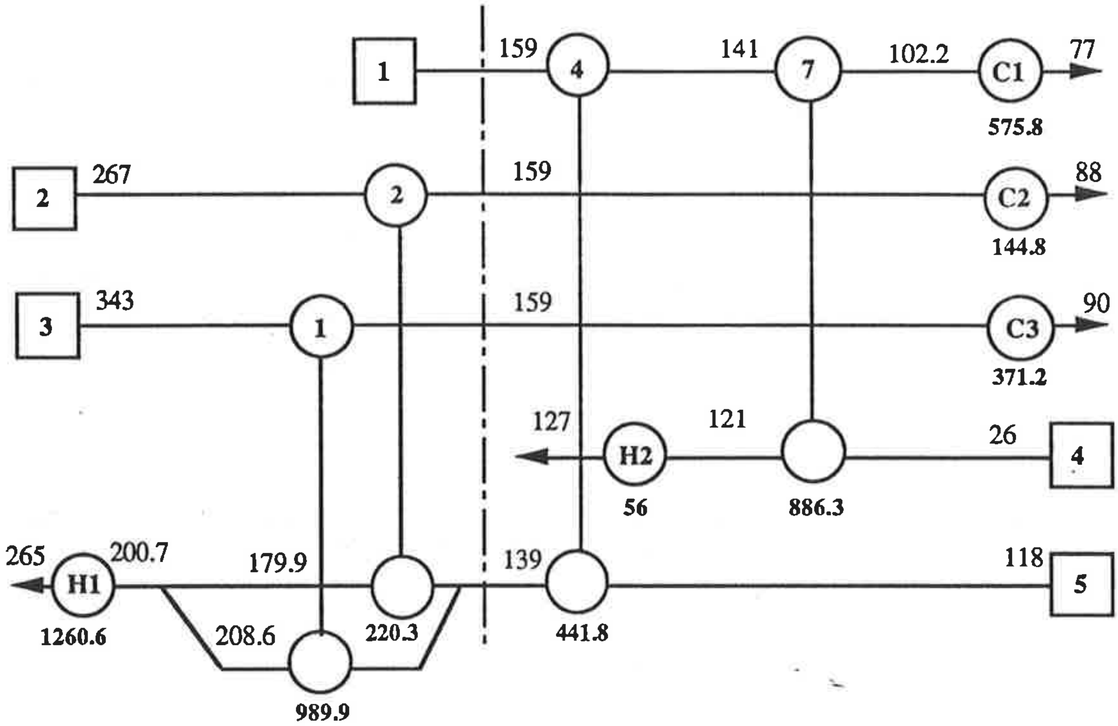
Figure 6.12: Initial MER Network for Case Study 2 (Pethe et al, 1989)



Energy penalty = 31.3 kW with removal of units 3 and 5

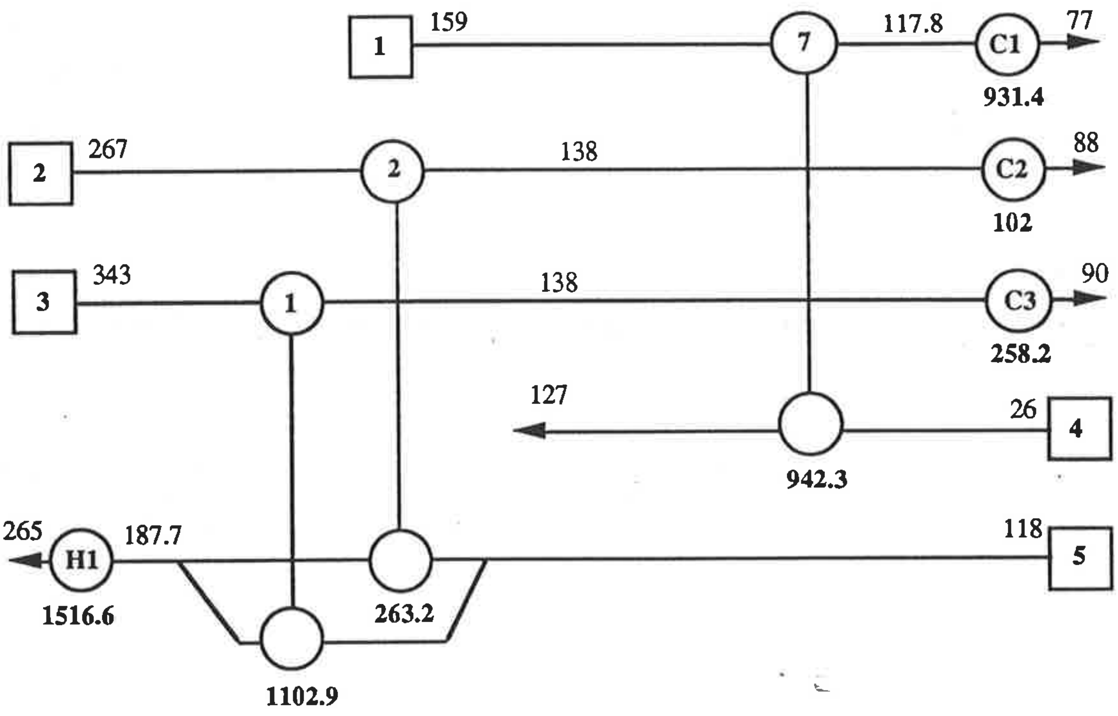
Figure 6.13: Evolved network 1 for Case Study 2

At least three units must be removed in order to break the three loops. Only two units (3 & 5) are removed so far. Clearly, a process-process loop remains in this network, namely (1, 4, 7, 6). The minimum energy penalty is 24.7 kW for breaking this loop by removing unit 6. Hence, the final network with minimum total energy penalty of 56.0 kW is evolved as illustrated in Figure 6.14.



Energy penalty = 24.7 kW by removing unit 6
Figure 6.14: Evolved Network 2 for Case Study 2

Though this network achieves minimum number of process-process exchangers, it requires three more utility exchangers. Thus, while focusing on U_{min} design, the network needs to be simplified further. The unit 4 is identified as the one which incurs lest energy penalty after removal. Again, unit 4 is not the smallest unit but its removal incurs lest energy penalty. Thus, it is selected for removal. The removal of unit 4 brings another benefit in allowing the removal of heater H2. The resultant network is given in Figure 6.15. This simplification of network incurs the energy penalty of 199.8 kW. It may need investigation to assess the worth of removing unit 4 because of the large energy penalty incurred. This network still has one more unit than the target. However, any further network simplification from Figure 6.15 will incur a large energy penalty.



Energy penalty = 199.8 kW with removal of unit 4

Figure 6.15: Evolved Network 3 for Case Study 2

From this example, it may be observed that in some cases, a design may achieve minimum process-process exchangers but needs more utility exchangers than the minimum (typically two for non-threshold problems). Since these utility exchangers are placed to ensure the satisfaction of ΔT_{min} constraints, thus the only way to achieve an U_{min} target is to reduce process-process exchangers further less than the minimum number of process-process exchangers. Usually, such evolution incurs a large energy penalty. Therefore, one should be cautious to make a decision about whether it is worth to simplify a network further when it incurs a large energy penalty.

6.6 Conclusions

The application of Kirchhoff's law to heat exchanger network enables a prediction of actual energy penalties incurred by different strategies for loop breaking. This allows the minimum energy penalty for breaking a loop to be determined and the units removed to achieve this optimal solution are readily identified. To reduce the size of the possible search space, a simple heuristic is introduced. The loops to be considered initially are then readily identified.

During the loop-breaking process additional utility exchangers may need to be added to avoid violation of the strict ΔT_{min} constraint. The final network can be evolved to contain the minimum number of process-process exchangers but extra utility units may be required to restore the minimum approach temperatures. These units will provide benefits in terms of improved operability.

Chapter 7

Conclusions and Recommendations for Future Works

A number of useful new concepts namely blocks, quasi-composites, matching matrix, block-based stream structure, block-based superstructure etc. have been introduced in this work. The basic concept is the 'block', which provides the physical insight of how to achieve the near-minimum area and near-maximum energy recovery with a small number of units and shells. The consequence of the application of this concept is the development of the block method. The block method overcomes the two drawbacks of the Pinch Design Method (PDM), i.e. the strict pinch decomposition associated with the MER constraint and the use of a single ΔT_{min} for all exchangers in a network. As well, this new method combines the advantages of both thermodynamic approaches and optimization techniques. There are also advantages when the block concept is applied successfully to optimization by mathematical programming and thus it links thermodynamic principles with mathematical programming approaches. These strong features make the block method very promising for practical applications. In summary, the block concept is simple to understand, readily implemented and it yields low cost and simple solutions.

7.1 The Block Method

It has been noted from the analysis of the composite curves that streams in different composite regions may have totally different driving force requirement. This calls for different treatment of streams located in such different regions. This observation forms the basis of the block concept. By defining blocks, i.e. distinct regions, a complex design problem is decomposed into several simple sub-problems. Designs for these sub-problems become relatively simple tasks. The connections between blocks are made by employing the import or export rules in the block method. With the use of the block decomposition, the pinch decomposition (either 'hard' decomposition which does not allow criss-crossing at pinch or 'soft' decomposition which permits criss-crossing at pinch with same amount of heat) is not a requirement though the pinch may be used as a block boundary if desired.

The block decomposition makes it possible to calculate the heat transfer areas for any possible matches and thus the match selection is more deterministic and more rigorous. With areas calculated for all possible matches, a set of matches can be determined simultaneously according to the minimum area principles or the minimum total cost principles. The advantage of match selection by the simultaneous approach is, that the best set of matches can be selected at one time and the back tracking which usually occurs in the sequential choice of matches is avoided.

There are also advantages when NLP optimization techniques are applied with this method. The application of the NLP optimization techniques in this case is different from the pure mathematical programming which merely relies on the optimization methods without the aid of thermodynamic methods. In the block method, an important improvement in searching for the global optimum is to find a very good initial network (near-minimum area, near-MER and near-minimum units), that is already relatively close to the optimum. Such initial designs are provided as the starting point of optimization. This strategy enhances the advantages of both thermodynamic and mathematical programming approaches.

As a result of such synthesis, the network will achieve a low total cost, i.e. low capital cost and good energy efficiency, and simple network structure. The simplicity of a network is the important feature for operation and control.

7.2 The Extended Block Method for Unequal Film Coefficients

The novelty of the *extended* block method lies in the incorporation of the diverse pinch approach (Rev and Fonyo, 1991) so that the more promising stream structures may be chosen prior to design. Then the block method is used for synthesis. It has been proved that the combination of the diverse pinch approach and the block method generates improved solutions to problems involving significantly different film coefficients compared with currently available methods.

The important discovery of this work is that the stream structures can be screened prior to design which provides more opportunities for a designer to choose promising candidates for detailed synthesis and thus increases the possibility of finding globally optimal solutions.

The another interesting phenomenon is that with block decomposition after individual stream-shifting, the boundary temperatures of streams of one type within a same block may be significantly different. The distribution of these temperatures obeys the general rule: the streams with high film coefficients are assigned with low driving forces and vice versa. With such a temperature distribution, the possibility for a match with a large area penalty is avoided, especially when a stream of one type with a high film coefficient matches the other type of a stream with a low film coefficient. In this manner, the difference in film coefficients is effectively exploited. The additional benefit of such arrangement of stream temperatures is that topology traps can be effectively avoided.

7.3 NLP Optimization Based on the Block Decomposition

Non-linear problem (NLP) optimization methods are very powerful in search of optimal solutions providing a good initial solution is given. Thus, how to best apply these techniques in solving heat exchanger network synthesis (HENS) problem is of great interest and importance. Recently, the research in this area has been making great progress and the application of NLP optimization techniques seems very promising. However, researchers in this area have mainly been concerned about how to improve the optimization techniques and how to simplify the mathematical formulations. Relatively little effort has been made to provide physical insights into the mathematical programming. In this study, the block concept has been applied successfully to the mathematical programming to decompose the synthesis problem into a small number of blocks. Although the block concept leads to similar superstructure approaches as that by the stage method (Yee et al, 1990), the block concept provides physical insights into the superstructures and makes them not only physically realizable but approach the minimum overall area.

The another physical insight is provided to the mathematical programming through the application of the supertargeting approaches (Linnhoff and Ahmad, 1986 a & b; Zhu et al, 1994) which give a good initial estimate of an 'optimal' HRAT through 'optimal' trade-off between energy and capital prior to design. This 'optimal' HRAT can be used as a good starting point for mathematical formulation. Therefore, together with a good starting point and simplified overall superstructures based on the block decomposition, the solution efficiency and quality can usually be improved.

The non-linearities in the model may lead to more than one local optimal solution due to their non-convexities. In addition, in a case with a bad initial solution, a nonlinear model may fail to find a feasible solution though such a solution exists. In order to overcome these problems and improve the quality of NLP solutions, a LP model for area targeting and a simple NLP model for cost targeting for an initial solution are also presented. These two models are formulated based on the block-superstructure with fixed block boundary temperatures. As the simple models provide excellent initial solutions (e.g. compare Figures 5.11 and 5.12), good solutions from NLP models can be found with ease and the likelihood of finding the global optimum is increased.

7.4 Kirchhoff's Law and Loop Breaking

The previous methods for loop breaking are usually based on heuristic rules which can only provide suboptimal solutions. However, in the method presented, the loop breaking is carried out based on the detailed calculation of the energy penalty for breaking a loop. This is obtained by applying the well known Kirchhoff's law to problems of heat exchanger networks. As a result of the prediction of the minimum energy penalty which may be incurred in loop-breaking, a designer can evolve a network with more confidence.

The use of Kirchhoff's law to represent a heat exchanger network may find an important application in the analysis of dynamic behavior or transient processes associated with HEN operation. This is because a network can be represented by a set of linear equations by employing Kirchhoff's law. When some parameters in the network change with time, the changes in other parameters can be calculated by solving the set of linear equations.

7.5 Recommendation of Future Work

The development of the block method has opened a lot of options for investigation which include the following projects:

(1) To examine the feasibility of the application of the general block method to the analysis of process integration. While the initial design synthesis and subsequent optimization are important themselves, they are part of a much wider problem, which is the complete process integration of the total processing system, e.g. including reactors and distillation columns. Thus, it is important to examine whether the insight gained from the development of the block method can be applied to problems associated with complete process integration. Another facet of the work will be to examine the feasibility of adopting the block method to batch processing systems.

(2) To examine the application of the block method to retrofit problems would be very interesting work. It would include:

- developing a general strategy for solving retrofit problems, e.g. how to effectively use existing exchangers, how to add new exchangers etc;
- developing methods to identify controlling constraints as a basis for heuristic development by applying the block decomposition to current mathematical models for retrofit problems;
- developing appropriate cost functions for removal of exchangers and piping modifications;
- developing methods of analysis for assessing the heat transfer area utilization in existing installed plant;
- examining the interaction between pressure drops and heat transfer coefficients.

(3) To investigate the possibility of doing part of a detailed design (thermal or mechanical design) at the stage of conceptual design. Process integration is regarded as conceptual design. However, if more information can be generated from the conceptual design, it would be of great benefit for the subsequent detailed design. The level of the knowledge extracted from the conceptual design depends on the depth of

such conceptual design. The information associated with a design produced by current available methods only contains the temperatures, the pairs of streams, heat loads and approximate heat transfer areas. The total cost of a network is calculated based on a pre-assumed exchanger cost model which applies to the whole network. However, when moving on to the thermal design and mechanical design, more detailed decisions are involved requiring selection of the material of construction, type of exchanger, exchanger geometry, pressure drop limitations etc. Consideration of the former two facts is unavoidable, particularly when special streams (high temperature, high pressure, high corrosion, explosion potential etc) are used in a process. The outcomes of such detailed design are more precise cost models which apply to individual exchangers. These cost models may significantly differ from the previously assumed cost models. Thus, the so–called optimal design from the conceptual design stage is really questionable.

In order to overcome the above drawbacks existing in the current methods, the conceptual design should involve a deeper level of design, e.g. thermal and part of mechanical design at some stage. Thus, the pre-assumed cost model can be modified in the design process. This interaction will affect the decisions about which alternatives are more attractive in terms of total cost. Obviously, the decisions made in such a manner should be more reliable and deterministic.

Since the block method is based on the block decomposition, when one investigates and analyzes possible matches in a block, the information about pairs of streams, temperatures and heat loads is all available. Thus, the proper materials for the corresponding exchanger can be determined based on the physical properties of each pair of streams. As well, the type of the exchanger, the number and size of the shells, the exchanger geometry (e.g. the tube length, diameter and pitch for tube-and-shell exchangers), etc can be determined. These considerations would provide more reliable costs for individual exchangers which can be used in the subsequent NLP cost optimization. Obviously, the total cost of such a final optimized design from this procedure should be closer to that provided by the manufacturer and it would help designers to make final decisions more confidently and convincingly.

APPENDICES

APPENDIX A DERIVATION OF EQS. (3.8a) AND (3.9a)

The simple splitting formulae (Eq. (3.9a)) can be derived based on a practical example. Consider the situation of two hot streams (j and k) and one cold stream i. These three streams form an independent optimization problem. Clearly, the ratio of the slopes of the associated composite curves can be expressed as $\frac{CP_j+CP_k}{CP_i}$.

First, split the cold stream to force one of the splits to mimic the composite curves, namely

$$\frac{CP_j}{CP_i^1} = \frac{CP_j+CP_k}{CP_i} \tag{A1}$$

Cross multiplication gives

$$CP_i \times CP_j - CP_i^1 \times (CP_j+CP_k) = 0 \tag{A2}$$

Conservation implies

$$CP_i = CP_i^1 + CP_i^2 \tag{A3}$$

Combining (A2) and (A3) yields

$$(CP_i^1 + CP_i^2) \times CP_j - CP_i^1 \times (CP_j+CP_k) = 0 \tag{A4}$$

or

$$CP_i^1 \times CP_j + CP_i^2 \times CP_j - CP_i^1 \times CP_j + CP_i^1 \times CP_k = 0 \tag{A5}$$

Thus, equation (A5) yields

$$CP_i^2 \times CP_j - CP_i^1 \times CP_k = 0 \tag{A6}$$

or

$$\frac{CP_j}{CP_i^1} = \frac{CP_k}{CP_i^2} \tag{A7}$$

As stated earlier, CP_i is split forcing

$$\frac{CP_j}{CP_i^1} \text{ equal to } \frac{CP_j+CP_k}{CP_i}$$

Hence, from equation (A8), it is inferred that

$$\frac{CP_k}{CP_i^2} \text{ also must equal } \frac{CP_j+CP_k}{CP_i}$$

Therefore, the split ratios determined by equation (A8) can ensure that the resulting two matches precisely mimic the profiles composite curves.

For the splitting case with one hot and two cold streams, the optimal split ratios for the hot stream determined by Eq. (3.8a) can be derived similarly.

APPENDIX B Case: Vertical (Ideal) Matching Driving Force Calculations – Hot Stream 'Tick Off'

1) For a particular match H_i, C_j, an 'ideal vertical matching' area can be calculated based on the quasi–composite curves , viz.

$$(A_{ij,\text{quasi ideal}})_{Hi} = \frac{Q_{ij}}{U_{ij}[\Delta T_{lm-ij}]_{\text{vertical match}}} \qquad \text{(B1)}$$

where with reference to Figure B1,

$$[\Delta T_{lm-ij}]_{\text{vertical match}} = \frac{(T_{c'} - T_{d'}) - (T_c - T_d)}{\ln\left[\frac{(T_{c'} - T_{d'})}{(T_c - T_d)}\right]} \qquad \text{(B2)}$$

The H_i is assumed to be subsumed into the hot quasi–composite curve for the appropriate temperature range and direct vertical matching then follows. The Q_{ij} value used is identical to that for the actual area calculation for the H_i, C_j match.

2) The required known temperatures are

$T_{a'}$, T_a $(= T_{c'})$, T_b $(= T_c)$, T_f and $T_{f'}$.

while the temperatures to be determined are $T_{d'}$ and T_d .

The basic identities are:

(i) For the individual streams

$$T_b = T_c = T_a + \frac{Q_{ij}}{CP_{Hi}} \qquad \text{(B3)}$$

$$T_e = T_f + \frac{Q_{ij}}{CP_{Cj}} \qquad \text{(B4)}$$

(ii) For the quasi–composite curves

$$(T_c - T_{a'})CP_{\text{hot quasi–composite}} = (T_d - T_{f'})CP_{\text{cold quasi–composite}} \qquad \text{(B5)}$$

$$(T_c - T_{c'})CP_{\text{hot quasi–composite}} = (T_d - T_{d'})CP_{\text{cold quasi–composite}} \qquad \text{(B6)}$$

From equation (B5)

$$T_d = T_{f'} + (T_c - T_{a'}) \left. \frac{CP_{\text{hot quasi-composite}}}{CP_{\text{cold quasi-composite}}} \right|_{\text{block}} \tag{B7}$$

Similarly, from equation (B6)

$$T_{d'} = T_d - (T_c - T_{c'}) \left. \frac{CP_{\text{hot quasi-composite}}}{CP_{\text{cold quasi-composite}}} \right|_{\text{block}} \tag{B8}$$

3) Similar temperature points are calculated when 'ticking off' a cold stream except that the cold stream C_j is first projected onto the cold quasi–composite and the resultant vertical match is then projected up to the hot composite with the resultant area being $(A_{ij,\text{quasi ideal}})_{Cj}$.

4) Appendix C contains an example calculation.

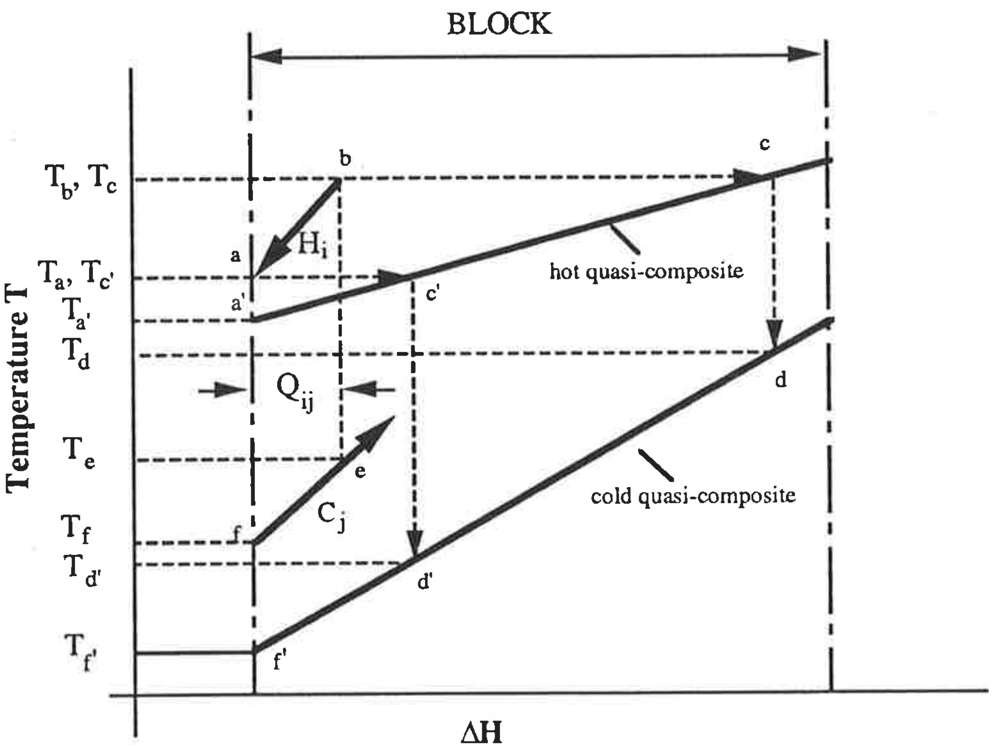


Figure B1: Illustration of calculation of 'ideal area'

APPENDIX C EXAMPLE CALCULATION OF 'IDEAL AREA'

Consider the following diagram (Figure C1) summarizing conditions in the block 2 of case study 1 (Figures 3.12b & 3.14). The 'ideal area' requirement for the match between streams 1 and 4 in the block above the pinch is illustrated. Two scenarios are possible:

1. Vertical matching based on the hot stream

The enthalpy change for the hot stream 1 being cooled from 150 °C to 90 °C is 12000 kW. To achieve vertical heat transfer based on the hot stream, the cold 'quasi composite' rises from 80 °C to 100.3 °C. hence the 'ideal area' may be computed.

$$(A_{14,\text{quasi ideal}})_1 = \frac{Q}{U\Delta T_{lm}} = \frac{12000\text{x}10^3}{100\text{x}24.76} = 4847 \text{ m}^2$$

2. Vertical matching based on the cold stream

For this case an energy input of 12000 kW raises the cold stream temperature from 80 °C to 104 °C. The corresponding fall in the hot 'quasi–composite' temperature is 161 °C to 90 °C. Hence, the ideal area is:

$$(A_{14,\text{quasi ideal}})_4 = \frac{Q}{U\Delta T_{lm}} = \frac{12000\text{x}10^3}{100\text{x}27} = 4445 \text{ m}^2$$

These values may be now used to determine an estimate of the ideal area for the match between streams 1 and 4 :

$$A_{14,\text{quasi ideal}} = \frac{(A_{14,\text{quasi ideal}})_1 + (A_{14,\text{quasi ideal}})_4}{2} = 4646 \text{ m}^2$$

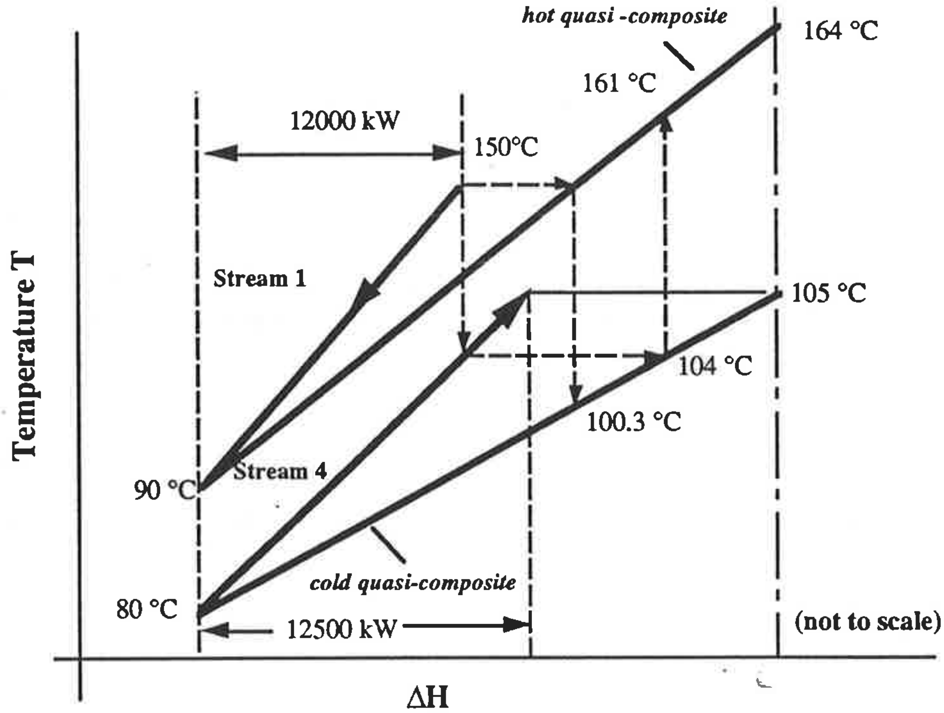


Figure C1: Example of calculation of the 'ideal area'

APPENDIX D Initialization Procedure for Solving the NLP Models (Yee et al, 1990)

The strategy is to provide reasonable initial values to favor the minimization of the various costs involved. The notations for the equations for the equations below are same as the nomenclature presented earlier in Chapter 5. Also, the expression .Init following the variable represents the initialization for the particular variable.

First, the temperatures variables are bounded and initialized to that they provide a high driving force for the exchangers to minimize area:

$$t_{ik} \leq T_{in,\,i}, \quad t_{ik} \geq T_{out,i} \quad i \in I, \quad k \in ST,$$
$$t_{jk} \leq T_{out,j}, \quad t_{jk} \geq T_{in,j} \quad j \in J, \quad k \in ST,$$
$$t_{ik}.\text{Init} = T_{in,i}, \quad i \in I, \quad k \in ST,$$
$$t_{jk}.\text{Init} = T_{in,j}, \quad j \in J, \quad k \in ST. \qquad \text{(D1)}$$

where ST is a set of stages.

Next, the heat load for each exchanger can be initialized to a value which spreads out the heat transfer amongst the NOK stages. Note that in the following, the maximum heat transfer for a particular pair of hot and cold streams is the minimum of either the hot or the cold stream heat loads:

$$q_{ijk}.\text{Init} = \min(CP_i(T_{in,i} - T_{out,i}),\ CP_j(T_{out,j} - T_{in,j}))/NOK,$$
$$i \in I, \quad j \in J, \quad k \in ST. \qquad \text{(D2)}$$

Finally, the variables for hot and cold utility loads can be initialized to small values so as to favor the minimization of the utility costs. For the area targeting case, though, where the utility requirement is fixed, these variables can be initialized to evenly distribute the required utility heat loads amongst the streams.

APPENDIX E Initialization Procedure for Solving the MINLP Models (Yee and Grossmann,1990)

The following is an initialization procedure that reduces the MINLP to an LP by assuming fixed temperature driving forces for each match:

1. Estimate a value of HRAT.

2. Estimate a driving force for each match by:

   (a) determining the $LMTD_n$ for each enthalpy interval n using its corresponding temperatures;

   (b) using the following weighting equation to calculate an average driving force for each match (i,j):

$$ALMTD_{ij} = \frac{\sum_n q_{ijn} LMTD_n}{\sum_n q_{ijn}} \tag{E1}$$

where q_{ijn} is the maximum heat transfer that can occur between hot stream i and cold stream j in enthalpy interval n.

3. For each match (i,j) in different stages for superstructure, set the driving forces in the MINLP model (equation (9) in the paper by Yee and Grossmann (1990)) with the fixed value of the average driving force ALMTDij, and replace the nonlinear cost term of the area by a linear approximation with a fixed charge. This reduced the MINLP to an MILP.

4. Solve the relaxed LP of the MILP in step 3.

5. Use the LP solution along with the estimated driving forces ($ALMTD_{ij}$) as an initial guess for the relaxed NLP problem.

APPENDIX F Calculation of the Number of Distinct Acyclic Solutions

A heat exchanger network may be represented as a graph *(G)* composed of arcs (matches) and nodes (streams). The number of fundamental loops in a connected graph with n nodes and a arcs is given by the expression $(a - n + 1)$.

In particular, for the energy relaxation problem from a particular connected structure, the upper bound of the number of possible distinct acyclic solutions in the graph after compete removal of the loops is equal to the number of distinct spanning trees that may be produced from the graph. In reality, the number of acyclic solutions for a network may be lower than this as some solutions may be thermodynamically infeasible. The number of spanning trees is readily calculated as follows (Wilson and Beinke, 1979):

$$\textit{no. of spanning trees} = \det(B \cdot B^T) \qquad \text{(F1)}$$

where B = reduced (i.e. one node removed) incidence matrix.

The reduced incidence matrix is defined by:

$$b_{ij} = 1, \text{ if edge i is connected to vertex j.}$$
$$b_{ij} = 0, \text{ if edge i is not connected to vertex j.} \qquad \text{(F2)}$$

As an example consider the following problem involving 2 hot and 3 cold streams (Figure F1). Converting this specification to a graph produces the following result (Figure F2). If, for example, vertex 1 is removed, the following graph results (Figure F3).

The corresponding reduced matrix is:

$$B = \text{Vertices} \begin{array}{c} \\ 2 \\ 3 \\ 4 \\ 5 \end{array} \overset{\text{Edges} \quad a \; b \; c \; d \; e \; f}{\begin{bmatrix} 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 1 & 1 \end{bmatrix}}$$

$$B^T = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 \end{bmatrix} \text{ and } B \cdot B^T = \begin{bmatrix} 2 & 0 & 0 & 1 \\ 0 & 2 & 0 & 1 \\ 0 & 0 & 2 & 1 \\ 1 & 1 & 1 & 3 \end{bmatrix}$$

Hence

$$\text{no. of spanning trees} = |B \cdot B^T| = 12 \qquad \text{(F3)}$$

For this simple problem the number of possible acyclic solutions is substantial. Clearly, it is unrealistic to generate all the possible solutions even for very simple problems.

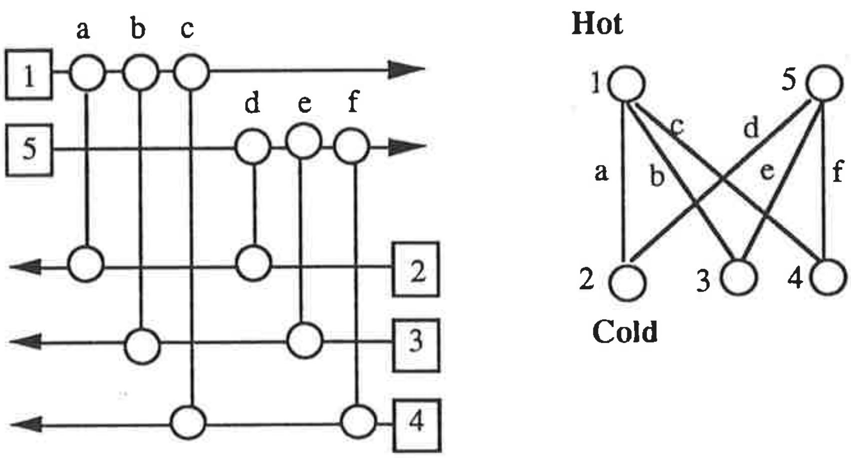


Figure F1: A simple HEN problem including potential matches

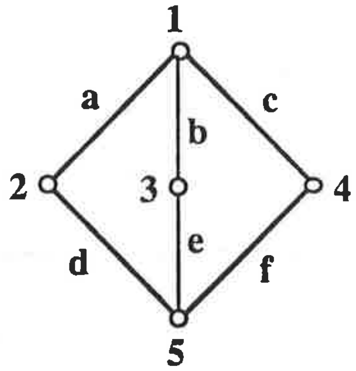


Figure F2: Graph of simple HEN

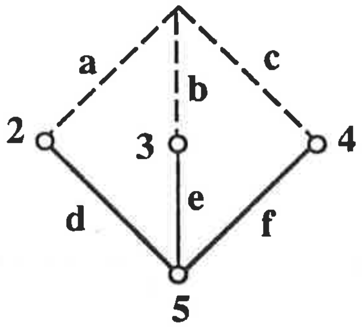


Figure F3: Reduced graph after removing vertex 1

APPENDIX G: PROGRAM LIST

The following is a list of programs* used for this work:

1. Targeting program

This optimization software is coded in C++ using objected oriented programming techniques. The program provides utility targets, the unit target, the shell target, and area targets for networks with either counter–current heat exchangers or with 1–2 type of exchangers subject to a maximum area limit. This program also incorporates the diverse pinch approach (Rev and Fonyo, 1991; Zhu et al, 1994).

2. MIP program for match selection

This program is coded (as an input file) using GAMS (Brooke et al, 1988) to implement ideas in Eq. (3.15) to solve problems with match selection.

3. NLP program for optimization mainly concerning parameters

This is also a GAMS program; the problem for optimizing an initial network is formulated as a NLP problem. The program mainly involves optimization of parameters (temperatures and heat loads) in a network although some exchangers may be effectively removed when the heat loads are set to zero after optimization. A detailed discussion of the mathematical formulation is given in Section 3.7 of this thesis.

4. NLP program for optimization with variable topologies

This is another GAMS program. The mathematical formulation (see Chapter 5) based on the block concept and the block–based superstructure is implemented in this program. The program has a general formulation which can be used for different problems relating to mathematical programming and includes both parameter and topology optimization.

---

* Copies of these files are available in the Department of Chemical Engineering, The University of Adelaide, Australia.

NOMENCLATURE

a	defined as $\frac{A}{Q}$ [Eq.(3.15)]
A	heat exchanger area
A'	heat exchanger area
a_m	heat exchanger area of match *m*
B	cost coefficient of an installed capital cost model
C	cost exponent of an installed capital cost model
C_C	annual cost for a cold utility stream
C_H	annual cost for a hot utility stream
cp	heat capacity flow rate
CP	heat capacity flow rate
DTA	Dual Temperature Approaches
DFP	Driving Force Plot
EI	enthalpy interval
EMAT	Exchanger Minimum Approach Temperature
F	fixed cost of an installed capital cost model
F_n	LMTD correction factor
FPDM	Flexible Pinch Design Method
h	film coefficient
H	enthalpy on the composite curves
HEN	Heat Exchanger Network
HRAT	Heat Recovery Approach Temperature
L	number of loops
LMTD	logarithmic temperature difference
lmtd	logarithmic temperature difference
LP	Linear Programming

M	number of blocks
M	large integer number
MER	Maximum Energy Recovery
MIP	Mixed Integer Linear Programming
MINLP	Mixed Integer Non Linear Programming
n	plant lifetime
n	number of units
N	number of units
N	number of shells
NLP	Non Linear Programming
NOK	number of stages (Eq. (5.A2)
NS	number of splitting branches
PDM	Pinch Design Method
P	energy penalty
PPDM	Pseudo Pinch Design Method
PTA	Problem Table Analysis
q	heat load
Q	heat load
Q''	heat flux
r	annual interest rate
R	annual recovery factor
RPA	Remaining Problem Analysis
S	number of disconnected subnetworks
S	number of streams at an enthalpy interval boundary
ST	stage Eq. (5.A1)
t	temperature
$\tilde{t}$	temperature

T	temperature
TCU	temperature of a cold utility stream
THU	temperature of a hot utility stream
TI	temperature interval
T_{in}	supply temperature of a stream
T_{out}	target temperature of a stream
U	overall heat transfer coefficient
U	total number of units
U_{min}	minimum number of units
x	binary variable assigned to a match
X	heat load
X_p	thermal effectiveness ratio
Y	energy penalty
z	exponent in the diversity relation [Eq. (4.4)]

Greek letters

α	constant [Eq. (4.3)]
δ	small positive number
δ	fitness of an actual match to the composite curves [Eq. (3.55)]
ΔA	area difference
ΔH	enthalpy change
Δt	approach temperature
ΔT	approach temperature
κ	factor in the diversity relation [Eq. (4.4)]

Indices

i	denotes a process-process exchanger

j	denotes a heater
k	denotes a cooler
Note:	above indices are used in Section 3.7 of Chapter 3.
i	denotes a hot process stream
j	denotes a cold process stream
k	denotes a block in the superstructure
s	denotes a hot utility
w	denotes a cold utility
Note:	above indices are used in Chapter 5.
i,j,k	running indices used in other chapters.

SUPERSCRIPTS

1	branch 1 of a stream after splitting
2	branch 2 of a stream after splitting
L	lower bound
U	upper bound

SUBSCRIPTS

1–M	number assigned to a block
1	hot end of a block
2	cold end of a block
C(c)	cold streams including cold utility
cu	cold utility
H(h)	hot streams including hot utility
hu	hot utility
in	supply temperature
max	maximum

min	minimum
minf	minimum flux
lm	logarithmic temperature difference
out	target temperature
r,m	remaining problem after selecting match *m*
sf	shifted
s	supply
t	target
t	total
p	process

REFERENCES

Ahmad S. and B. Linnhoff. Overall cost targets for heat exchanger networks. *IChemE Annl Res. Mtg.* Bath. (1984).

Ahmad S. Heat exchanger networks: cost trade-offs in energy and capital. *Ph.D. Thesis,* University of Manchester, Inst. of Sci. and Technol, U.K. (1985).

Ahmad S., B. Linnhoff and R. Smith, Design of multipass heat exchangers: An alternative approach. *Trans of the ASME: Journal of Heat Transfer*, 110, 304–309 (1988).

Ahmad S and R.Smith, Targets and design for minimum number of shells in heat exchanger networks, *Chem. Eng. Res. Des,* Sep. (1989).

Ahmad S. and B. Linnhoff. SUPERTARGETING: different process structures for different economics. *Transactions of ASME: Jl of Energy Resources Technology*, 111, 131136 (1989).

Ahmad S., B. Linnhoff and R. Smith. Cost optimum heat exchanger networks-2. Targets and design for detailed capital cost models. *Comput. chem. Engng.* 14, 751-767 (1990).

Beautyman A.C. and A.R.H. Cornish, The design of flexible heat exchanger networks. *IChemE Symp. Ser.* 86, 547 (1984).

Boland D. and B. Linnhoff. The preliminary design of networks for heat exchange by systematic methods. *The Chem. Engr.* April 9-15 (1979).

Bowman R.A, A.C.Mueller and W.M.Nagle, Mean temperature difference in design, *Tr ASME*, 62:283, (1940).

Brooke A, Kendrick, D and A. Meeraus *"GAMS: A User's Guide"* . Scientific Press, (1988).

Calandranis J. and G. Stephanopoulos. Structural operability analysis of heat exchanger networks. *AIChE Mtg.* Houston (1985).

Cerda J. and A.W. Westerberg. Synthesizing heat exchanger networks having restricted stream/stream matches using transportation problem formulations. *Chem. Engng. Sci.* 38, 1723-1740 (1983).

Cerda J., A.W. Westerberg, D. Mason and B. Linnhoff, Minimum utility usage in heat exchanger network synthesis. *Chem. Engng. Sci.* 38, 373-387 (1983).

Challand T.B., R.W. Colbert and C.K. Venkatesh. Computerized heat exchanger networks. *Chem. Engng. Prog.* 77, 65-71 (1981).

Chen B., J.Shen, Q. Sun and S. Hu. Development of an expert system for synthesis of heat exchanger networks. *Comput. chem. Engng.* 13, 1221-1227 (1989).

Ciric A.R. and C.A. Floudas. Application of the simultaneous match-network optimization approach to the pseudo-pinch problem. *Comput. chem. Engng.* 14, 241-250 (1990).

Ciric A.R. and C.A. Floudas. Heat exchanger network synthesis without decomposition. *Comput. chem. Engng*. 15, 385-396 (1991).

Colberg R.D. and M. Morari. Area and capital cost targeting for heat exchanger network synthesis with constrained matches and unequal heat transfer coefficients. *Comput. chem. Engng*. 14, 1-22 (1990).

Colbert R.W. Industrial heat exchange networks. *Chem. Engng. Prog*. 78, 47-54 (1982).

Dolan W.B., P.T. Cummings and M.D. LeVan. Heat exchanger network design by simulated annealing. *Proc. First Int. Conf. on Foundations of Computer Aided Process Operations*, Park City, UT (1987).

Dolan W.B., P.T. Cummings and M.D. LeVan. Process optimization via simulated annealing: application to network design. *AIChE Jl* 35, 725-736 (1989).

Edgar T.F.and D.M.Himmelblau, "*Optimization of Chemical Processes*", McGraw–Hill Book Company, (1988).

Floudas, C.A., I.E. Grossmann and R.M. Wood, automatic synthesis and optimization of heat exchanger networks. *CHEMECA 85, Australia* (1985).

Floudas C.A., A.R. Ciric and I.E. Grossmann. Automatic synthesis of optimum heat exchanger network configurations. *AIChE Jl* 32, 276-290 (1986).

Floudas C.A. and A.R. Ciric. Strategies for overcoming uncertainties in heat exchanger network synthesis. *Comput. chem. Engng.* 13, 1133-1152 (1989).

Floudas C.A., A. Aggarwal and A.R. Ciric. Global optimum search for nonconvex NLP and MINLP problems. *Comput. chem. Engng.* 13, 1117-1132 (1989).

Floudas C.A. and V. Visweswaran. A global optimization algorithm (GOP) for certain classes of nonconvex NLPs-theory. *Comput. chem. Engng.* 14, 1397-1417, (1990).

Fraser, D.M., The use of minimum flux instead of minimum approach temperature as a design specification for heat exchanger networks, *Chem. Engng. Sci.*, 44, 1121-1127, (1989a).

Fraser, D.M., The application of minimum flux specification to the design of heat exchanger networks, *European Symposium on the use of computers in the chemical industry:* Erlangen, 23-26 April, DECHEMA Monogram, 116, 253-260, (1989b).

Grimes L.E., M.D. Rychener and A.W. Westerberg. The synthesis and evolution of networks of heat exchange that feature the minimum number of units. *Chem. Engng. Commun.* 14, 339-360 (1982).

Grossmann I.E. and M. Morari, Operability, resiliency and flexibility–process design objectives for a changing world. *Proceedings of the Second International Conference on Foundations of Computer-–aided Process Design* (A.W.

Westerberg and H.H. Chien, Eds), p. 931, CACHE publications, Ann Arbor (1984).

Grossmann I.E. *Personal Communication*. Carnegie-Mellon University, Pittsburgh (1985).

Grossmann I.E. and C.A. Floudas, A new approach for evaluating flexibility in chemical process design. *IChemE Symp. Ser.* 92, 619 (1985).

Gundersen T. and L. Naess. The synthesis of cost optimal heat exchanger networks - An industrial review of the state of the art. *Comput. chem. Engng.* 12, 503-530 (1988).

Gundersen T. and I.E. Grossmann. Improved optimization strategies for automated heat exchanger network synthesis through physical insights. *Comput. chem. Engng.* 14, 925-944 (1990).

Halemane K.P. and I.E. Grossmann, Optimal process design under uncertainty. *AIChE Jl* 29, 425 (1983).

Hohmann E.C. Optimum networks for heat exchange. *Ph.D. Thesis*, Univ. of Southern California (1971).

Hohmann E.C., Heat exchanger technology, network synthesis. *Kirk–Othmer Encyclopedia of Chemical Technology*, 3rd Ed., Supplement Volume, John Wiley & Sons, New York, pp. 521–545 (1984).

Jezowski J. A simple synthesis method for heat exchanger networks with minimum number of matches. *Chem. Engng. Sci.* 14, 1928-1932 (1990).

Jezowski J. A note on the use of dual temperature approach in heat exchanger network synthesis. *Comput. chem. Engng.* 15, 305-312 (1991).

Jones S.A. and D.W.T. Rippin. The generation of heat load distributions in heat exchanger network synthesis. Proc. Int. Conf. *Process Systems Engng (PSE-85)*, Cambridge, 157-177 (1985).

Johns S.A., Methods of the Generation and Evaluation of Alternative Heat Exchanger Networks. *Ph.D. Thesis*, Eidgenössischen Technischen Hochschule, Zürich, Switzerland (1987).

Kobayashi S., T. Umeda and A. Ichikawa, Synthesis of optimal heat exchange systems–an approach by the optimal assignment problem in linear programming. *Chem. Engng. Sci.* 26, 1367–1380 (1971).

Linnhoff B. and J.R. Flower. Synthesis of heat exchanger networks: I. Systematic generation of energy optimal networks. *AIChE Jl* 24, 633-642 (1978a).

Linnhoff B. and J.R. Flower. Synthesis of heat exchanger networks: II. Evolutionary generation of networks with various criteria of optimality. *AIChE Jl* 24, 642-654 (1978b).

Linnhoff B., D.R. Mason and I. Wardle. Understanding heat exchanger networks. *Comput. chem. Engng* 3, 295-302 (1979).

Linnhoff B. and J.A. Turner. Heat-recovery networks: New insights yield big savings. *Chem. Engng.* 88, 56-70 (1981).

Linnhoff, B., *et al. User Guide in Process Integration for the Efficient Use of Energy*, Inst. Chem. Engrs., U.K. (1982).

Linnhoff B. and E. Hindmarsh, The pinch design method for heat exchanger networks. *Chem. Engng. Sci.* 38, 745–763, (1983).

Linnhoff B. and D.R. Vredeveld. Pinch technology has come of age. *Chem. Engng. Prog.* 80, 33-40 (1984).

Linnhoff B. and S. Ahmad, SUPERTARGETING, or the optimization of heat exchanger networks prior to design. *World Congress II, Chem. Engng*, Tokyo (1986a).

Linnhoff B. and S. Ahmad, SUPERTARGETING: optimum synthesis of energy management systems. *ASME Meeting*, Anaheim, California (1986b).

Linnhoff B. and S. Ahmad, Cost optimum exchanger networks – I. Minimum energy and capital using simple models for capital cost. *Comput. chem. Engng.* 14, 729–750, (1990).

Masso A.H. and D.F. Rudd, The synthesis of system design II: heuristic structuring. *AIChE Jl* 15, 10 (1969).

McGallard R.L. and A.W. Westerberg, Structural sensitivity analysis in design synthesis. *Chem. Engng Jl* 4, 127-138 (1972).

Niida K, J.Itoh, T. Umeda, S. Kobayashi and A. Ichikawa, Some expert system experiments in process engineering. *IChemE, Chem. Engng Res. Des.* 64, 372-380 (1986).

Nishida N., S. Kobayashi and A. Ichikawa. Optimal synthesis of heat exchange systems: Necessary conditions for minimum heat transfer area and their application to systems synthesis. *Chem. Engng. Sci.* 26, 1841-1856 (1971).

Nishida N., Y.A. Liu and L. Lapidus. Studies in chemical process design and synthesis: III. A simple and practical approach to the optimal synthesis of heat exchanger networks. *AIChE Jl* 23, 77-93 (1977).

Nishida N., G. Stephanopoulos and A.W. Westerberg. A review of process synthesis. *AIChE Jl* 27, 321-351 (1981).

Nishimura, H., Theory on optimal synthesis of heat exchange systems, *Japan-USA Joint Seminar,* Kyoto, Japan, (1975).

Nishimura H. A theory for the optimal synthesis of heat exchanger systems. *J. Optimization Theory Applic.* 30, 423 (1980).

O'Neill B.K., J.R.Roach, R.M.Wood and K.K.Trivedi, Design of heat exchanger networks employing pseudo–pinch concepts, *Proceedings of the 17th Australia*

Chemical Engineering Conference (CHEMECA' 89), Broadbeach, Australia, August, (1989).

Papoulias S.A. and I.E. Grossmann. A structural optimization approach in process synthesis -II. Heat recovery networks. *Comput. chem. Engng.* 7, 707-721 (1983).

Paterson, W.R. A replacement for the logarithmic mean. *Chem. Engng. Sci.* 39, 1635, (1984).

Polley G.T, M.H. Panjeh Shahi.and F.O. Jegede, Pressure drop considerations in the retrofit of heat exchanger networks. *Trans IChemE*, 68, Part A, 211–220 (1990).

Polley G.T. and Panjeh Shahi M.H., Interfacing heat exchanger network synthesis and detailed heat exchanger design. *Trans IChemE*, Institution of Chemical Engineers, 69, Part A, 445–457 (1991).

Ponton J.W. and R.A.B. Donaldson. A fast method for the synthesis of optimal heat exchanger networks. *Chem. Engng. Sci.* 29, 2375-2377 (1974).

Ptacnik R. and J. Klemes, An application of mathematical optimization methods in heat-exchange network synthesis. *Comput. chem. Engng* 12, 231–235 (1988).

Quesada I. and I.E. Grossmann. A global optimization algorithm for heat exchanger networks. *Industrial and Engineering Chemistry Research*, Vol. 132, 487-499 (1993).

Rather R.N.S. Process resequencing for energy conservation. *Chem. Engng. Prog.* 78, 7582, (1982).

Rev E. and Z. Fonyo. Hidden and pseudo pinch phenomena and relaxation in the synthesis of heat-exchange networks. *Comput. chem. Engng.* 10, 601-607 (1986).

Rev. E. and Z. Fonyo, Diverse pinch concept for heat exchange network synthesis: the case of different heat transfer conditions, *Chem. Engng. Sci.*, 46, 1623-1634, (1991).

Rev. E. and Z.Fonyo, Comments on diverse pinch concept for heat exchanger network synthesis, *Comput. chem. Engng.* 48, 627–628, (1993).

Saboo A.K. and M. Morari, Design of resilient processing plants–IV. Some new results on heat exchanger network synthesis. *Chem. Engng Sci.* 38, 579 (1984).

Saboo, A.K. and M. Morari, RESHEX: An interactive software package for the synthesis and analysis of resilient heat–exchanger networks – I. Program description and application. *Comput. chem. Engng.* 10, 577–589, (1986).

Saboo A. K., M. Morari and R. D. Colberg. RESHEX-an interactive software package for the synthesis and analysis of resilient heat exchanger networks-II. Discussion of area targeting and network synthesis algorithms. *Comput. chem. Engng* 10, 591-599 (1986).

Shah J.V. and A.W. Westerberg, Evolutionary synthesis of heat-exchanger networks. *AIChE Mtg*, Los Angeles (1975).

Shah J.V. and A.W. Westerberg, EROS: a program for quick evaluation of energy recovery systems. *Comput. chem. Engng*. 4, 21-32 (1980).

Shiroko K. and T. Umeda, A practical approach to the optimal design of heat exchange systems. *Proc. Econ. Int.* 3, 44-49 (1983).

Siirola J.J., Status on heat exchanger network synthesis. *AIChE Mtg*. Tulsa (1974).

Stephanopoulos G. Industrial Energy-Conservation Manual – *4. Synthesizing Networks of Heat Exchangers*. The Massachusetts Institute of Technology (MIT) press (1982).

Su L.J., A loop-breaking evolutionary method for the synthesis of heat exchanger networks. *M.S. Thesis*, Sever Institute of Washington University (1979).

Su J.L. and R.L. Motard, Evolutionary synthesis of heat exchanger networks. *Comput. chem. Engng*. 8, 67-80 (1984).

Pethe, S., Singh, R. and Knopf, F.C. A Simple Technique for Locating Loops in Heat Exchanger Networks. *Comput. chem. Engng*, Vol 13, No. 7, 859-860, (1989).

Suaysompol K. Synthesis of optimal energy recovery networks applying a flexible pinch design embedded in artificial intelligence. *PhD Thesis,* The University of NSW, Australia, (1991).

Suaysompol K. and R.M. Wood. The flexible pinch design method for heat exchanger networks: Part I. Heuristic guidelines for free hand designs. *Trans. IChemE*, 69, 458-464, (1991a).

Suaysompol K. and R.M. Wood. The flexible pinch design method for heat exchanger networks: Part II. Heuristic searching guided by the A~ algorithm. *Trans. IChemE,* 69, 465-470, (1991b).

Swaney R.E. and I.E. Grossmann, An index for operational flexibility in chemical process design. *AIChE Jl* 31, 621 (1985).

Terrill D.L., Heat Exchanger Network Design and Operability Evaluation. *Ph.D Thesis,* The University of Massachusetts (1985).

Townsend D.W and M. Morari, Resiliency of heat exchanger networks: an objective compatible with minimum cost. *AIChE Ntl Mtg*, San Francisco (1984).

Townsend D.W. and B. Linnhoff. Surface area targets for heat exchanger networks. *IChemE Annual Res. Mtg*, Bath. U.K. (1984).

Townsend D.W. Surface area and capital cost targets for heat exchanger networks. *PhD. Thesis*, University of Manchester, Inst. of Sci. and Technol, U.K. (1989).

Trivedi K.K, J.R. Roach and B.K. O'Neill, Shell targeting in heat exchanger networks. *AIChE Journal,* 33, 2087–2090 (1987).

Trivedi K.K., B.K. O'Neill, J.R. Roach and R.M. Wood. A new dual-temperature design method for the synthesis of heat exchanger networks. *Comput. chem. Engng.* 13, 667-685 (1989).

Trivedi K.K., B.K. O'Neill, J.R. Roach and R.M. Wood. Systematic energy relaxation in MER heat exchanger networks. *Comput. chem. Engng.* 14, 601-611 (1990).

Umeda T., J. Itoh and K. Shiroko. Heat exchange system synthesis. *Chem. Engng. Prog.* 74(7) 70-76 (1978).

U.S National Research Council. *Frontiers in Chemical Engineering* - Research Needs & Opportunities. National Academy Press, 143-145 (1988).

Viswanathan M. and L.B. Evans. Development of an expert system to synthesize heat integration systems for process plants. *Energy Engng Sci. Symp.* Chicago (1986).

Viswanathan M. and L.B. Evans. Studies in the heat integration of chemical process plants. *AIChE Jl* 33, 1781-1790 (1987).

Viswanathan J. and I.E. Grossmann. A combined penalty function and outer-approximation method for MINLP optimization. *Comput. chem. Engng.* 14, 769-782 (1990).

Visweswaran V. and C.A. Floudas. A global optimization algorithm (GOP) for certain classes of nonconvex NLPs-II. application of theory and test problems. *Comput. chem. Engng.* 14, 1419-1434 (1990).

Wilson, R.J. and L.W. Beinke *Applications of Graph Theory*, Academic Press, (1979).

Wood R.M., R.J. Wilcox and I.E. Grossmann. A note on the minimum number of units for heat exchanger network synthesis. *Chem. Engng. Commun.* 39, 371-380 (1985).

Wood R.M., K. Suaysompol, B.K. O'Neill, J.R. Roach and K.K. Trivedi. A new option for heat exchanger network design. *Chem. Engng. Prog.* 38-43, September (1991).

Yee T.F. and I.E. Grossmann. A screening and optimization approach for the retrofit of heat exchanger networks. *Annual AIChE Meeting*, Washington, D.C. (1988).

Yee T.F., I.E. Grossmann and Z. Kravanja. Simultaneous optimization models for heat integration-I. Area and energy targeting and modelling of multi-stream exchangers. *Comput. chem. Engng.* 14, 1151-1164 (1990).

Yee T.F. and I.E. Grossmann. Simultaneous optimization models for heat integration-II. Heat exchanger network synthesis. *Comput. chem. Engng* 14, 1165-1184 (1990).

Zhu X. X., B.K.O'Neill, J.R Roach and R.M.Wood. A new method for the synthesis of heat exchanger networks using area-targeting principles. accepted for publication *Comput. chem. Engng*.(1993a)

Zhu X. X., B.K.O'Neill, J.R.Roach and R.M.Wood. Area-targeting methods for the direct synthesis of variable film coefficient heat exchanger networks. accepted for publication. *Comput. chem. Engng*.(1994)

Zhu X.X., B.K. O'Neill, J.R. Roach and R.M. Wood, A method for cost and area targeting based on block decomposition and non-linear optimization. Submitted for publication, *Comput chem. Engng* (1993b).

Zhu X.X., B.K. O'Neill, J.R. Roach and R.M. Wood, Kirchhoff's law and loop-breaking for the design of heat exchanger networks. Accepted for publication, *Comput, chem. Comm* (1993c).

PUBLICATIONS

Journal Publications

Zhu X. X., B.K.O'Neill, J.R Roach and R.M.Wood. A new method for the synthesis of heat exchanger networks using area-targeting principles. accepted for publication, *Comput. chem. Engng.* (1993a)

Zhu X. X., B.K.O'Neill, J.R.Roach and R.M.Wood. Area-targeting methods for the direct synthesis of variable film coefficient heat exchanger networks. accepted for publication, *Comput. chem. Engng.* (1994)

Zhu X.X., B.K. O'Neill, J.R. Roach and R.M. Wood, A method for cost and area targeting based on block decomposition and non-linear optimization. Submitted for publication, *Comput chem. Engng* (1993b).

Zhu X.X., B.K. O'Neill, J.R. Roach and R.M. Wood, Kirchhoff's law and loop-breaking for the design of heat exchanger networks. Accepted for publication, *Comput chem. Comm* (1993c).

Conference Proceedings

Zhu X. X., B.K.O'Neill, J.R Roach and R.M.Wood. The synthesis of heat exchanger networks using area–targeting principles. Presented at *Australian CHEMICA 92*, Canberra (1992).

Zhu X. X., B.K.O'Neill, J.R Roach and R.M.Wood. Area and Cost targeting using block decomposition and non-linear optimization. Presented at *Australian CHEMICA 93*, Melbourne (1993).

Wood R.M., X.X.Zhu, N.Al–Fakir, B.K.O'Neill and J.R.Roach. Criteria for area minimization of heat exchanger network for streams with unequal film coefficients. Submitted to *Australian CHEMICA 94*, Perth (1994).

Auresenia J., Wood R.M., X.X.Zhu, B.K.O'Neill and J.R.Roach. Use of the diverse pinch and flexible pinch methods to synthesis hear cost–optimal heat exchanger networks. Submitted to *Australian CHEMICA 94*, Perth (1994).