SUPPLY AND TARGET-BASED SUPERSTRUCTURE SYNTHESIS OF HEAT AND MASS EXCHANGE NETWORKS

A thesis submitted for the degree of

DOCTOR OF PHILOSOPHY

In the Department of Chemical Engineering

UNIVERSITY OF CAPE TOWN

by

OLUWATOSIN SARAFA AZEEZ

Under the supervision of

Professor Duncan Fraser

December 2011

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Whereas, there is no reward for good other than good, and any individual that is not grateful to his fellow human being for one good received will never be grateful to God. In line with this tradition, I will like to express gratitude to God who created man from a clinging substance and taught him by the pen. Glory be to God for his mercies in the course of this research, he teaches man that which he knew not. I will then go on to thank the people that will be mentioned below.

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ABSTRACT

This study presents three new methods for superstructure synthesis of heat exchanger networks (HENs) and mass exchanger networks (MENs) that involve the use of key parameters in HEN and MEN to define superstructure intervals. The key parameters are the stream supply and target temperatures/compositions. The Supply-Based Superstructure (SBS) uses the supply temperatures/compositions of both the hot/rich streams and the cold lean streams. The Supply and Target-Based Superstructure (S&TBS) uses the supply temperatures/compositions of hot/rich streams and the target temperatures/compositions of cold/lean streams for the definition of the superstructure intervals. The Target and Supply-Based Superstructure (T&SBS) uses the target temperatures/compositions of hot/rich streams and the supply temperatures/compositions of cold/lean streams for the definition of the superstructure interval boundaries.

These aforementioned superstructures are all modelled as Mixed Integer Non Linear Programmes (MINLP) with the objective of minimising the Total Annual Cost (TAC) of the HEN/MEN. The intermediate temperatures/compositions in each of these superstructures are variables in the optimisation processes. The ability of each stream to exchange heat/mass in any interval in the superstructure is subject to thermodynamic heat/mass transfer feasibility. These superstructures generally have the potential to give more intervals than previous superstructures presented in the literature, allowing for more opportunities for heat/mass exchange between streams. These superstructures are not partitioned at the pinch as is done in pinch technology and they offer the opportunities of matches being either preferred or forbidden.

The newly developed superstructure synthesis techniques have been applied to five HENS problems. They include a HEN with forbidden /restricted matches and one of significantly different heat transfer coefficient. The superstructures were also applied to two multiple utility HENS problems and four MENS problems. The MENS problems include a continuous contact column, those involving stagewise columns and a MEN involving regeneration of the mass separating agent (MSA).The superstructures presented are compared with other HEN and MEN superstructures in terms of formulation and the solutions they returned. The solutions obtained are also compared with the solutions of other synthesis techniques that are not superstructure based. Nine of the eleven solutions obtained in this study are in the same range as the best ones in the literature with one solution given by SBS being the best of all, for the ammonia removal MEN problem.

It is observed in this study that the inclusion or the exclusion of the isothermal/isocomposition mixing assumptions at HEN/MEN partition boundaries does not necessarily translate to structures of lowest TAC. The comparison of the solutions of these superstructures with previous techniques shows that no single technique has been able to obtain the lowest TAC for all the HEN/MEN problems presented in the literature. Most importantly, this study shows that different superstructure partitioning techniques have the tendency to impose a limitation on the solution space in HEN and MEN. The solutions obtained in this study also show that the use of a larger number of intervals in superstructures does not necessarily translate to a lower TAC in HENs/MENs. This study again shows that a network with the minimum number of units does not necessarily translate to the minimum TAC in HENs/MENs.

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CHAPTER 1

INTRODUCTION

CHAPTER ONE: INTRODUCTION

1.1 BACKGROUND TO PROCESS SYNTHESIS

Process synthesis is concerned with the conversion of raw materials into finished products. This conversion is achieved through various stages such as reaction, separation, mixing, heating, drying, cooling and size reduction. The process elements involved have to be suitably integrated and the process flowsheet generated for the system to meet the desired objectives. El-Halwagi (1997) states that this holistic approach to chemical process design can enhance and reconcile process objectives like yield improvement, effective energy use, cost reduction and pollution prevention.

The task before the process designer is to first identify the stages required for the process, then work out suitable integration of those stages to form a complete process that gives the desired output. This integration is a holistic approach to process design, retrofitting and operation with emphasis on the overall process (El-Halwagi, 1997). Process integration offers the designer the opportunity to set targets for the process streams and to have the understanding of the interactions among various units, which enables the designer to achieve the targets.

The synthesis process leads to industrial activities which are important in meeting current global needs. However, it should also take care of the needs of future generations (Smith, 1995). In effect, chemical process design should use raw materials economically and efficiently, and should be manipulated to avoid the production of waste and inefficient use of energy. This study focuses on the synthesis of cost effective heat exchanger networks (HENs) and mass exchanger networks (MENs) with the ultimate aim of reducing the total annual cost (TAC) of the production processes.

In the process of transforming raw materials into products in chemical industries, there is a hierarchy of different levels that can be represented as an onion diagram (Smith, 1995), as shown in Figure 1.1. Reactor is a basic piece of equipment needed for the reaction of the species; the reactor is thus the centre of the onion. After the reaction, the main products then come out of the reactor along with unreacted feed and the by products go into the separator in order to separate the main products in their pure form from the mixture while the unreacted feed is recycled. This means that in the system, reactor, separator and the recycle system have to be designed together. Energy is needed to drive the reaction, effect the separation, drive pumps and compressors in the process line. The products also have to be cooled before collection, among other cooling requirements in the process. This calls for energy integration in the form of heat exchanger network (HEN) design. In the integration process, the external heating and cooling utilities will be identified. Two major techniques that have been used in the recent time for such energy integration are the pinch technology and the mathematical programming approaches.

In process design, mass optimisation in terms of the mass separating agents (MSAs) needed to effect transfer of certain component(s) from one stream to another, or to be used to remove pollutants and other unwanted materials from the process line is also gaining prominence in the recent years. This is also necessary because environmental regulations stipulate the concentration limits for waste products emanating from process industries which are to be discharged into the environment. Pinch technology and mathematical programming have as well been used to accomplish these tasks in the form of MEN design. In pinch technology, the designer exploits physical and thermodynamic insights to evaluate the performance characteristics of the process system which enables him to set targets without prior commitments to its design. The designer, however, completes the process by evolving a design to meet the set target. Mathematical programming approach involves the setting up of the HEN or MEN task as mathematical model equations and constraints with the aim of optimising the process.

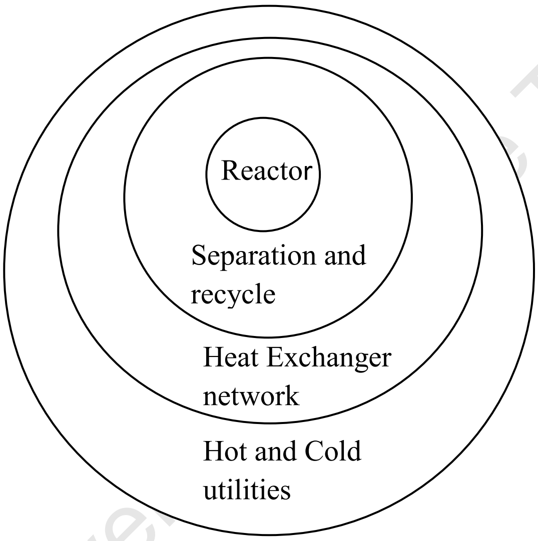


Figure 1.1 The Onion diagram model showing the hierarchy of chemical process design for the transformation of raw materials to products (Smith, 1995).

1.2 PINCH TECHNOLOGY

Pinch technology evolved in the early 1970s, due to the energy crisis of the time, as a tool for HEN design (Hohmann, 1971; Linnhoff & Flower, 1978). It has, however, been used for other chemical engineering processes such as distillation and heat pumps among others and it has been extended to MEN by El-Halwagi and Manousiouthakis (1990a). Pinch technology involves two steps - targeting and design. The early technique in pinch technology involves the prediction of the optimum energy performance achievable in a process in the first step, while the minimum number of units and minimum exchanger area that satisfy the energy predicted are used in the second step to target the capital cost. Operating and caqital costs may be traded off against each other to find the minimum Total Annual Cost (TAC), a procedure known as supertargeting, which is presented in Section 2.3.5. Pinch technology has been used for the costs targeting and design sequentially in HEN and MEN. Pinch technology has the advantage that the designer is involved in the process, making it possible for the screening of different options at the targeting stage and as such, the design performance can be well monitored. It does, however, have the limitation that it is sequential. This is because the trade-off between the utility and capital costs can not be accounted for simultaneously which usually results in suboptimal networks in HEN and MEN design.

1.3 MATHEMATICAL PROGRAMMING

The application of mathematical programming to heat exchanger network synthesis (HENS) and mass exchange network synthesis (MENS) (which entails sequential and simultaneous approaches) involves the setting up of mathematical models where the heat/mass exchange problem is defined using mathematical equations and constraints. The model is subsequently optimised so as to achieve the desired objectives. The sequential models that have been presented for HENS and MENS are the mathematical implementation or interpretation of the pinch technique. The most prominent of such models is the Linear Programming (LP) and the Mixed Integer Linear Programming (MILP) transhipment model of Papoulias and Grossmann (1983) which is used to determine the pinch points and the minimum number of units respectively in HENS. The transhipment model was later adapted by El-Halwagi and Manousiouthakis (1990a) for MEN. The simultaneous approaches, on the other hand, are those models where the HENS or the MENS task is formulated either as a non linear programming (NLP) or mixed integer non linear programming (MINLP) to enable all the competing cost in the synthesis task to be traded off in a single step (Ciric & Floudas, 1991; Yee & Grossmann, 1990; Papalexandri *et al*., 1994).

1.4 MOTIVATION

Temperatures of streams have been used by various workers over the years in partitioning of HENS problems (Papoulias & Grossmann, 1983; Floudas *et al*., 1986; Colberg & Morari, 1990; Ciric & Floudas, 1990). The foremost is the Linear Program (LP) and Mixed Integer Linear Program (MILP) transshipment model of Papoulias and Grossmann (1983). The model is an automated version of the Pinch Technology approach to HENS; it can be used to target the minimum utility cost and minimum number of units. Some workers have consequently based their studies on the concept of the transhipment model. They include Colberg and Morari (1990) in targeting for area and capital cost for HENs using non linear programming and the MILP Superstructure of Floudas *et al*. (1986). The studies of Ciric and Floudas (1990) in the simultaneous match–network optimisation approach to the pseudo-pinch problem where the assumption of no heat flow across the pinch in HEN was relaxed and the mixed integer non linear programming (MINLP) hyperstructure of Ciric and Floudas (1991) for simultaneous optimisation of utility consumption and stream matches were based on the temperature partitioning approach. The Interval based mixed integer non linear programming (IBMS) model of Isafiade and Fraser (2008a; 2008b) was also based on the temperature partitioning approach.

These temperature based partitioning approaches guarantee feasible heat transfer in HEN intervals (Papoulias & Grossmann, 1983). In this study, it is observed that in all the above optimisation techniques, none has exploited the use of the supply temperatures of hot streams or the target temperatures of hot streams or the combinations of supply temperatures of hot streams and the target temperatures of cold streams or even the combination of target temperatures of hot stream and the supply temperatures of cold streams in HEN to develop superstructures that can optimise all the competing costs in HEN simultaneously using MINLP. A similar observation is made regarding MENS superstructures.

This thesis presents new approaches for the synthesis of heat and mass exchange networks. The techniques presented use insights from pinch technology to generate superstructures for heat and mass exchange network design. The first superstructure developed, which is known as the Supply Based Superstructure (SBS), is partitioned using supply temperature/composition which is a key parameter for the optimum use of driving forces in exchangers. Temperature/composition locations in the superstructure are defined by the supply values of the process and utility streams. The intermediate temperatures/compositions of the streams are variables to be optimised within the intervals created by their supply values. The ability of each process/utility stream to exchange heat/mass within each interval is, however, subject to thermodynamic feasibility. The SBS which is an MINLP model simultaneously optimises competing costs in heat and mass exchange networks by minimising the Total Annual Cost (TAC).

The conception of SBS gave rise to the second and third superstructures known as the Supply and Target Based Superstructure (S&TBS) and the Target and Supply Based Superstructure (T&SBS) respectively for the synthesis of heat and mass exchanger networks. The HENS part of this study are similar to the stagewise superstructure (SWS) of Yee and Grossmann (1990) and the IBMS of Isafiade and Fraser (2008a) while the MENS part are similar to the IBMS of Isafiade and Fraser (2008b) and the stagewise-like superstructure ('SWS') of Szitkai *et al*. (2006). The studies presented in this thesis offer the opportunity of a higher number of intervals which offer more and effective combinations of streams in the use of superstructure for the synthesis of HENS and MENS.

1.5 OBJECTIVES, METHODOLOGY, SCOPE AND STRUCTURE OF THIS THESIS

This study presents three different superstructures for the synthesis of heat and mass exchanger networks as highlighted in the motivation. Each of the superstructures was developed and modelled as an MINLP for the simultaneous optimisation of the operating and capital costs in HEN/MEN in turn. The fourth possible superstructure, which is the conception of superstructures based on the target temperature/composition of hot/rich streams and the target temperature/composition of cold/lean streams to define the superstructure boundary has some limitations in its applications to HENS and MENS. These limitations are discussed in this thesis.

The three superstructures shall be applied to HENs problems involving restricted matches, those involving significantly different heat transfer coefficients and problems with multiple utilities, and MENS problems, including one with simultaneous mass exchange and regeneration networks, and those with multiple MSAs. The results obtained in this study will be comprehensively compared with all stage/interval based approaches and with other studies that are not interval based. The effects of the nature of partitioning on the total annual costs (TACs) of HENS and MEN will be highlighted

Chapter 2

This chapter presents the review of literature relevant to this study starting from the advent of the pinch technique and mathematical programming for HENS and MENS. The review links the sequential mathematical programming technique to pinch from where it originates, and the link between sequential and simultaneous methods are also highlighted. The SWS of Yee and Grossmann (1990), the 'SWS' of Szitkai *et al*. (2006), and the IBMS of Isafiade and Fraser (2008a; 2008b) are reviewed extensively in this chapter because of their similarities with this study.

Chapter 3

The development of SBS, S&TBS, T&SBS and TBS for both HENS and MENS are presented in this chapter. The problems encountered in the use of TBS for the synthesis of HENS and MENS are also presented. The superstructures presented in this chapter are also compared with various HENS and MENS superstructures as previously presented by various researchers.

Chapter 4

Following the development of the superstructures in Chapter 3 is the presentation of HENS and MENS variables and model equations for SBS, S&TBS and T&SBS in this chapter.

Chapter 5

The SBS, S&TBS and T&SBS are applied to various HENS and MENS literature problems in this chapter. A HEN problem involving significantly different heat transfer coefficients and others involving multiple utilities and one involving forbidden/restricted matches are considered. MENS problems including those of multiple MSA and a MEN with simultaneous mass exchange and regeneration network are considered. The solutions obtained using the SBS, S&TBS and the T&SBS are compared with the solutions of the SWS and its derivatives in this chapter. The features of the superstructures are also presented in this chapter.

Chapter 6

This chapter presents the discussions of results obtained in Chapter 5 with the results of all other researchers that have obtained solutions for the problems solved in Chapter 5. The effects of how intervals are defined on the TAC as obtained by various researchers are discussed in this chapter.

Chapter 7

The key findings in this research and proposed future work are presented in this chapter.

CHAPTER 2

LITERATURE REVIEW

CHAPTER TWO: LITERATURE REVIEW

2.1 INTRODUCTION

This section presents the review of relevant literature with respect to this study. The first part dwells on various studies by different sets of workers on the advent and the application of the pinch technique to process synthesis as it applies to heat exchanger networks (HENs). This is followed by the development of mathematical programming in HENS. The application of Mathematical programming to HENS is subdivided into sequential and simultaneous approaches depending on whether it is developed and applied to only utility targeting followed by matching or the total annual cost of heat exchanger networks (HENs). The latter part of the review deals with mass exchanger network synthesis (MENS) in order of pinch technique, followed by mathematical programming. The contributions and shortcomings of the methods presented by various workers are highlighted all along in this review. The results obtained by various sets of workers whose work is reviewed are then compared with the present study in later chapters of the thesis.

2.2 HEAT EXCHANGER NETWORK SYNTHESIS (HENS)

The tasks of synthesising cost effective heat exchanger networks have been extensively studied in process synthesis over the years (Lee *et al*., 1970; Hohmann, 1971; Linnhoff & Flower, 1978; Linnhoff, 1979; Gundersen & Naess, 1988; Gundersen & Grossmann, 1990). For example, Lee *et al.* (1970) formulated HENS problems using the branch and bound technique of Lawler and Wood (1966) with the aim of optimal energy exchange to obtain a network of minimum cost.

The HENS design problem to be considered is as defined by Masso & Rudd, 1969; Floudas, 1995; Krishna & Murty, 2007; Isafiade & Fraser, 2008a; Azeez *et al*, 2011. It is stated as follows:

The HENS problem statement:

> *There are a number of hot and cold process streams (to be cooled and heated respectively). The task is to synthesise a heat exchanger network which can transfer heat from the hot streams to the cold streams in order to get a minimum total annual cost network. Specified also are the heat capacity flowrates, heat transfer coefficients, and supply and target temperatures of each process stream. Available for service are cooling and heating utilities whose costs, heat transfer coefficients, supply temperatures, target temperatures are also given, along with annual operating time, heat exchanger costs and the annual capital cost factor.*

2.3 APPLICATION OF PINCH TECHNOLOGY TO HENS

Pinch Technology emerged as a tool for the design of heat exchanger networks against the background of the energy crises of the nineteen seventies (Hohmann, 1971; Linnhoff & Flower, 1978). It involves two steps, namely targeting and design. In the targeting step, using the graphical approach or the problem table analysis (algebraic approach) of Linnhoff and Flower (1978), the pinch is identified as a temperature level in the process which is a bottle neck to further energy recovery. The graphical tool is shown in Figure 2.1 and it is known as the heat exchange composite curves (Umeda *et al*., 1979). The identification of the pinch as shown in Figure 2.1 gives the minimum energy (hot and cold utilities) needed to satisfy the energy requirements of the process (Linnhoff *et al*., 1982). This is equivalent to the annual operating cost (AOC) target. The corresponding total heat exchange area needed to satisfy the energy targets, and hence the cost of this area, can also be predicted ahead of the design step in a procedure known as capital cost targeting (Linnhoff & Ahmad, 1989).

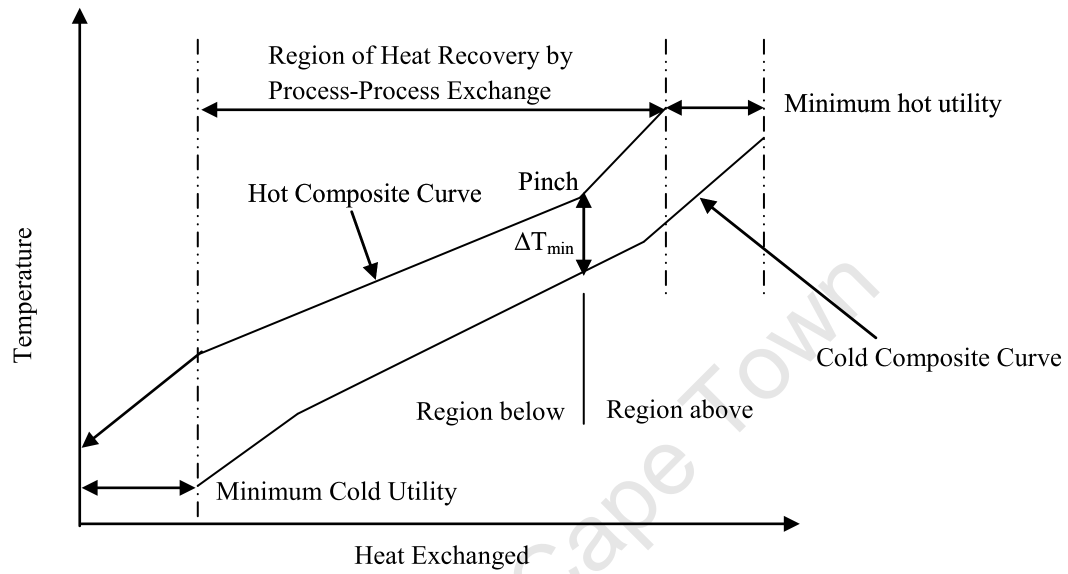


Figure 2.1: The hot and cold streams heat exchange composite curves (Shenoy, 1995).

2.3.1 Energy Targeting and Annual Operating Cost.

The energy targeting process in pinch technology is demonstrated in the heat exchange composite curve shown in Figure 2.1 above. The curve is a plot of a composite of the hot process stream against the cold process streams on the same temperature versus enthalpy axes (Linnhoff *et al.*, 1982). The point of closest approach between the two curves is the minimum temperature difference (ΔT_{min}); this point is referred to as the pinch (Umeda *et al.*, 1978; Linnhoff & Flower, 1978; Linnhoff *et al.*, 1979; Linnhoff & Hindmarsh, 1983). The pinch point divides the process into two thermodynamic regions; it is the most constrained area for energy recovery.

In Figure 2.1, the area of vertical overlap of the two composite curves gives the region of maximum heat recovery from the hot streams to the cold streams. Heat recovery is not possible in the area where the cold composite curve overshoots the hot composite curve. The energy need of the cold streams in this area is satisfied with external hot utility, which is the target for the minimum hot utility as shown in Figure 2.1. Similarly, heat recovery is not possible where the hot composite overshoots the cold composite, the energy need of the hot streams in this area is satisfied with external cold utility, this is the targeting for the minimum cold utility. Thus, the process demonstrated in Figure 2.1 above ensures maximum energy recovery (MER) among process to process hot and cold streams in the process. The identification of the pinch gives the minimum energy (hot and cold utilities) needed to satisfy the heat requirement of the process (Linnhoff *et al*., 1982). The above process is valuable in the evaluation of utility costs (Shenoy, 1995) since it corresponds to the annual operating cost (AOC) target, the pinch message in HENS is that this target should be established before any conception of heat exchanger network design.

2.3.2 Capital Cost Targets in HENS

In HENS, the factors that contribute to capital cost targeting are the exchanger surface area target, number of heat exchange units, number of shells, materials of construction, exchanger pressure rating and the type of heat exchanger (Smith, 2005).

2.3.2.1 *Heat Exchanger Area Targeting and Capital Cost*

Exchanger area targets is key in capital cost estimation prior to network design, this involves the calculation of minimum surface area of heat transfer for all the participating streams in the vertical heat exchange (the heat exchange within intervals) on the composite curve with counter flow assumption (Shenoy, 1995). It is important to note that the process gives minimum area only if the heat transfer coefficients of all streams including those of utilities are equal (Nishimura, 1980). However, if the heat transfer coefficients differ by one order of magnitude, the area targeted by this process from the minimum area shall falls within 10% of the actual area (Linnhoff and Ahmad, 1990).

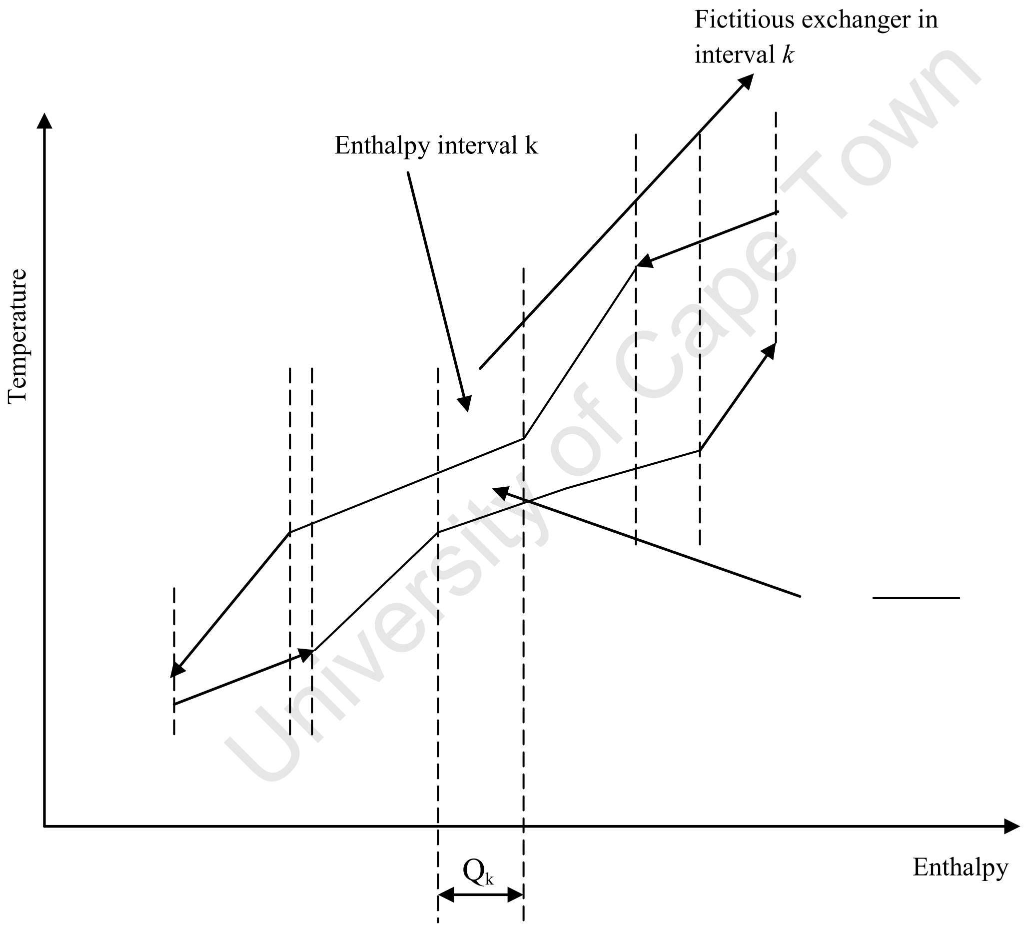


Figure 2.2: Balanced composite curves divided into enthalpy intervals for network area determination (Smith, 2005)

In the use of composite curves to calculate the network area, the temperatures and enthalpy changes information of utility streams are included with those of process streams to obtain a balanced composite curve shown in Figure 2.2.

The balanced composite curves are divided into enthalpy intervals as shown in Figure 2.2 at the inflection points and each interval treated as a fictitious exchanger. The minimum total area between the balanced composite curves is the sum of the areas of all the fictitious exchangers from all enthalpy intervals. For a constant heat transfer coefficient U, with the counter flow heat transfer assumption, the expression for the area for enthalpy interval can be written as:

where

is the exchanger area in interval

is the enthalpy change in interval

is the logarithmic temperature difference in interval

is the overall heat transfer coefficient

The sum of all the area contributions from each enthalpy interval gives the total network area over the whole enthalpy range as shown in the equation below (Townsend & Linnhoff, 1984):

where is the minimum heat exchange area for the total network over the whole intervals and is the total number of enthalpy intervals. It is important to note that Equation 2.2 above only holds for the situation where the overall heat transfer coefficient is constant for the whole process, otherwise, the effect of each stream film transfer coefficient should be included in the equation as presented by Townsend and Linnhoff (1984) as follows:

Where are the enthalpy changes for hot stream , cold stream *j* and heat transfer coefficients for hot stream , cold stream , in interval *k* respectively.

In Figure 2.2, counter current heat transfer is manifested as vertical heat transfer as mentioned earlier. This is ensured by the division of the balanced composite curve into vertical enthalpy intervals. The matching of hot and cold streams within an enthalpy interval was proposed as follows (Linnhoff & Ahmad, 1990): Firstly, that there should be the same number of hot streams as there are cold streams, otherwise, streams with fewer numbers should split to the same number of streams as there are in opposite kind. Secondly, each of the hot streams should match with each cold stream once.

Note that the matches appear vertical on the balanced composite curves since each match occurs between the temperature limits of the enthalpy interval (Shenoy, 1995). If this proposition is applied to enthalpy interval *k* in Figure 2.2 and we consider a case where the hot composite goes from temperatures to while the cold composite goes from temperatures to on the hot and cold composite curves respectively. Then, the proposition of Linnhoff and Ahmad (1990) is applied as follows: if there is one hot stream

(H1) and two cold streams (C1 and C2) in enthalpy interval *k*, then, H1 must split into two to match with C1 and C2 as shown in Figure 2.3. If there are two hot streams (H1 and H2) and two cold streams (C1 and C2) in the enthalpy interval *k*, then each of the streams must split into two to be able to match once with the streams of opposite kind as shown in Figure 2.4, this is always necessary as network design becomes complex, this is the spaghetti design network concept of Ahmad and Smith (1989).

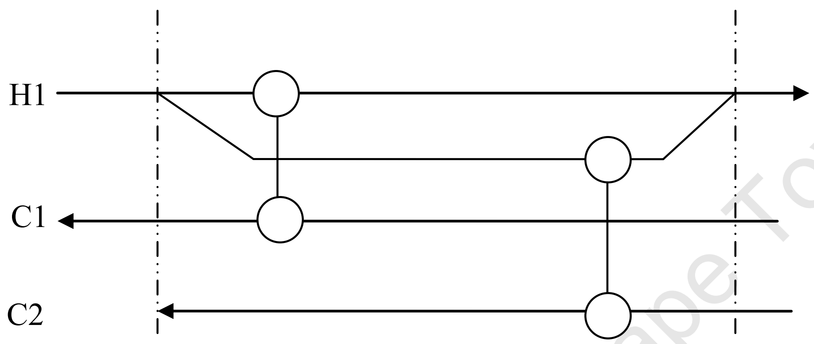


Figure 2.3: The counter current vertical heat transfer in enthalpy interval *k* showing the split of H1 to match with cold streams C1 and C2

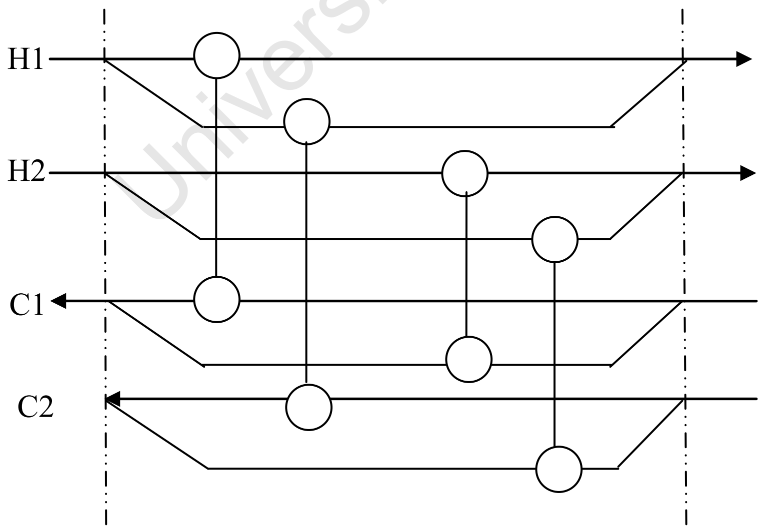


Figure 2.4: Figure showing two hot streams and two cold streams where every stream is split into two to obtain the spaghetti design network of Ahmad and Smith (1989) in enthalpy interval *k*

In spaghetti networks shown in Figures 2.3 and 2.4, each of the matches between a pair of hot and cold streams within interval *k* has exactly the same temperature profiles as the streams on the composite curves in interval *k*. This implies that the spaghetti design networks make maximum use of available driving force ( ) in the network. Non vertical or crisscrossed heat transfer on the composite curves was considered by Colberg and Morari (1990) as shown later in this review.

2.3.2.2 *Targeting for Number of Exchanger Units*

The minimum number of exchanger units required for a synthesis is the total number of streams presents (hot, cold and utilities) minus one (Smith, 2005). Thus, if the number of units is represented by *N*, total number of stream represented by *S*, then, the relation can be expressed as

(2.4)

But in pinch technology, targeting for below and above pinch separately is more correct (Fraser, 1991), Equation 2.4 should then be applied below and above pinch separately as follows.

$$- 2 \qquad (2.5)$$

2.3.2.3 *Capital Cost Evaluation in HENS*

The correlation for the prediction of an installed heat exchanger capital cost with surface area *A* is given by Smith (2005) as follows:

where *a*, *b* and *c* are constants for a particular type of exchanger. The cost function in Equation 2.6 is non linear because the exponent *c* is usually less than 1. At the targeting stage, the area distribution among the conceived exchangers in the network is unknown, it is thus necessary to assume the area is evenly distributed in the proposed exchangers; this still gives good prediction of the capital cost (Ahmad *et al.*, 1990). Equation 2.6 thus becomes

where *N* is the minimum number of units.

For consistency, Equation 2.7 above applies to region below and above pinch separately, the addition then gives the total network capital cost.

2.3.3 Network Total Annual Cost

The energy cost that constitutes the operating cost is unstable though, capital cost is invested once and for all, the life expectancy of the plant should therefore be taken into consideration when calculating the annual costs. Shenoy (1995) gives the expression for total annual cost as follows:

In Equation 2.8 and 2.9, AOC is the annual operating cost, CC is the network capital cost and is the annualisation factor, *r* is the interest rate of return and *t* is the expected plant life.

2.3.4 Network Design

A basic rule in pinch methodology is that the network design must not transfer energy across the pinch either through process to process heat transfer or by wrong use of utilities. If this rule is violated, the design will not achieve the energy target. It is therefore necessary to divide the design process into below and above pinch, and the design be started at the pinch, which is the most constrained region for energy recovery, and also, adhere to the following criteria to avoid difficulty in the design process.

1. Stream population rule.

In the matching of hot stream with cold stream, directly above the pinch, the number of hot streams, should be less than the number of cold streams, and vice versa for stream distribution below the pinch, this can be presented as:

This is known as stream number criterion (Smith, 2005). This rule may require stream splitting to avoid violation of the constraint at pinch.

2. The stream capacity flow rate (CP) inequality rule.

Since the occurs at the pinch, the temperature difference should increase as we move away from the pinch, the feasible matches should thus have a temperature difference that starts with at the pinch, and then increases as it moves away from the pinch. This condition will only be satisfied if

This condition can also require stream splitting at the pinch (Smith, 2005).

Having observed the above rule around the pinch, the design should then continue in a way that minimises cost. A number of heuristics are available to aid this process.

2.3.5 Limitations of the Application of Pinch Technique to HENS.

The main feature of pinch based HENS is that the synthesis approach decomposes the task to sub-tasks that can be handled much more easily than the main task. The targeting of the optimum energy and the corresponding capital cost as done in pinch is obtained at a particular ΔT_{min}. If this targeting is done at a lower value of ΔT_{min}, the energy cost decreases while the capital cost increases. On the other hand, if the targeting is done at a higher value of ΔT_{min}, the energy cost increases while the capital cost decreases. This implies that the minimum TAC (sum of annual operating and annual capital cost) in pinch is obtained at a ΔT_{min} where the trade off between the utility cost and the capital cost gives the minimum TAC. This process of targeting the minimum TAC in pinch technique is called Supertargeting. This approach, however, has the disadvantage that the trade off between the operating cost and the capital cost cannot be accounted for simultaneously; hence, it usually produces sub optimal solutions (networks). Furthermore, the fact that the area obtained using the pinch area targeting method (shown in Figure 2.2) is the true minimum only if the heat transfer coefficients of all streams are equal is another limitation of the pinch technique because this is not always the case., Finally as pointed out by Sagli *et al*. (1990), the assumption that for a given number of units, optimum HEN is possible with one unit less than the number of streams is another limitation of the pinch technique.

2.4 APPLICATION OF MATHEMATICAL PROGRAMMING TO HENS

The application of mathematical programming (which can be sequential or simultaneous) to HENS involves the use of mathematical models (Floudas, 1995) to define the heat exchange problem using mathematical equations and constraints. The resulting model is then subject to optimisation to achieve the desire goal. The key contribution in this respect to HENS is the Linear programming (LP) transhipment model for energy targeting and the Mixed Integer Linear programming (MILP) model for the minimum number of units targeting of Papoulias and Grossmann (1983). The LP model of Papoulias and Grossmannis the implementation of the problem table algorithm (PTA) of Linnhoff and Flower (1978), as such, the model can as well recognise the pinch division of the HENS task. The approach of Papoulias and Grossmann (1983), however, has the same limitation as the pinch technique due to it's sequential.

Floudas *et al*. (1986) subsequently presented a non linear programming (NLP) superstructure based model for the synthesis of HENs using insights from the LP and MILP of Papoulias and Grossmann (1983). The main idea of the Floudas *et al*. (1986) method is to decompose the HENS task into subtasks of minimum utility and minimum number of units from which the network that features a minimum investment cost will be developed. The superstructure was then formulated as an optimisation problem whose solution seeks to minimize the investment cost. Apart from the fact that the NLP model of Floudas *et al*. is sequential, it is also a non convex model because it contains bilinear inequalities in the mixers and the exchanger model formulations. Thus the solutions obtained may not be optimum (Floudas & Ciric, 1989).

Colberg and Morari (1990) also used insights from the models of Papoulias and Grossman (1983) to present an NLP model for targeting the minimum area for specified utilities in HENS. The NLP model of Colberg and Morari (1990) is based on the concept that the sphageti design structure is not necessarily required to achieve the minimu area target in HENS. The authors thus presented network structures where criss crossed heat transfer is accommodated to allow for the targeting of the area for streams with unequal heat transfer coefficients. The sequential decomposition into separate targets of utilities, units and area in the models disposes the approach of Colberg and Morari to give non optimal solutions (Shenoy, 1995). Moreover, the main objective of the HENS task should be the TAC, and not the minimum area, this is because the minimum TAC includes the area as well, and it is not always correct that the minimum area network is equivalent to the minimum TAC (Floudas, 1995).

Floudas and Ciric (1989) presented a hyperstructure based MINLP model that can treat the competing tasks in HENS simultaneously. The simultaneous matches-network optimisation approach of Floudas and Ciric represented all the matches and the entire possible alternative HEN configuration in the hyperstructure which is formulated as an MINLP whose objective function seeks to minimise the total annual cost of the HEN. Floudas and Ciric then adopted a decomposition technique of the non convex formulation into a set of convex subproblems to be able to obtain a global optimum solution. In the approach, Floudas and Ciric identified uncertainties associated with the sequential technique of Floudas *et al.* (1986) and similar sequential approaches as follows:

i) Even though there will be an increase in utility cost if heat is allowed to flow across the pinch, the designer needs to be certain whether or not such cross pinch flow results in overall investment savings in the network.

ii) The designer needs to be certain of the actual matching of streams in situations where there are various match combinations that can satisfy the minimum cost network configuration instead of narrowing the matching to only the combination of streams that satisfies the targeting criteria.

iii) The non convexity associated with the NLP model of Floudas *et al*. has the tendency to give several local optima solutions in the network optimisation process.

The hyperstructure of Floudas and Ciric (1989) is meant to search globally for the optimum network to overcome the uncertainties in (ii) and (iii) stated above. The proposed search used the Generalized Benders Decomposition algorithm (Floudas & Ciric, 1989) to decompose the non convex networks into a set of convex subtasks that represent the upper and lower bounds in a hyperstructure. The hyperstructure contains all possible matches and all possible network configurations in a simultaneous match-network optimization as opposed to the superstructure of Floudas *et al*. (1986) that contains only the matches based on the minimum number of matches criterion. The proposed hyperstructure is formulated as a MINLP problem to give a solution network with the objective of producing a global minimum TAC.

Ciric and Floudas (1990) presented the application of the simultaneous match-network optimisation of Ciric and Floudas (1989) to the pseudo-pinch problem (where heat was allowed to flow across the pinch) to address the uncertainty in (i) by reducing the total number of units in HENS. In this approach, the assumption of no heat flow across the pinch was relaxed. The authors adopted the heat recovery approach temperature (HRAT) to calculate the minimum utility levels and to locate the pinch point in the transhipment model of Papoulias and Grossman (1983). The authors thus determined the maximum amount of heat that flows across the pinch in HENS for a particular (HRAT) value and then formulated the HEN problem as the simultaneous-match network of Floudas and Ciric (1989) for the minimisation of TAC.

Ciric and Floudas (1991) treated the HENS task as a single optimisation problem (i.e. without decomposition) and presented an MINLP formulation where all the competing alternatives (operating cost and capital cost) are treated simultaneously. Ciric and Floudas used the hyperstructure of Floudas and Ciric (1989) for the selection of optimal HEN and a modified form of the transhipment model of Papoulias and Grossmann (1983) for the selection of heat loads using continuous variables and selection of stream matches using binary variables. The simultaneous approach of Ciric and Floudas (1991) can be applied as a single network either to the strict pinch formulation of Floudas and Ciric (1989) or the pseudo pinch formulation of Ciric and Floudas (1990).

In the model formulation of Ciric and Floudas (1990) and Ciric and Floudas (1991), the objective functions contain the exchanger areas while the energy balance expressions are contained in the mixers and heat exchangers. These introduced non convexities in both the objective functions and the constraints equations. Floudas (1995) pointed out that as a result of these non convexities, the solutions obtained by Ciric and Floudas are local optima.

Yee and Grossmann (1990) presented a simplified superstructure based MINLP model with isothermal mixing assumptions for the simultaneous optimisation of HENs to be able to do away with non linear mixing equations in the mixers and exchangers in the constraints equations. The isothermal mixing assumption led to a linear set of constraints and a robust MINLP model, though not without its disadvantages that will be mentioned in due course in the detailed discussion of the simplified superstructure (SWS) model of Yee and Grossmann.

An Evolutionary Algorithm (EA) approach has also been used for the simultaneous synthesis of HENs. For example, Lewin (1998) presented a generalised simultaneous method for HENS using a stochastic optimisation based on a Genetic Algorithm (GA), a form of Evolutionary Algorithm (Goldberg, 1989), using NLP. In the model formulation, both the objective function and the constraints are non linear. The author presented a solution based on the observation that an optimal network doest not usually involve many stream splits. The solution of the NLP model was based on a cascaded algorithm involving an upper level non linear optimisation of the stream split flows, and a lower level pseudo-linear optimisation of the heat exchanger duties. The non linearities in both the objective function and the constraints in the EA of Lewin (1998) result in non convex models that may produce sub-optimal solutions (Floudas, 1995).

Krishna and Murty (2007) applied a differential evolution method (DEM), another version of EA, to HENS. The model considered stream splitting but did away with the simplifying assumption of isothermal mixing of the split streams of Yee and Grossmann (1990). Their model can also handle compulsory and forbidden matches in optimization of HENs. The

DEM is suitable for optimisation problems with continuous variables but HENS problems comprise both continuous variables in the form of heat duties and temperatures on one hand and integer variable in terms of process matches or process-utility matches on the other hand. Therefore, Krishna and Murty (2007) had to modify the DEM approach. Price and Storn (1997) observed that the DEM approach is only more likely to find the true optimum than the Genetic Algorithm approach.

The State Space Approach is another technique that has been used for the minimisation of TAC in HENS. Bagajewicz *et al*. (1998) adopted the application of the State Space Approach to HENS and MENS using NLP, the authors demonstrated the flexibility of the approach in HEN and MEN synthesis formulation through the use of various operators. Details of the State Space Approach are contained in Manousiouthakis and Sourlas (1992), Bagajewicz and Manousiouthakis (1992) and Roxenby and Manousiouthakis (1994). Bagajewicz *et al*. (1998) show that the State Space Approach is a special case of either network superstructures or hyperstructures, but the approach can only guarantee local optimality (Azeez *et al*., 2011).

Martin and Manuosiouthakis (2001) synthesised heat and mass exchanger networks using the State Space Approach. The authors employed a variation induced minimisation (VIM) technique to generate an NLP that can recognise the state variables that are zero at optimal solution as a method of reducing the size of the HENS task. The authors developed a hybrid algorithm that consists of branch and bound underestimation with interval analysis to identify the minimum TAC of the HENS. However, the criterion for network optimality only holds under the conditions that the bypass streams and the recycle streams of such HENs vanish at minimum TAC of the networks (Martin & Manuousiouthakis, 2001).

An Infinite-Dimensional State-Space (IDEAS) approach has also been used to minimize heat exchange area requirement with fixed utility in HENs (Martin & Manuosiouthakis, 2003), as well as identification of minimum area target for single component MEN and the synthesis of HEN (Manuousiouthakis & Martin, 2004). The (IDEAS) approach can generate models that are convex, but it has been earlier stated that the minimum area network is not synonymous to the minimum investment cost (Floudas, 1995).

2.4.1 The Use of Superstructures in HEN Design

The pinch approach to HEN design is meant to produce an irreducible structure, however, the network structure can be optimised to remove unwanted features in the network (Smith, 2005). The superstructure approach in HENS is a deliberate attempt to include redundant features in the network, and then subject the network to an optimisation process to pick the optimum design. This has been demonstrated by Floudas *et al*. (1986) where a HEN superstructure that includes a wide range of possible structures was presented, and then subject to optimisation to minimise the cost. Other workers that have presented superstructures for HENS include Yee & Grossmann, 1990 and Isafiade & Fraser, 2008a.

The stagewise superstructure (SWS) of Yee and Grossmann (1990) and the interval based mixed- integer non linear programming superstructure (IBMS) of Isafiade and Fraser (2000a) will be discussed in detail in Sections 2.4.2 and 2.4.3 respectively because the superstructures presented in this thesis namely: the supply based superstructure (SBS), the supply and target based superstructure (S&TBS) and target and supply based superstructure (T&SBS) for the synthesis of heat exchanger networks are similar to SWS and IBMS.

2.4.2 Stagewise Superstructure of Yee and Grossmann (1990)

Yee and Grossmann (1990) presented a simplified stage wise superstructure (SWS) for HENS, the SWS is an extension of the superstructure developed by Grossmann and Sargent (1978) where within each stage, heat exchange between hot streams and cold streams is possible. In the SWS, heat exchange can occur between each hot stream and each cold stream in each of the stages of the superstructure. The SWS is also similar to the spaghetti design concept of Linnhoff and co-workers (Linnhoff *et al*., 1979; Linnhoff & Ahmad, 1990) where division of composite curves was shown in sections, this division was viewed by Yee and Grossmann (1990) as a series of stages.

In the SWS, Yee and Grossmann (1990) fixed the number of stages required to model heat integration at max where represents the number of hot streams and number of cold streams. In the superstructure, all hot process streams start at the first temperature location and end at the last temperature location, the reverse is the case for cold streams. The utilities are placed at the ends of the superstructure. In the superstructure, all streams can participate in every stage. In each stage, each of the streams can split into the number of streams of the opposite kind for the purpose of heat exchange. The split streams are assumed to mix isothermally after leaving the heat exchangers in a stage before moving to the next stage. This procedure is repeated until each of the streams gets to the last stage of the superstructure (if hot) and to the first stage of the superstructure (if cold).

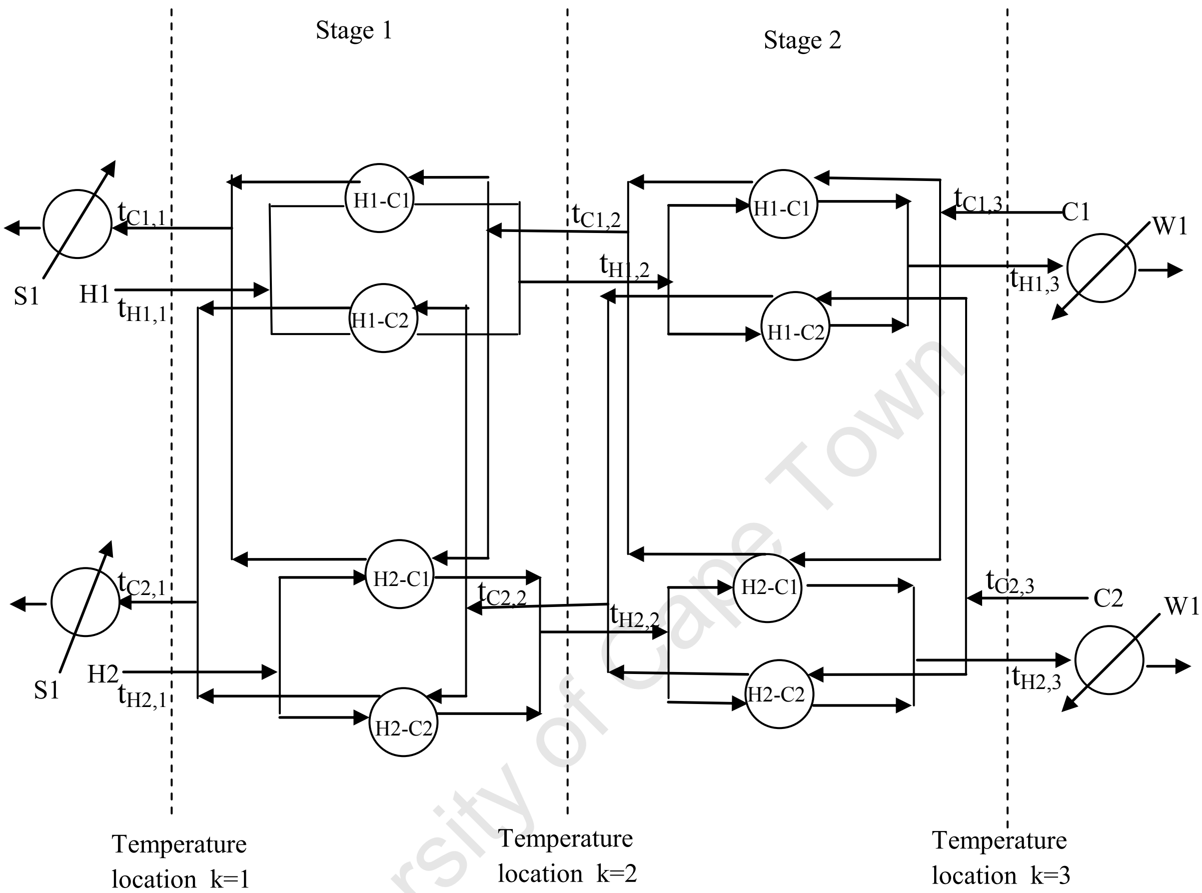


Figure 2.5: The Simplified Stagewise Superstructure of Yee and Grossmann (1990).

Figure 2.5 illustrates the SWS with two hot streams (H1 and H2) and two cold streams (C1 and C2). In the illustrative diagram, all the hot process streams begin at the first temperature location, k = 1 and end at the last temperature location, k = NK+1, where NK is the number of stages. Similarly, all cold streams begin at the last temperature location k = NK+1 and end at the first temperature location k = 1. In SWS, each of the streams can split into a number of streams of opposite kind in each stage for heat exchange. For instance in Figure 2.5, the hot stream 1, H1, has a temperature of $t_{H1,1}$ at temperature location k = 1, which is its supply temperature. In the first stage of the superstructure, H1 can split into two streams to exchange heat with the two available cold streams, C1 and C2 in exchangers and respectively. These split streams are assumed to mix isothermally after leaving these exchangers. The exchanger exit streams thus assume the temperature of the mixer, $t_{H1,2}$ at temperature location k = 2. Stream H1 enters Stage 2 with temperature $t_{H1,2}$ and the same splitting pattern in Stage 1 is repeated in Stage 2. Hot stream 2 goes through the same process of splitting and heat exchange in exchangers and . If H1 and/or H2 does not reach its target temperature at the last stage, a cold utility placed at the end of the superstructure will be used to effect this. Each of the cold streams goes through the same process from the last stage to the first stage, and if any of the cold streams does not reach its target temperature by the end of first stage, a hot utility is used to effect this.

The assumption of the isothermal mixing at the stage junctions by Yee and Grossmann (1990) eliminates the inclusion of non linear energy balances of the mixing junction equations around the exchangers. This results in the reduction of the problem dimensionality, linearity in the set of constraints equations and robustness in the model. The SWS of Yee and Grossmann (1990) also offer the following advantages:

- It is possible to synthesize a minimum cost HEN structure where utilities, units and exchanger area are simultaneously optimized (i.e, as they combine to affect the TAC).
- The calculation of capital costs considered the actual area of the exchangers, this makes it possible to handle problems with different heat transfer coefficients.
- The model can also handle problems with multiple utilities, different cost laws and those with constraints on forbidden/preferred matches (Shenoy, 1995).

The SWS as presented by Yee and Grossmann (1990), however, has the following limitations:

- The isothermal assumption can lead to an overestimation of the area cost for structures with split streams.
- This assumption in some cases can exclude network structures that are only possible without isothermal mixing.
- The SWS does not include structures having split streams going through exchangers in series and stream bypasses.
- An NLP suboptimisation step is often needed to determine the split flow ratio and temperature.
- The SWS is conceptually similar to a spaghetti design. However, the number of stages is typically much smaller than the number of enthalpy intervals in SWS, whereas, the number of stages and enthalpy intervals are necessarily equal in sphagetti designs. Choosing a large number of stages will allow for more combinations of stream matches (Shenoy, 1995).

The last two limitations of SWS highlighted above will be addressed in this thesis by using either the supply temperatures or the combinations of the supply and target temperatures of streams in HENS to define the interval locations of HEN superstructures. This temperature interval approach ensures that splitting and mixing of streams takes place in an interval defined by a temperature value, and it ensures more intervals/stages in the superstructure in resemblance to spaghetti design. The model equations of the SWS of Yee and Grossmann (1990) are presented next.

Overall stream heat balance equations

Overall enthalpy balances for each of the hot streams and each of the cold streams in the superstructure stages are given as stated in Equations 2.14 and 2.15 respectively.

Where and , refer to supply and target temperatures respectively, refers to heat capacity flow rate, and represents the heat exchanged between hot stream and cold stream , the index represents temperature locations at the stage boundaries, while *H* and *C* are the set of hot and cold streams respectively.

Stage heat balance equations

The stage heat balance, which refers to the heat exchanged by hot stream with cold stream in stage were calculated using the Equations 2.16 and 2.17 for hot and cold streams respectively.

and are continuous variables, they represent intermediate stream temperatures of hot stream *i* and cold stream *j* at temperature locations *k*.

Assignment of superstructure inlet temperatures

In the SWS, the supply temperatures of hot streams are assigned to the first temperature location designated as , while the supply temperatures of cold streams are assigned to the last temperature location designated as . These are represented as:

(2.18)

Temperature feasibility along the superstructure

Temperatures of hot and cold streams decrease monotonically from left to right along the superstructure in order for them to reach their target values. This was ensured using the feasibility constraints in Equations 2.20 and 2.21 for hot and cold streams respectively.

Logical Constraints

Logical constraint and binary variables $Z_{i,j,k}$, were used in logical constraint equations to determine the existence or otherwise of match *i,j* in stage *k*. $Z_{i,j,k}$ takes on a value of '1' if match *i,j* exists in stage *k* and a value of '0' if not. The amount of heat that can be exchanged between stream *i* and *j* is restricted to the smaller of the heat duties of the two streams involved in the match using the parameter

Calculation of approach temperature

Calculation of the area requirement of each match requires the determination of the approach temperatures, , along with introduction of binary variables. The binary variables are then used to either activate or deactivate the constraints in Equation 2.23 and 2.24 for approach temperatures:

The binary variables in the above equations ensure that nonnegative driving forces are present for an existing match (Shenoy, 2005). When a match (*i*,*j*) occurs in stage k, the binary variable is equal to one and the constraints is activated for the calculation of the approach temperature. In cases that the match does not occur, the binary variable equals zero and the upper bound in Equations 2.23 and 2.24 renders the equations inactive.

In order to avoid including exchangers of infinite areas, an exchanger minimum approach temperature (EMAT) is included in the model as given in Equation 2.25:

where is a small positive number.

Objective function

The objective function in SWS was defined as the total annual cost of the network, comprising the total annual operating cost and the annualized capital cost of the network. To avoid the singularity when calculating the logarithmic mean temperature difference, LMTD, in case the driving forces are equal, Chen's first approximation (Chen, 1987) is used in the calculation of the LMTD as shown below.

The objective function is given by:

Where HUC and CUC are defined as per unit costs for hot and cold utilities respectively. *AC, AE, CF* are the area cost coefficient, area exponent cost and the fixed charge for an exchanger respectively, and U is the over all heat transfer coefficient.

The errors of the various log-mean approximations (Underwood, 1970, Paterson, 1984, Chen, 1987) over a range of $\Delta T_2/\Delta T_1$ between 1.0 and 10.0 are compared in Figure 2.6. Chen (1987) did not compare the errors that arise from his two approximations, but pointed out that his second approximation was better than that of Paterson over the range of $\Delta T_2/\Delta T_1$ values from 1.5 to 10.0. Paterson (1987) compared Chen's (1987) second approximation with Underwood's (1970) and noted that Chen's second approximation is much more accurate than Underwood's around 10.0 but somewhat less accurate at a ratio of 1.5 (Shenoy and Fraser, 2003). Figure 2.6 shows that Chen's second approximation is a bit worse than Underwood's below a ratio of 5.0 but a bit better from 5.0 upwards. Chen's first approximation is the worst of all at ratios above 2.0 but unfortunately, it was adopted in the

SWS model of Yee and Grossmann (1990) and most of other workers have done the same. This thesis adopts Chen's first approximation as done by Yee and Grossmann (1990) and most of other researchers. This will be done for the purpose of a fair comparison with other results since most workers based their results on it, unlike Chen's second approximation which gives more accurate LMTD.

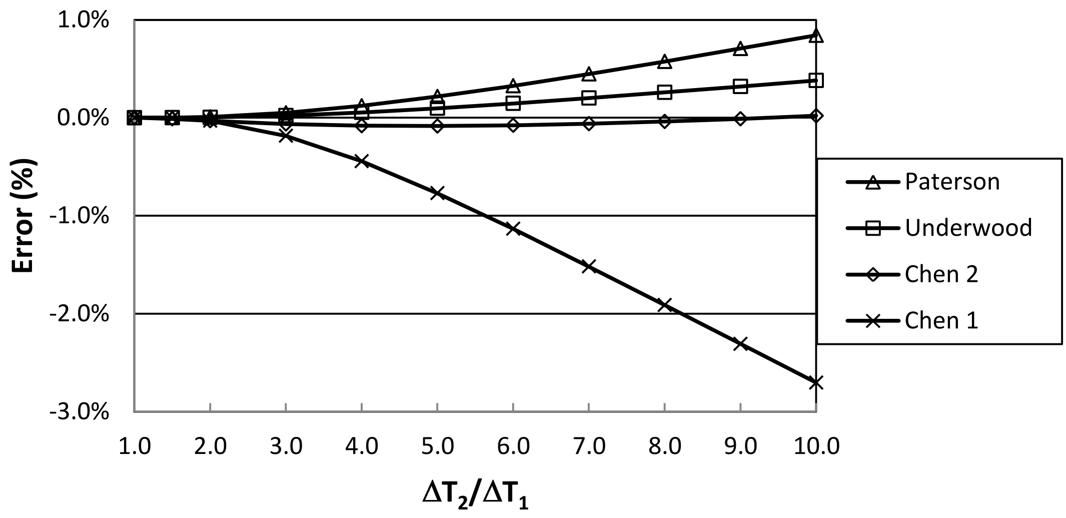


Figure 2.6: Comparison of Log-mean approximation errors

A framework similar to that of SWS of Yee and Grossman (1990) has been used to construct interval based mixed integer non linear programming superstructure (IBMS) for HENS (Isafiade and Fraser, 2008a). The construction of the IBMS and its mathematical model are discussed next.

2.4.3 The Interval Based Based MINLP Superstructure (IBMS) of Isafiade and Fraser (2008)

Isafiade and Fraser (2008a) used a framework similar to the SWS of Yee and Grossman (1990) to optimize the design of heat exchange networks. The authors presented the Interval Based MINLP Superstructure (IBMS) which is constructed using the supply and target temperatures of either the hot or the cold set of streams. If the intervals are defined by hot streams (i.e., a hot stream based superstructure) then the cold streams are assumed to participate (or be made to float) in all the intervals created by the hot streams. The reverse would be the case for a cold stream based superstructure. The exchange of heat between hot streams and cold streams in an interval is, however, subject to thermodynamic feasibility.

An illustration of the hot stream based superstructure of Isafiade and Fraser (2008a) having two hot streams (H1 and H2) and two cold streams (C1 and C2) is shown in Figure 2.7. Note that in the superstructure, the hot utility and the cold utility are treated as process streams (if both these utilities were needed there would need to be two extra streams in the superstructure – this is not shown in Figure 2.7). In Figure 2.7, the supply temperature, of H1 is higher than the supply temperature, of H2. The target temperature, of H1 is also higher than the target temperature, of H2 but lower than the supply temperature of H2. These temperatures were sorted from highest to lowest and used to construct the superstructure with intervals k =1, 2, 3 and 4 in Figure 2.7 where defines k=1, defines k=2, defines k=3 and defines k=4.

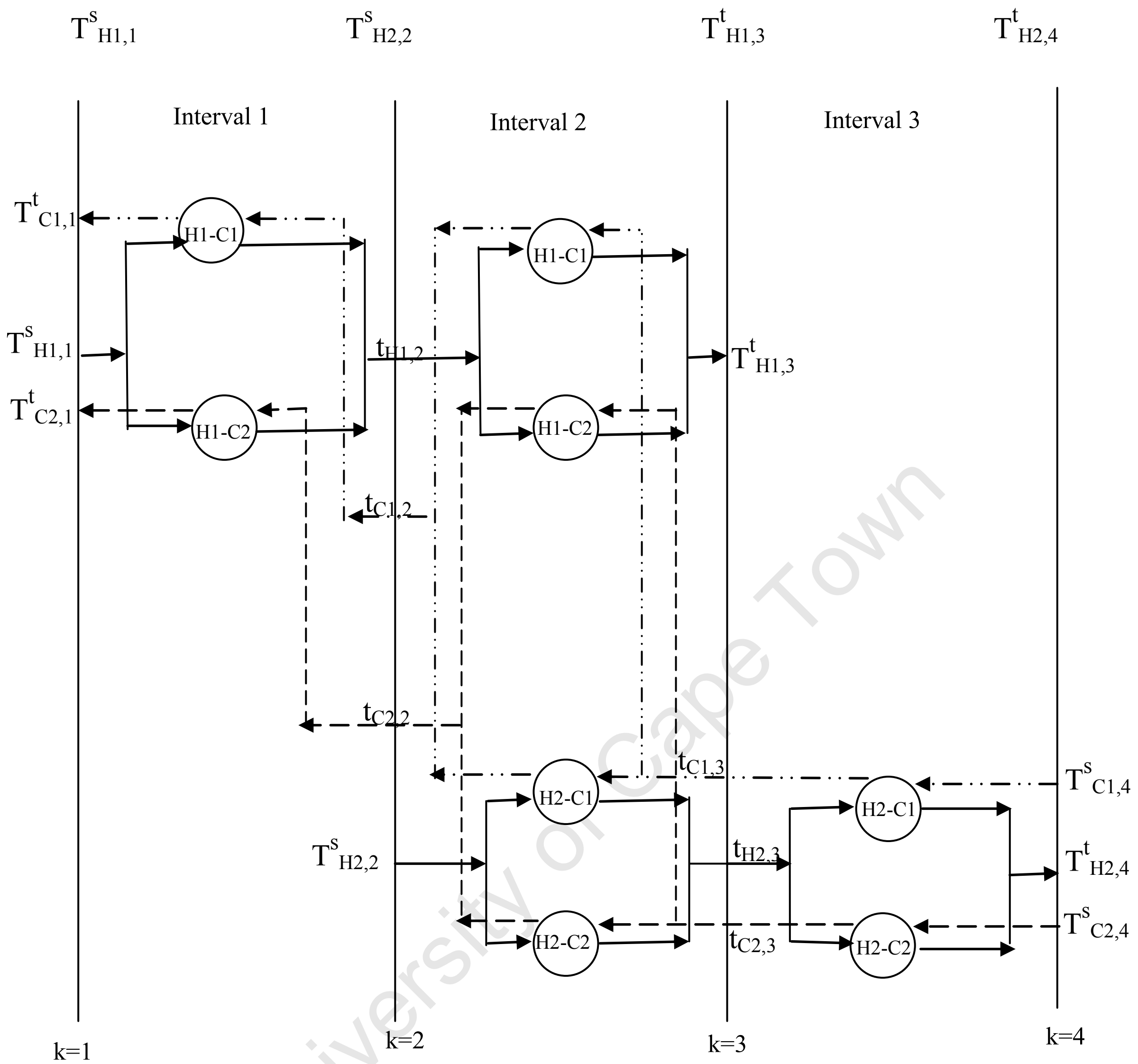


Figure 2.7: A Hot Stream based IBMS superstructure.

In Figure 2.7, the temperature of H1 in temperature location k=1 is its supply temperature value, . Its temperature at any other location in the superstructure is a variable to be optimised, for example, the temperature of H1 at k=2 is . This value is not necessarily equal to the temperature value, , that defines the interval location at this position. The same condition applies to other streams, both hot and cold, in the superstructure. It should, however, be noted that the temperatures of cold streams C1 and C2 do not define any temperature interval location in the superstructure. These cold streams are simply assumed to participate in all intervals where the hot stream(s) is/are present. The reverse would be the case in a cold stream based IBMS, that is, the supply and target temperatures of cold streams will be sorted and used to define the temperature intervals of the superstructure, while the hot streams will be participating (or made to float) in the superstructure to be able to exchange heat with cold streams in intervals where cold stream(s) may be present.

The ability of a hot stream and a cold stream to exchange heat in an interval depends on thermodynamic feasibility. In the IBMS, the equations that involve the calculation of the intermediate temperatures are modelled using existence coefficients conditionals in the form of constraints. Isafiade (2008) observed that defining coefficients in terms of stream existence and using the temperature of the streams to define the temperature locations ensures that split streams are mixed at equal temperatures in the intervals defined using temperatures of streams.

The SWS technique of Yee and Grossman (1990) and the IBMS technique have the isothermal mixing assumption in common. In addition, the IBMS derives its basis from the SWS of Yee and Grossman (1990), which is conceptually similar to a spaghetti design. However, in spahgetti design, the numbers of stages and enthalpy intervals are necessarily equal, but in SWS and the IBMS, the numbers of stages are usually much smaller than the numbers of enthalpy intervals. The SWS technique and the IBMS therefore suffer from the problem that they cannot guarantee a global optimal solution, due to the non-convexity of HENS problems. Moreover, the SWS cannot guarantee minimal consumption of utilities that is obtainable with the composite curves since the number of intervals in the approach is not equal to number of enthalpy intervals (Daichendt and Grossmann, 1994). This study will present superstructures that are capable of generating more intervals for more effective combinations of stream matches to be able to derive more optimal networks by minimising the TAC.

2.5 SYNTHESIS OF HENs INVOLVING MULTIPLE UTILITIES

The pinch balanced composite curve shown in Figure 2.2 is only applicable when one hot utility and one cold utility are being considered. Linnhoff *et al*. (1982) developed the grand composite curve (GCC), which is a plot of interval temperatures (adjusted by −) against the cumulative heat on temperature-enthalpy axes. This GCC is able to present the multiple utilities at different optimum temperature levels in their consumption process. Other workers have presented their studies based on GCC (Jezowski & Friedler, 1992; Sachdeva, 1993; Fraser, 1994). In all the pinch based studies included above for multiple utilities, the utilities were sequentially considered and the TAC was not targeted.

Shenoy *et al*. (1998) also presented a pinch based optimization methodology known as the cheapest utility principle (CUP) for the optimisation of HENs involving multiple utilities. The CUP was based on the concept that the optimal use of utility will be obtained through the increase of the load of the cheapest utility while the load of the expensive utilities is kept constant in the process of increasing the total utility consumption. Shenoy *et al*. kept the temperature driving forces constant at the utility pinches while the minimum approach temperature $\Delta Tmin$ at the process pinch is varied in the utility optimisation process represented on the optimum load distribution (OLD) diagram. The energy-capital trade off was then done using the supertargeting technique to determine the minimum TAC.

The major problem observed with the CUP of Shenoy *et al*. (1998) is that the utility optimisation process was done sequentially, as only one utility (the most expensive) was used to determine the total utility needed for the process before successive replacement of this most expensive utility with cheaper ones. A further problem with this technique is that the energy-capital trade-off was done on the balanced composite curve, which can only give the true TAC if the heat transfer coefficients of all the streams are the same. This is rarely possible because problems involving multiple utilities often have different heat transfer coefficients. Shenoy *et al*. used the uniform Bath area targeting formula presented by Townsend and Linnhoff (1984). Another problem is that the technique of Shenoy *et al*. becomes impracticable when a large number of utilities are involved, because the process of successive replacements of the utilities becomes cumbersome with increasing numbers of utilities. The final optimisation process also involves carrying out the replacement of utilities at various $\Delta Tmin$ which were sequentially chosen. For these reasons, the CUP of Shenoy *et al*. cannot give the global optimum solution for HENS involving multiple utilities.

Jose *et al.* (2010) developed a SWS based MINLP model where exchange of heat between process streams and utilities is possible in each stage of the superstructure as opposed to the SWS of Yee and Grossmann where the utilities are placed at the ends of the superstructure. This is aimed at the determination of the optimal location of hot and cold utilities at any stage of the superstructure through the use of a disjunctive programming formulation. The SWS of Jose *et al.* is similar to that of Yee and Grossmann in many respects, including the isothermal assumption at the stage borders to avoid the nonlinear heat balances. The observation by Jose *et al* that the intermediate location of the utilities along the superstructure can lead to reduction in the TAC of the networks can not always be true because the manner of superstructure partitioning in SWS may not allow the optimum stream matches and combinations as obtained in spaghetti design. Moreover, the objective function of their model is non linear and as such, predisposes the model to be nonconvex. This implies that the solutions obtained from such a model can not be the global optimum.

2.6 MASS EXCHANGE NETWORK SYNTHESIS (MENS)

Mass Exchange Network Synthesis (MENS) was introduced by El-Halwagi and Manousiouthakis, (1989a) as a concept of identification of a cost effective network of mass exchangers that can selectively transfer certain species from a set of rich streams to a set of lean streams or Mass Separating Agents (MSAs). The process of mass exchange can be through absorption, adsorption, leaching, ion exchange, solvent extraction, or stripping, among other unit operation processes. The MEN problem statement can be defined as follows (El-Halwagi, 1997):

> *Given a number of rich streams and a number of MSAs (lean streams), the task is to synthesize a network of mass exchangers that can preferentially transfer certain species from the rich streams to the MSAs in order to achieve a minimum total annual cost network. Given also are the flowrates of each rich stream and their supply and target compositions. In addition, the supply and target compositions for each MSA together with the mass transfer equilibrium relations are also given for each MSA and each species. The flowrate of each MSA is unknown and is to be determined as part of the synthesis task. Also given are the annual operating time, mass exchanger sizing and cost information and the annual cost of capital*

The candidate MSAs can be classified as process and external MSAs. The process MSAs are available virtually free since they exist on site. However, the amount of each process MSA that can be used for mass exchange is bounded by its availability on site. On the other hand, the external MSAs can be purchased from the market and their flowrates are to be determined by economic considerations.

The key questions that the designer needs to answer to be able to design a cost effective network includes the following (El-Halwagi, 1997):

- the mass exchange process/operation to be used (e.g absorption, adsorption, stripping, etc)
- the MSA to be used and its optimal flow rate
- the matching/pairing of the rich streams and the MSAs
- the optimal mass exchanger networking
- the optimal sizing parameters of the mass exchange equipment

El-Halwagi and Manousiouthakis (1989a) answered some of these questions by presenting the mass exchange composite curve for minimum MSA targeting and the minimum number of mass exchanger units targeting. The mass exchange composite curve was achieved by using the concept of corresponding composition scales to establish a one to one correspondence among the composition of streams where mass exchange is thermodynamically possible through the introduction of a minimum composition difference, ε, an analogue of the minimum temperature difference in HENS. This is necessary because the equilibrium relation that governs mass transfer is not as direct as the thermodynamic relation that governs heat transfer in HENS.

2.7 APPLICATION OF PINCH TECHNOLOGY TO MENS

The early stages of the application of pinch technology to MENS dwell on the maximization of the use of process MSAs subject to thermodynamic equilibrium relations before the introduction of external MSA, and thereafter, the network with minimum number of units was synthesised (El-Halwagi & Manousiouthakis, 1989a). Hallale and Fraser (2000a; 2000b) in their quest for capital cost targeting developed the y-y* tool for targeting the mass exchanger area for both stage-wise and continuous contact columns in their applications of pinch technique to MENS in the latter part.

2.7.1 The Use of the Pinch Diagram for Mass Separating Agent Targeting in MENS

The graphical approach termed the 'pinch diagram' was introduced by El-Halwagi and Manousiouthakis, (1989a) to target for the minimum MSA required for a synthesis task. This was accomplished by plotting the composite of all the rich streams on a graph of mass exchange against their compositions. The composite lean stream was obtained by first establishing one to one corresponding scales between each of the lean streams and the rich streams to obtain a global representation of all process MSAs, and then, plot the mass of the pollutants transferable to an MSA against the composition scale of such MSA as shown in Figure 2.8. This was done by introduction of the minimum composition difference, ε, into the equilibrium relation that governs the transfer of mass from a rich stream to a lean stream in MEN as shown in Equation 2.28.

where

is the composition of pollutant in the rich stream

is the composition of pollutant in the lean stream

is the slope of the lean composite stream

is the minimum composition difference between the operating line and equilibrium line in the lean phase of the mass exchanger

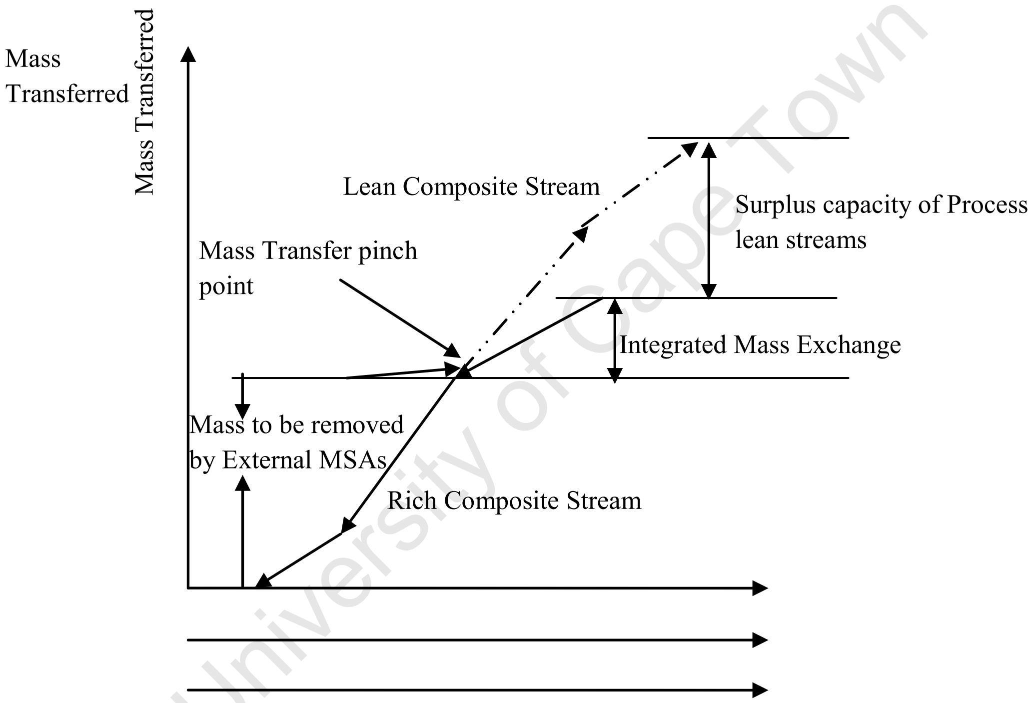


Figure 2.8: The mass transfer pinch diagram (El-Halwagi and Manousiouthakis, 1989a).

El-Halwagi and Manousiouthakis (1989a) termed the point of contact between the rich and the lean composite curves the mass transfer pinch point, and aver that there should be no mass transfer across this pinch point as in HENS. The two composite curves touch at the pinch in Figure 2.8 because ε is built into the lean stream compositions using Equation 2.28, this is unlike the pinch point shown in the heat exchange composite curve in Figure 2.1 for HENs where there is no such contact. This point nevertheless is the bottle neck for mass recovery in the mass transfer in MENs. Similarly to HENs, however, the region of vertical overlap of the rich composite curve over the lean composite depicts the region of maximum process to process mass exchange. The overshoot of the lean composite over the rich indicates the surplus capacity of the process lean streams that can not be used because it can not remove mass from the process rich stream due to thermodynamic infeasibility. El-Halwagi and Manousiouthakis recommend such surplus be removed by reducing the flowrate and/or the outlet composition of some process lean streams. The overshoot of the rich composite streams over the lean indicate the mass to be removed by external MSAs, this is MSA targeting, corresponding to the utility targeting for HENS. MSA targeting can also be achieved by the algebraic approach, the analogue of the problem table algorithm in HENS (El-Halwagi, 1997). The tool is called the composition interval diagram (CID), the use of which also requires the construction of corresponding composition scales for the MSAs. El-Halwagi (1997) called any design that features the minimum cost of MSAs the Minimum Operating Cost (MOC) solution.

2.7.2 Minimum Number of Units Target in MENS

The pinch point in MENS divides the synthesis task into below and above pinch in the MSA targeting process as in HENS utility targeting, and it produces the MOC solution. The minimum number of mass exchangers that can achieve the MOC is obtained from the equation stated below (El-Halwagi & Manousiouthakis, 1989a).

Where N is the number of units and S is the total number of rich and lean streams.

2.7.3 Capital and Total Cost Targets in MENS

El-Halwagi and Manousiouthakis have presented various aspect of MENS , some of which are, MENs involving single component (1990a), multicomponents MENs (1989b), MENs involving regeneration (1990b) and MENs involving non-isothermal operation (1990c), among others. In all of these studies, capital cost targeting was not done, as such, the TAC of the networks of those studies could not be obtained.

The gap of capital cost and total cost targets in MENS was bridged by Hallale and Fraser, (1998; 2000a; 2000b). This was done through the development of a tool known as the *y-y** composite curve shown in Figure 2.9. This tool is a better analogy between the heat exchange composite curve and the mass exchange composite curve. The *y-y** tool can be used to target the minimum number of stages and the minimum packed height for stagewise and packed exchangers respectively in MENS. The AOC and ACC can also be traded off using the minimum composition difference in the rich phase, Δy_{min}. This process is supertargeting for MENS (Hallale & Fraser, 2000b). The use of Δy_{min} to initiate design in MENS gives structures which usually need little or no evolution in order to arrive at an actual TAC that meets the target TAC in design (Hallale & Fraser, 2000a). The design rules are the analogues of those for HENS mentioned earlier.

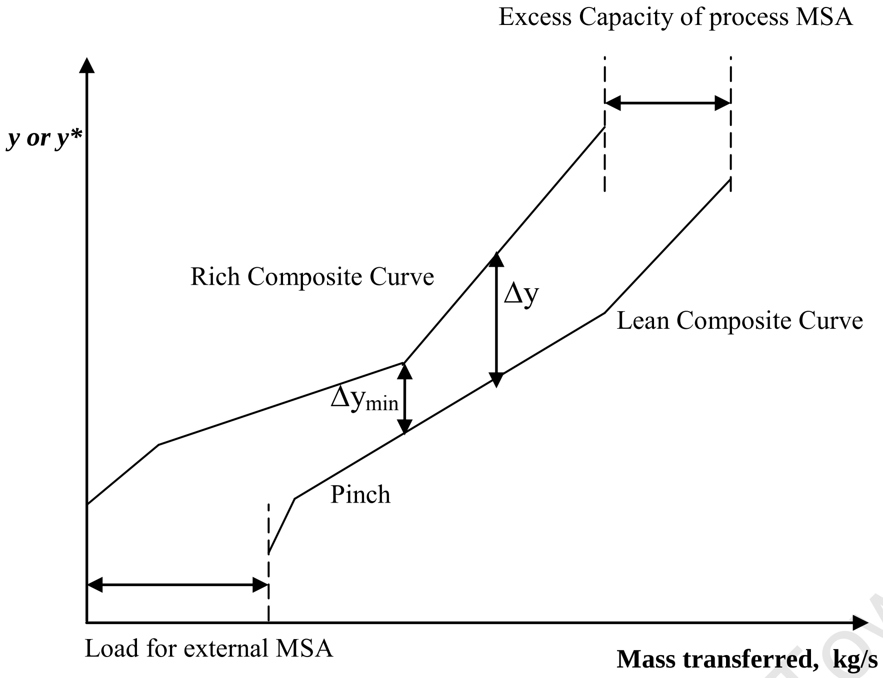


Figure 2.9: Mass transfer Composite Curves (Hallale and Fraser, 2000a).

2.7.4 The *y-y** Composite Curve for Capital Cost Targets in MENS.

Figure 2.9 above is a modification of the MSA targeting method of El-Halwagi and Manousiouthakis, (1989a) shown in Figure 2.8. The graph was obtained by plotting the mass transfer composite curves which shows the MSA composition (y*), in equilibrium with rich stream (y), versus mass exchanged. Note that y* is used in place of the *x* used by El-Halwagi and Manousiouthakis Thus, all MSA compositions are in common terms regardless of how many MSAs are present. Hallale and Fraser (2000a), in Figure 2.9, adopted Δy_{min} as the minimum composition difference between the composite rich and composite lean streams since ε was defined in terms of MSA by El-Halwagi and Manousiouthakis (1989a). This vertical distance, Δy is the driving force for mass transfer. The point of closest approach between the rich and lean composite curves, Δy_{min}, , is called the pinch point, which divides the network into below and above the pinch in Figure 2.9.

The mass transfer composite curve in Figure 2.9 can be used to size mass exchangers, which account for capital costing in MENs. The requirement for sizing continuous contact columns is Δy values (for exchanger height targeting), which is clearly shown in Figure 2.9. For staged columns, the graphical method or the Kremser equation can be used to determine the number of stages using the *y-y** information, as described later. The mass transfer composite curve can is demarcated into compositon intervals and such intervals treated as imaginary mass exchangers as done in HENS for area targeting.

The target for the total number of stages is obtained by adding the contributions from the targeting for below the pinch and above the pinch separately, since it is more correct to target for the region below the pinch and above the pinch separately (Fraser, 1991).

The number of equilibrium stages shown in Equation 2.30 can be targeted using Kremser equation shown in its traditional form in Equations 2.31 and 2.32 or by using the stepping off on the *y-y** using the McCabe Thiele method (Treyball, 1981; Hallale, 1998). Where necessary, the number of real trays can be obtained by dividing the equilibrium number of trays by the column efficiency.

A is called the absorption factor.

In the case of continuous contact columns, Hallale and Fraser (2000a) treated the packed height required for MENS analogously to the pseudo-Bath formula for HENS. The authors based their targeting for minimum height, H_{min}, on the overall mass transfer coefficient in the rich phase as follows:

where

is the lumped overall coefficient for each rich stream,

is the mass load transfer for a rich stream

is the area of cross section of the mass exchanger

It is important to note that Equation 2.33 above is comparable with the Bath formula where the target is premised on vertical heat transfer. Thus, the formula will predict the exact minimum height, provided the values are all the same, and give a good approximation, if the variation in is not much (Hallale and Fraser, 2000a).

Equation 2.33 above can be expressed as follows:

where NTU is the number of transfer units and HTU is the height of a transfer unit, and H_k is the unit height in interval *k*. Equation 2.34 above holds provided, that the composite operating lines and the equilibrium lines are straight lines, and that the network stream flow rates are constant. It is recommended by Hallale and Fraser (2000a) that the equilibrium lines be linearised over the region of interest if they are not straight, and that the flow rates of inert component in the stream be used if the flow rates change appreciably, in conjunction with using mass or mole ratios, instead of mass or male fractions. Equation 2.34 can as well be presented as sum of contributions from each stream as shown in the equation below:

where and are the starting and the ending points of the interval where the rich stream exists. This form of targeting allows the contributions of below and above the pinch, thus, the rich stream contribution in the targeting of H_{min} can be written as

The above equations form the basis for capital cost targeting in pinch based MENS as well as mathematical programming in MENS.

2.7.5 Network Design for MENs

El-Halwagi (1997) affirms the basic rule in pinch methodology that the network design must not transfer mass across the pinch, otherwise, the MOC solution will not be achieved. It is, therefore, necessary that the design be started at the pinch, which is the most constrained region for mass recovery, and then conform to the criteria stated below (the first of which is similar to the stream population rule in HENS) to guarantee MOC solution. The rules for network design as given by El-Halwagi and Manuousiouthakis (1989) are as follows:

1. Stream population rule.

   In the matching of rich streams with lean streams for MOC design above the pinch, the number of rich streams should be less than the number of lean streams and conversely for stream distribution below the pinch. This can be presented as:

   where and are the respective number of rich and lean streams. Equations 2.37 and 2.38 may require stream splitting of the lean stream(s) and of the rich stream(s) respectively in case the inequalities presented above are not met for the available stream data at the pinch.

2. Operating line versus equilibrium line rule

   In order to ensure match feasibility above the pinch, the slope of the operating line should be greater than or equal to the slope of the equilibrium line. This feasibility criterion is expressed as follows:

In order to ensure match feasibility below the pinch, the feasibility criterion that needs to be followed is stated as follows:

—

where and are the flowrates of lean stream and rich stream respectively and is the equilibrium constant in the relation that governs the transfer of mass from rich stream to lean stream .

Note that stream splitting may be required for Equation 2.39 and 2.40 to be feasible.

In the capital cost targeting method of Hallale and Fraser (2000a), some of the analogues of the HEN design rule were used for the MEN design to achieve the capital cost target. However, there are some differences due to the equilibrium relation in MENS. The driving force plots (DFP) for MENS using the *y-y** composite curve plot of Hallale and Fraser (2000a), which allow the designer to distinguish between good matches and bad matches, is one of those rules. Hallale and Fraser also used Remaining Problem Analysis (RPA) for MENS which evaluates the goodness of a match based on the penalty incurred during network synthesis (Linnhoff & Ahmad, 1990).

The problems associated with HENS using the pinch technique were also observed for MENSs using the pinch technique. Hence, mathematical programming methods have been adapted for the synthesis of MENS as will be discussed next.

2.8 MATHEMATICAL PROGRAMMING IN MENS

Similar observations (of sequential and simultaneous) made in pinch based HENS techniques are made for the pinch technology approach for MENS. Mathematical programming approaches have, therefore, been adopted by various researchers to address some MENS based issues such as determination of MOC solution and the location of mass exchange pinch point (El-Halwagi & Manousiouthakis, 1990a), simultaneous screening of MSAs (process and external) (Isafiade & Fraser, 2008b) among others.

The analogy of transhipment model of Papoulias and Grossmann (1983) in HENS has been drawn for MENS in a two stage automatic synthesis of MENs with single component targets (El-Halwagi & Manousiouthakis, 1990a). In the first stage, the MENS problem was formulated as an LP to locate the pinch point and to determine the minimum cost of the MSA. In the second stage, the authors solved an MILP model to determine the minimum number of mass exchange units that satisfied the minimum operating cost of the MSA in the first stage. The synthesis approach and the model formulations are based on the CID and a specified value of minimum composition difference.

El-Halwagi and Manousiouthakis (1990b) presented a two stage mathematical formulation for simultaneous synthesis of mass exchange and regeneration networks. The formulation was based on the same concept of CID and minimum composition difference; these are with the introduction of feasibility criteria for mass exchange below and above the pinch. In the first stage, an MINLP was used to identify the minimum MSA cost for both the primary and the regeneration networks. In the second stage, an MILP was solved to minimise the number of mass exchange units in the networks. The approach of El-Halwagi and Manousiouthakis (1990a; 1990b) recognises the pinch point which divides the network into subnetworks, and each is solved independently, as done in pinch based MENS. Thus, the approach suffers the same limitation as other sequential techniques of inappropriate consideration of utility cost and capital cost, and as such, can not guarantee a global optimum for the MENS task.

Papalexandri *et al*. (1994) presented an MINLP hyperstructure model (analogue of Ciric & Floudas, 1989) where all possible matches between rich and lean streams are feasible for the simultaneous determination of TAC in MENS. The adapted generalized match-network hyperstructure model of Papalexandri *et al.* has features that include the following:

- Each of the participating streams entering the network is split towards a potential mass exchange unit
- The consideration of multiple mass exchange between two streams, hence, the introduction of subnetworks in the hyperstructure where such exchange can take place and the subsequent introduction of binary variables to denote the existence or otherwise of a match between such two streams in the subnetworks. The number of matches between a pair of rich and lean streams is controlled by the number of subnetworks that are specified apriori in the model of Papalexandri *et al.*
- A mixer placed before each mass exchanger for the mixing of split streams from the splitter and bypass streams from other exchangers, these mixed streams serve as the feed for each of the mass exchangers
- A splitter placed after each exchanger to send the exchanger outlet stream to the final mixer and to the other exchangers

- The use of integer variables in the hyperstructure to determine the existence of stream matches or otherwise within a subnetwork as well as the splitting and mixing procedure in the network

One of the problems with the hyperstructure model of Papalexandri *et al*. (1994) is that the partitioning into many subnetworks increases the number of variables and the size of the model, which requires a large computational effort. Additionally, the mass balances for the exchangers are obtained by the multiplications of flow rates and concentrations. More over, the Kremser equation was used for the calculation of the number of stages of the exchangers. These problems results in non linear mixing and splitting equations in the constraints as well as the non linearity in the objective function, rendering the model highly non convex, and hence the model produced sub optimal solutions (Hallale and Fraser, 2000a).

Lee and Park (1996) adopted a two step procedure using process graph theory for MENS to generate two feasible MEN structures (maximal and solution) in the first step. The maximal structure contains all feasible structures in the network contained in the process graph while the solution structure contains the network operating conditions. The solution structure was then formulated as an NLP model in the second step to determine the characteristics of each of the networks generated in the first step. The NLP model is formulated for each of the feasible networks to identify the optimum structure with lowest TAC. Process graph theory has the characteristic that the feasible structures are determined a-priori and it does not utilise binary variables in match selection. The disadvantage, however, is that many programmes have to be generated since each of the feasible solutions has to be modelled using NLP.

Comeaux (2000) presented a reducible superstructure for MENS where the superstructure intervals were defined using the supply and target compositions of the rich streams and the equilibrium equivalent compositions of the lean streams in the rich phase. A stream extension rule was adopted for the lean streams to ensure that each lean stream can match at least once with each rich stream in the superstructure. The superstructure made use of the branch flow rates to determine the existence or otherwise of matches between rich and lean streams. The superstructure was then modelled as a nonlinear programme (NLP) to optimise the TAC of the network. However, the NLP formulation of Comeaux could not guarantee global optimality for MENS (Isafiade and Fraser, 2008b).

The MENS analogue of Yee and Grossmann's SWS (1990) was first presented by Chen and Hung (2005) for waste minimization. Similar to the SWS of Yee and Grossmann (1990), mass exchange is possible between any pair of rich and lean streams in any stage of the superstructure, and the superstructure does not require partitioning into below and above the pinch. The authors chose the number of stages in the superstructure as the maximum of the number of rich or lean streams present in the synthesis task as done by Yee and Grossmann (1990). However, the authors recommended an additional stage to be able to search for optimal networks for MENS. Both the process lean streams and the external lean streams are equally represented in the adapted superstructure. In the 'SWS' of Chen and Hung (2005), the outlets of each exchange unit from a split stream in the same stage are different in their compositions, because isothermal mixing is not assumed, as done by Yee and Grossmann (1990) for HENS. Hence, the inclusion of non linear mass balances of the stream splits and the mixing junction equations around the exchangers increase non linearity in the equations, predisposing the model to produce suboptimal solutions.

Szitkai *et al*. (2006) used the key idea of Yee and Grossmann (1990) together with the pinch technique and the mixed integer non linear programming (MINLP) formulation of Papalexandri *et al.* (1994) to develop a MENS superstructure similar to Yee and Grossmann's HENS model. The MEN superstructure of Szitkai *et al* (2006) maintains most of the characteristics of the SWS superstructure of Yee and Grossmann (1990). The number of stages in the adapted SWS is arbitrarily chosen but Szitkai *et. al.* (2006) recommended a number of stages that is large enough to accommodate the MENS problem.

Emhamed *et al*. (2007) used a hybrid method for the optimisation of mass exchange networks. The main idea of Emhamed *et al.* involves the use of integer cuts and bounds to the lean stream to exclude non optimal solutions. The authors employed the driving force plot (DFP) supertargeting technique of Hallale (1998) to determine the initial flow sheet in the first step, and the flow sheet is then optimized using the MINLP model of Szitkai *et al*. (2006) in the second step. Isafiade and Fraser (2008b) pointed out that the results obtained by Emhamed, *et al*. (2007) are not global optima.

The IBMS of Isafiade and Fraser (2008a) has been adapted for MENS in Isafiade and Fraser (2008b) using a framework similar to that of Szitkai *et al*. (2006). Contrary to the superstructure defining approach of Szitkai *et al*. (2006), the rich based IBMS is defined using the supply and target compositions of the rich streams while the lean based IBMS is defined using the supply and target composition of the lean streams. The process and external lean streams are equally represented in the adapted 'SWS' and the IBMS.

The SWS of Szitkai *et al*. (2006) and the mixed integer IBMS of Isafiade and Fraser (2008b) will again be discussed in detail because the SBS, S&TBS and T&SBS presented for MENS in this thesis were adapted for the synthesis of mass exchanger networks, and are similar to the 'SWS' and IBMS.

2.8.1 The Stagewise Superstructure (SWS) for MENS.

The 'SWS' of Szitkai *et al*. (2006) with two rich streams (R1 and R2) and two lean streams (S1 and S2) in two stages is illustrated in Figure 2.10. The rich and lean stream mole fractions are denoted as y and x respectively. The process lean streams and external lean streams are equally treated in the superstructure. In the superstructure, all rich streams run from the first composition location k = 1 to the last, k = 3, while the lean streams run from the last composition location to the first. In each stage, each of the streams can split into a number of streams to match with the streams of the opposite kinds for mass exchange. The split streams are assumed to mix in an iso- composition manner after leaving the mass exchangers in a stage before moving to the next stage. This procedure is repeated until each of the streams gets to the last stage of the superstructure (if rich) and to the first stage of the superstructure (if lean).

In the Figure 2.10, the composition of R1 at composition location k = 1 is , which is its supply composition. In Stage 1, R1 splits into two, to exchange mass with S1 and S2 in exchangers R1-L1 and R2-L2 respectively as indicated in Figure 2.10. These split streams are assumed to mix iso-compositionally in the mixer after leaving the exchangers. The exit streams of R1 assume the composition of the mixer, , at composition location k = 2, therefore, R1 enters Stage 2 with composition , where it experiences the same splitting pattern as in Stage 1. Similarly, R2 and the two lean streams go through the same mass exchange and splitting process as indicated for R1. Every composition along the superstructure is a variable to be optimised, as such, there is no vertical mass transfer as in the mass exchange composite curve.

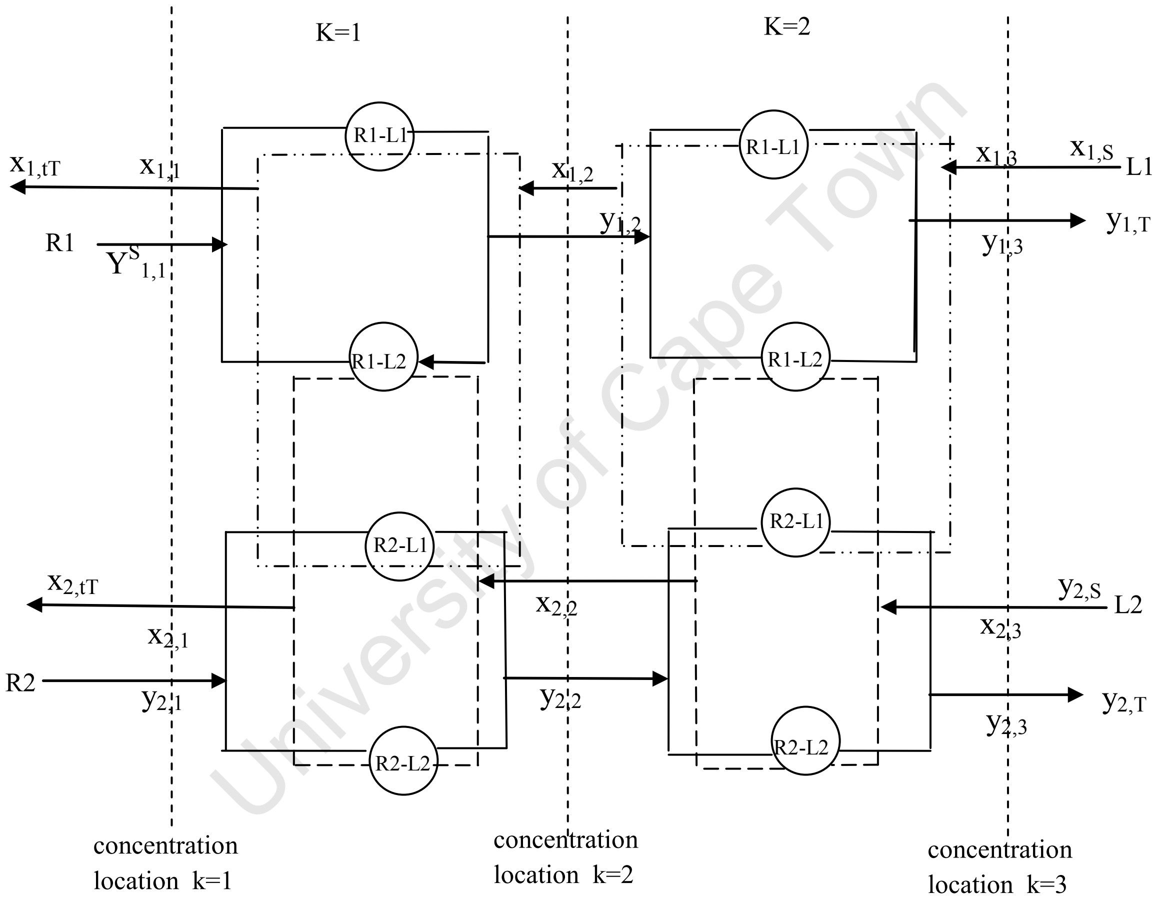


Figure 2.10: The 'SWS' of Szitkai *et al*. (2006)

The assumption of the isocomposition mixing of outlet streams recombining at the stage junctions eliminates the inclusion of non-linear mass balances of the stream splits and the mixing junction equations around the exchangers in MENS 'SWS'. This results in the fairly linear model (FLM) of Szitkai *et al*. (2006). Among the advantages of the 'SWS' of Szitkai *et al*. (2006) is that it is possible to synthesise a minimum cost MEN structure where the MSA cost and the capital cost can be optimised simultaneously. More over, the exclusion of non linear mass balance and mixing equation in the model results in a simplified fairly linear model, since non linearity is only present in the stage mass balance equations and the objective function.

The MENS SWS of Szitkai et al. however, has some limitations similar to the SWS of Yee and Grossmann (1990) which can be stated as follows:

- The isocomposition mixing assumption can lead to an overestimation of the area cost for structures with split streams.
- This assumption can exclude network structures that are only possible without isocomposition mixing.
- The SWS cannot account for cases of split streams going through two or more exchangers in series and those of stream by passes (Floudas, 1995).
- An NLP suboptimisation step will sometimes be needed to determine the split flow ratios and exchanger outlet compositions.
- The number of stages in MENS SWS is typically much smaller to obtain optimum MENs, as observed for the SWS HENS superstructure (Azeez *et al*, 2011).

The last two limitations in the SWS highlighted in the MENS superstructure of Szitkai *et al*. (2006) will be addressed in this thesis by using the supply compositions of streams to define the composition locations of the superstructure. It will also be addressed by using the supply and target compositions of streams to define the composition locations of the superstructure. This approach to defining the superstructure intervals ensures that splitting and mixing of streams takes place in an interval location defined by a composition value. It also guarantees more intervals in the superstructure in resemblance to the spaghetti design. The model equations that describe the superstructure of Szitkai *et al*. (2006) are presented next.

Overall Stream Mass Balance Equations

Overall mass balance equations ensuring that each rich and lean streams reach their target compositions by exchange of mass with opposite kind of stream in the superstructure stages are given below.

Where , , , are the supply composition of rich stream , target composition of rich stream r, the equilibrium supply composition of lean stream in the rich phase and equilibrium target composition of lean stream in the rich phase respectively. G_r, and are the rich and lean stream flow rate respectively, while is the mass exchanged between the rich stream and the lean stream in interval .

Stage Mass Balances

The mass balances for the rich and lean streams in each stage are presented in Equations 2.43 and 2.44 below.

Where and are the composition of rich stream and the equilibrium composition of lean stream, in the rich phase in composition location .

Assignment of Superstructure boundary Compositions

Similar to the approach of Yee and Grossmann (1990), the first composition location, = 1, is assigned the supply composition of rich streams while the last composition location, = NK + 1 is assigned the lean streams supply compositions as shown in the equations below.

Feasibility of Composition in the Superstructure

Constraints are used to ensure monotonic decrease of composition from the first composition location to the last in the superstructure, i.e. a decrease in composition from supply to target and target to supply for each rich and each lean stream respectively.

Logical Constraints

The existence of a match *r,l* in stage *k* is represented using a binary variable, Z_{rlk} in a logical constraint equation. If a match exists, Z_{rlk} takes on a value of '1', otherwise it is '0'. An upper bound, **Ω**, is used to limit the mass which can be exchanged in each match to the smaller of the mass loads of the rich and lean streams participating in each match.

Calculation of Exchanger Driving Forces

The variables and , which are the exchanger rich and lean end composition differences respectively, are used together with the logical constraints Z_{rlk} in the equations to calculate exchanger driving forces. These equations also incorporate a parameter Γ_M which is set as the maximum of '0' and the composition differences between rich stream *r* and lean stream *l* in stage *K* (Shenoy, 1995). This is to avoid numerical errors due to negative approach compositions for matches that do not exist in the optimal network.

The integer infeasible path MINLP (IIP-MINLP) formulation of Sorsak and Kravanja (2002) which enables the solver to search for feasible solution is used by Szitkai *et al*. (2006) as stated in Equation 2.54.

where is the relaxed form of the real variable while are positive and negative tolerances respectively, these tolerances equal to zero eventually.

Logarithmic mean concentration difference

To avoid the problem of singularities associated with mass exchanger sizing, the first approximation of Chen (1987) was used for the calculation of the logarithmic mean composition difference (LMCD) in Szitkai *et al. (*2006) model as follows.

Capital Costs estimation

The exchanger mass-based costing equation of Hallale (1998) in equation 2.56 was adopted for the capital cost estimation for the packed column.

In equation 2.56, is the estimated mass of mass exchanger in kg, is a problem specific term called the lumped mass transfer coefficient and is the amount of substance transferred from the rich stream to the lean stream in an exchanger.

Objective Function

The objective function of Szitkai *et. al*. (2006), which expresses the TAC (which comprises the annual operating costs and the annualised capital costs of the mass exchangers), is as shown below in Equation 2.57 for continuous contact columns.

In equation 2.57, is the per unit cost of the lean stream, *p* is a weighting factor while the two last two terms are the penalty terms derived from Equation 2.54. In the MINLP model presented above, the non linear equations are those that express the lean stream mass balances and the objective function, that is, Equations 2.42, 2.44 and 2.57. The model is, thus, fairly linear inthe case of packed column in MENs. For staged columns where the Kremser equations or its extensions were used, several additional variables and non linear inequality constraints will have to be introduced to the model (Szitkai *et al*., 2006). These additions will surely increase the non linearity in the model and can give non optimal solutions for MENS.

2.8.2 The MENS IBMS.

The HENS IBMS of Isafiade and Fraser (2008a) was adapted for MENS in Isafiade and Fraser (2008b) using a framework similar to that of Szitkai *et al*. (2006). The rich based IBMS is defined using the supply and target compositions of the rich streams while the lean based IBMS is defined using the supply and target compositions of the lean streams. An illustrative diagram of the rich based IBMS for MENS with two rich streams (R1 and R2) and two lean streams (S1 and S2) is shown in Figure 2.11. In MENS IBMS, no distinction is made between the process lean streams and external lean streams. In the illustrative Figure 2.11, the supply composition, , of R1 is higher than the supply composition of, of R2. The target composition, , of R1 is higher than the target composition of R2 but less than the supply composition, of R2. . These compositions sorted from highest to lowest are used to define the composition locations k = 1 to k = 4 in Figure 2.11. In analogy to the HENS IBMS, each of the rich streams runs between the interval boundaries that correspond to its supply and target compositions while the two lean streams participate in all the intervals created by the rich streams in the superstructure.

In Figure 2.11, the composition of R1 in composition location k = 1 is its supply composition, . Its composition at any other location in the superstructure is a variable to be optimized. For example, the composition of R1 at k = 2 is , this value is not necessarily equal to the composition value, , that defines the composition at this location. This situation also applies to other rich and lean streams at composition locations that are not defined by their supply or target values. The compositions of S1 and S2 do not define any composition

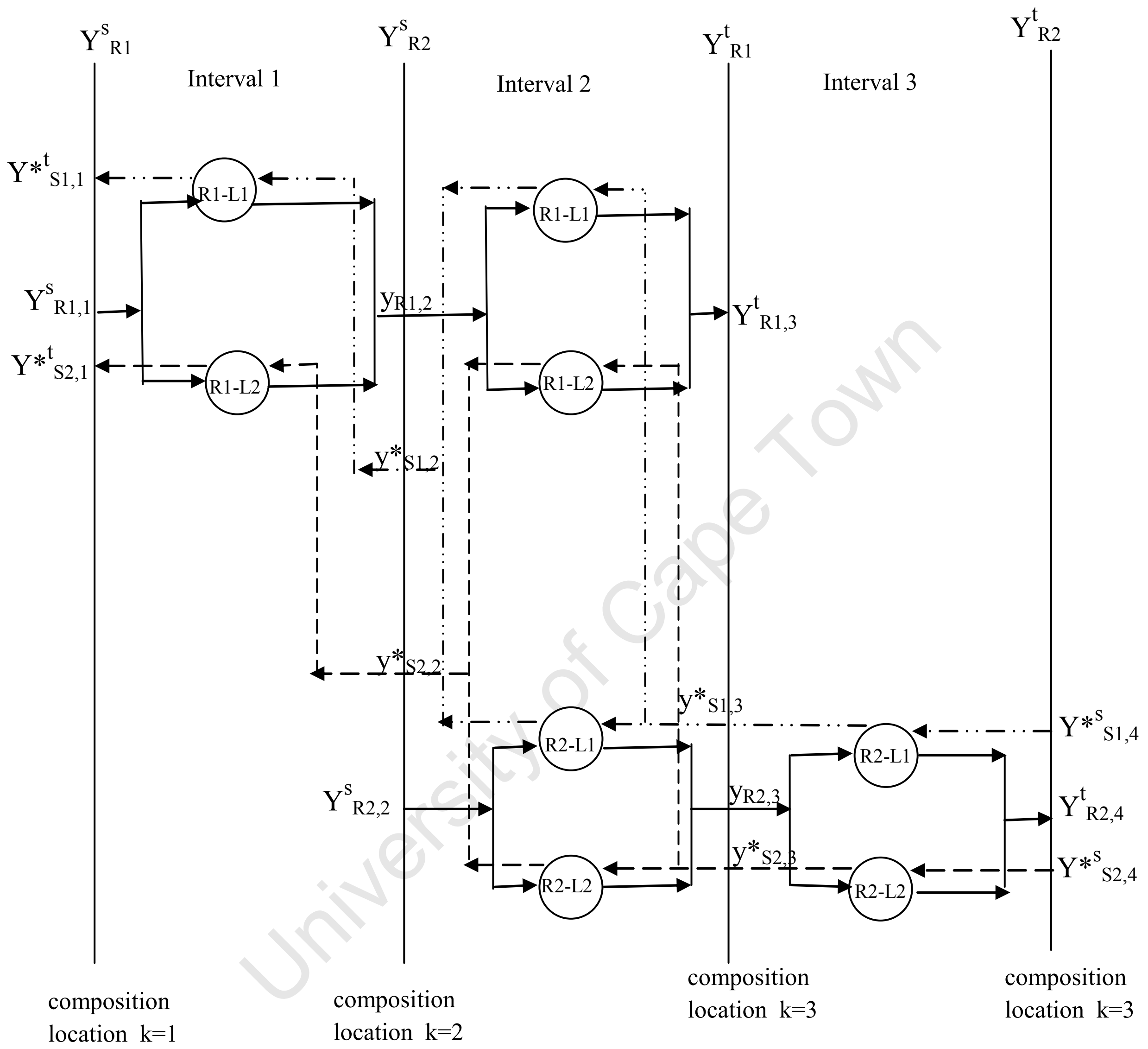


Figure 2.11: A rich stream based interval superstructure.

interval location in the superstructure, they are simply assumed to participate in all intervals where the rich stream(s) is/are present. If the superstructure is lean based, the supply and target compositions of the lean streams would be made to define the superstructure locations while the rich streams would merely participate in all the intervals, the ability to exchange mass between the rich and the lean streams is, however, dependent on thermodynamic feasibility.

2.9 LOGARITHMIC MEAN TEMPERATURE/COMPOSITION DIFFERENCE (LMTD/LMCD)

The basic equation for the logarithmic mean temperature difference has been modified by various researchers (Underwood, 1970, Chen, 1987) in order to handle the numerical difficulty that arises in the calculations of LMTD when equal temperature differences occur at both ends of an exchanger. Such an occurrence leads to an undefined function, i.e zero divided by zero in HENS models. Equal composition differences at both ends of mass exchangers introduce the same difficulty to MENS and the analogue of the LMTD approximations have been adapted for MENS (Shenoy & Fraser, 2003; Fraser & Shenoy, 2004) as shown in Equations 2.58 to 2.63. Shenoy and Fraser (2003) and Fraser and Shenoy (2004) employed the Kremser equation (see Equations 2.31 and 2.32) to derive their approximations for LMCD. The basic expression for the LMCD is presented in Equation 2.58.

The LMCD approximation in the form given by Underwood (1970) is shown in Equation 2.59:

while the approximation expressed in the form presented by Paterson's (1984) is stated in Equation 2.60

In the first approximation proposed by Chen (1987), the LMCD can be stated as given in Equation (2.61)

The LMCD in the second approximation of Chen (1987), which is a modification of the Underwood (1970) approximation, is as follows in the equation below:

Shenoy and Fraser (2003) presented a new formulation of the Kremser equation in order to overcome the problem of singularities that occurs when the Kremser equation is being used for the sizing of mass exchangers in mathematical models for MENS. The formulation of Shenoy and Fraser utilised the logarithmic mean approximation of Underwood (1970) and the second approximation of Chen (1987) to obtain a ratio of two logarithmic mean terms for the sizing of mass exchangers as presented in Equation 2.63.

where (see Figure 2.12)

rich stream concentration difference

lean stream equilibrium concentration difference rich end of the exchanger driving force

lean end of the exchanger driving force, and

(Underwood, 1970) and 0.3275 (Chen, 1987).

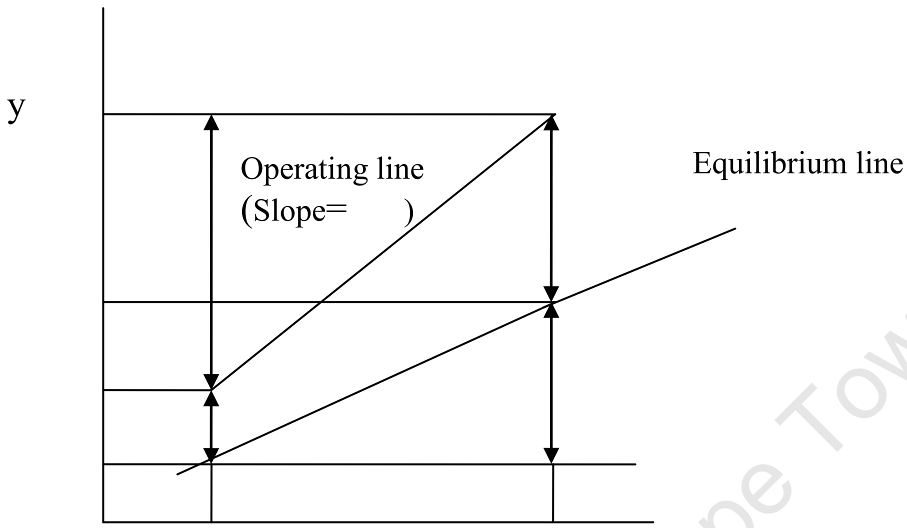


Figure 2.12: y-x plot for counter current mass exchanger (Shenoy and Fraser, 2003)

The formulation of Shenoy and Fraser (2003) in Equation 2.63 was applied to 71 different exchangers in some of the network designs of Hallale (1998) to see the extent of deviations of the approximations in the form presented by different workers as shown in Equations 2.59 to 2.62 from the true logarithmic mean. Shenoy and Fraser observed that the Chen's first approximations deviated most by always giving an overestimation of the number of stages with an average error of 4.67%. Chen's second approximation performed best with an average error of 0.53% followed by Underwood (1970) with error of 0.76% and then Paterson (1984) with error of 1.55%. It is also important to note that the error in using Equation 2.63 for calculating the number of stages is a function of the ratio of the driving forces . For example, at a ratio of 17.89, the Underwood and second Chen approximations produced errors of 0.87% and 0.34% respectively, while, at a ratio of 57.16, the errors are 2.74% and 1.92% respectively (Shenoy and Fraser, 2003).

2.10 CONCLUSION AND THESIS CONTRIBUTION

HENS and MENS have been reviewed in this part of the thesis, beginning with the pinch technique as a sequential synthesis tool. The pinch technique, which is based on vertical heat transfer through the use of the composite curves, is accomplished by a targeting step and a design step. It is shown to have been very well developed for HENS but less so for MENS. The achievements and limitations of the pinch technique for HENS and MENS were highlighted in this chapter.

This review also presented the mathematical programming approaches developed by various researchers for HENS and MENS. The mathematical approaches can be divided into two categories: sequential and simultaneous. Some are automations of pinch techniques and modelled sequentially for HENS and MENS. This sequential mathematical approach though introduced some automation in HENS and MENS but suffered the same limitations as observed for the pinch technique. The other category of mathematical approach is the simultaneous approach where the competing costs in HENS and MENS were optimised in a single step through combining them in the TAC. The simultaneous approaches as presented by various researchers have their shortcomings as presented in the review.

This review observed that for the most part, each of the mathematical programming approaches improves on a previous method. The main issue with the simultaneous mathematical approaches is the issue of non linearity in the model, which renders the search space non convex. As a result, the network costs presented by various researchers are not globally optimal. The issue of non linearity was pronounced in the early simultaneous mathematical approach presented by Ciric and Floudas (1991) for HENS and the analogue of it presented by Papalexandri *et al*. (1994) for MENS.

The review presented the alternative approach of the SWS by Yee and Grossmann (1990) to reduce the prominence of non linearity in the HENS model and the 'SWS' adaptation model by Szitkai *et al*. (2006) for MENS. The non linearity was reduced by assuming isothermal mixing of streams in the stage outlet for HENS and isocomposition mixing in the stage outlet for MENS. This assumption eliminates the mixing junction equations and the non linear heat/mass balances for the stream splits in HENS/MENS. The IBMS of Isafiade and Fraser (2008a) reviewed in this chapter attempted to redefine the SWS of Yee and Grossmann (1990) by using supply and target temperatures/compositions of either the hot/rich streams or the cold/lean streams to partition their superstructure for HENS and MENS instead of using the number of streams as done in the SWS.

The current author believes just as Shenoy (1995) that the conception of SWS was similar to the spaghetti design of the pinch approach. In the SWS, however, the number of stages created by the maximum of the hot or cold streams is not equal to the number of enthalpy intervals on the composite curves. This thesis thus presents new ways of defining superstructures to be able to have more intervals to give opportunities for more match combinations. The superstructures presented in this thesis are the supply based superstructure (SBS) synthesis of heat and mass exchange networks, the supply and target based superstructure (S&TBS) synthesis of heat and mass exchange networks and the target and supply based superstructure (T&SBS) synthesis of heat and mass exchange networks. These superstructures were applied to various HENS and MENS problems as illustrated in Chapters 3, 4 and 5 in this thesis. The current author will demonstrate that the manner of superstructure definition as done by various studies imposes restrictions on the solution space for feasible solutions in HENS and MENS. This leads to none of those techniques consistently generating solutions with the lowest TAC.

CHAPTER 3

SUPPLY BASED SUPERSTRUCTURE, SUPPLY AND TARGET BASED SUPERSTRUCTURE, TARGET AND SUPPLY BASED SUPERSTRUCTURE AND TARGET BASED SUPERSTRUCTURE SYNTHESIS OF HEAT AND MASS EXCHANGE NETWORKS

CHAPTER THREE: SBS, S&TBS, T&SBS AND TBS SYNTHESIS OF HEAT AND MASS EXCHANGE NETWORKS

3.1 I NTRODUCTION

This chapter presents four new ways of defining superstructure partitioning for the synthesis of heat and mass exchange networks. The technique adopted uses insight from pinch technology to generate superstructures for heat and mass exchange network design. The newly developed superstructures are partitioned using temperatures/compositions which are the key parameters for the optimum use of driving forces in exchangers. Temperature/composition locations on the superstructures are defined by either supply values, or target values, or combinations of supply and target values of the process and utility streams in HENS/MENS.

The first superstructure that will be presented is the Supply-Based Superstructure (SBS). The SBS is constructed using the supply temperatures/compositions of all the streams in the HENS/MENS task to define the superstructure interval boundaries. The second superstructure uses the supply temperatures/compositions of the hot/rich streams and the target temperatures/compositions of the cold/lean streams in HENS/MENS to define the superstructure interval boundaries. This superstructure is called the Supply and Target-Based Superstructure (S&TBS). In the third superstructure, the Target and Supply- Based Superstructure (T&SBS), the interval boundaries are defined using the target temperatures/compositions of the hot/rich streams and the supply temperatures/compositions of the cold/lean streams. The fourth superstructure is the Target-Based Superstructure (TBS) whose boundary intervals are defined using the target temperatures/compositions of the hot/rich streams and the cold/lean streams. In all these superstructures, both streams and utilities are treated as process streams. The first three superstructures are modelled as mixed integer non linear programmes (MINLP) with the objective of minimising the TAC in HEN/MEN task in Chapter 4 of this thesis. The fourth superstructure (TBS) can not be used for the synthesis of HENs/MENs because of the problem that will be highlighted in Section 3.2.5.

The intermediate temperature/composition values for the streams in all the superstructures presented are optimisation variables within the intervals created in the superstructures. This indicates that in all these superstructures there is no adherence to vertical heat/mass transfer as obtained on the composite curves. This makes the newly presented HEN superstructures suitable for the optimisation of streams with significantly different heat transfer coefficients. The ability of each process/utility stream to exchange heat/mass within each interval is, however, subject to thermodynamic feasibility.

3.2 MOTIVATION

It appears that the way superstructures are partitioned and the numbers of intervals used in a superstructure partitioning plays a part on the minimum TACs that have been obtained in HENS and MENS by different researchers. There is apparently an inherent limitation of the solution space that is available with each different way of partitioning that is imposed on HENS and MENS. This study will explore if perhaps a different partition technique would produce consistently lower TACs in HENS and MENS.

In all the transshipment based models and other simultaneous synthesis techniques developed for heat and mass exchange networks mentioned earlier in this thesis, none has exploited supply temperatures/compositions of both the hot/rich and the cold/lean streams, or the combinations of supply and target temperatures/compositions of hot/rich streams and cold lean streams to develop superstructures that can simultaneously optimise the TAC (AOC and ACC) in HENS and MENS using MINLP.

This study seeks to investigate the effect of the use of supply temperatures/compositions or combinations of supply and target temperatures/compositions in the definition of superstructure intervals on TACs in HENS and MENS. This is worthwhile since such interval definition approaches would seemingly lead to an increase in the number of intervals created in HENS and MENS when compared with the SWS and its derivatives. This should lead to more combinations of stream matches in the intervals created, and as such would produce networks that bear more resemblance to the spaghetti design network. The conceptual thought of the SBS led to the realisation that one or any of the combinations of the supply and/or target temperatures/compositions of HENs/MENs could conceivably be used to define the boundaries of the intervals in a superstructure for the minimisation of TAC in HENS and MENS. This results in four possible combinations of superstructure partitioning highlighted above.

This first part of this chapter presents the SBS for HENS and its adaptation to MENS, the second part will present the HENS and MENS S&TBS while the HENS and MENS T&SBS will be presented in the third part. The TBS will be presented in the fourth part and the problem associated with its use in HENS/MENS will be highlighted. All the HENS superstructures to be presented are alternatives for the synthesis of heat exchange networks that are similar to both the SWS of Yee and Grossmann (1990), and the IBMS of Isafiade and Fraser (2008a) approaches. The MENS SBS, S&TBS and the T&SBS can also serve as alternatives for the mass exchanger network synthesis as presented in the 'SWS' of Szitkai *et al*.(2006) and the IBMS of Isafiade and Fraser (2008b).

In a similar manner to the SWS and the IBMS, the SBS, the S&TBS and the T&SBS assume isothermal/isocomposition mixing at the junctions defined by the supply temperatures/compositions of streams in order to avoid the mixing junctions equations and the non linear heat/mass balances in the HENS/MENS task. This is to achieve reduction in non linearity and dimensionality problems in HENS and MENS.

3.2.1 Construction of the HENS Supply-Based Superstructure

The HENS SBS involving two hot and two cold streams is illustrated in the grid diagram in Figure 3.1. The supply temperatures of hot and cold streams are sorted and the streams are arranged in descending order from top to bottom, with the hot streams above the cold streams. The supply temperatures of all the hot and cold streams are then used to define the superstructure interval boundaries, with temperature decreasing from left to right. In Figure 3.1, the order of the supply temperatures of the hot and cold sets of streams is as follows: . Each of the hot streams terminates at the last temperature location (k = 4, i.e., the lowest cold stream supply temperature) while each of the cold streams terminates at the first temperature location (k = 1, i.e., the highest hot stream supply temperature).

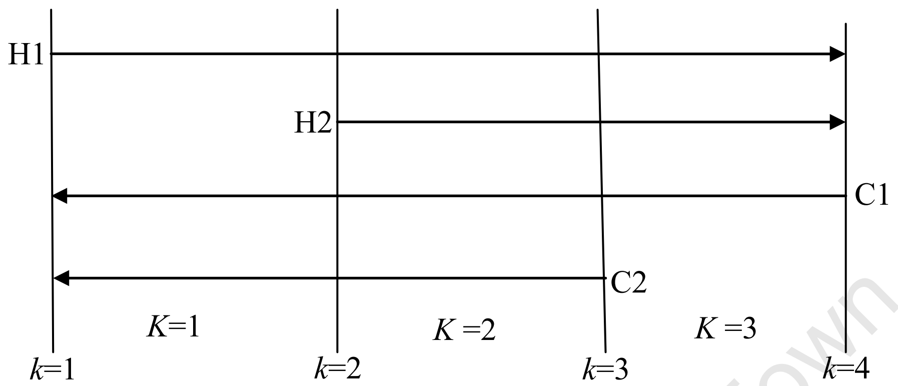


Figure 3.1: Grid diagram of the SBS superstructure for two hot and two cold streams.

In the HEN SBS, each hot stream begins from the interval boundary that corresponds to its supply temperature and extends across all successive intervals to be able to exchange heat with all streams of the opposite kind in these intervals, subject to thermodynamic feasibility. Likewise, each cold stream begins from the interval boundary that corresponds to its supply temperature and extends across all the successive intervals having temperatures greater than its supply value. The utility streams are included with the process streams in the SBS just as in the IBMS.

The participation and possible exchange of heat by streams in each of the SBS intervals in the grid diagram shown in Figure 3.1 is illustrated in Figure 3.2.

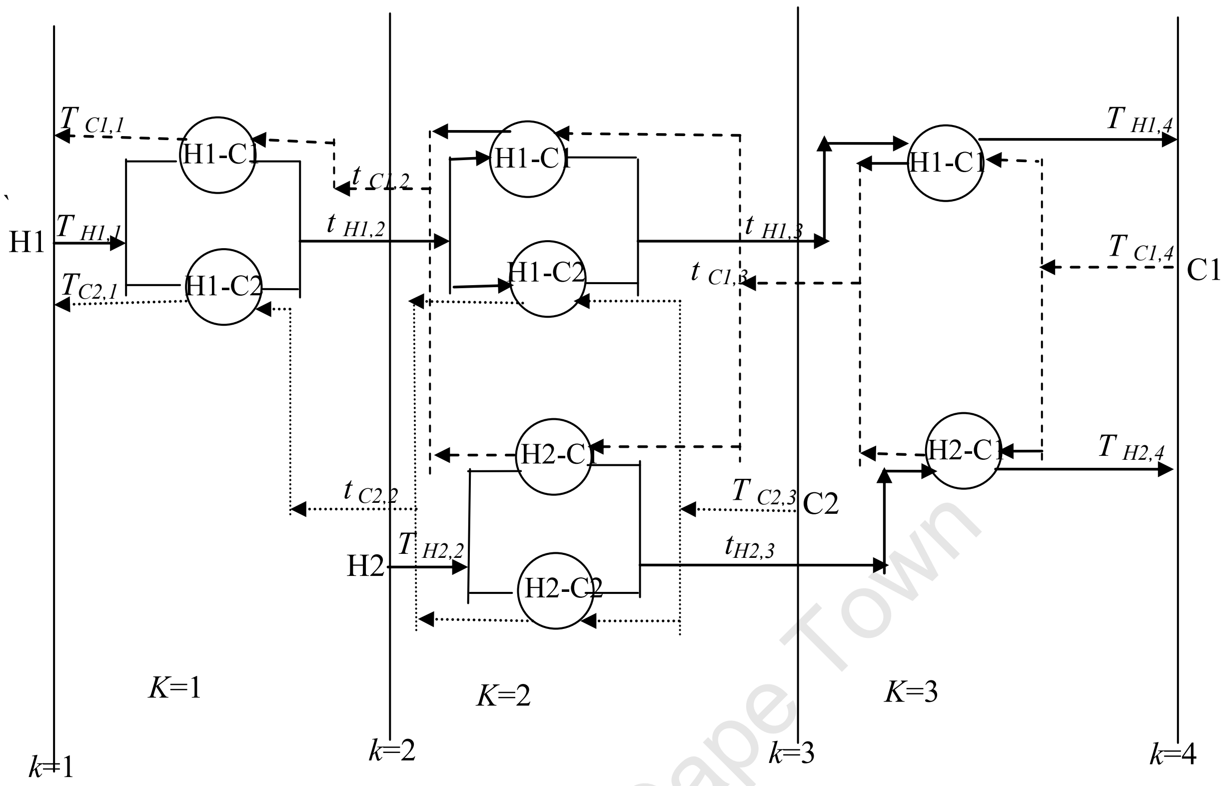


Figure 3.2: SBS for HENS for two hot streams and two cold streams

In Figure 3.2, defines the first temperature interval boundary k = 1, defines k = 2, defines k = 3, and defines the last temperature interval boundary k = 4. If two or more supply temperatures are the same, only one value is used to define the interval boundary for such streams. Circles denote heat exchange between two streams and each pair of circles represents a heat exchanger.

Heat exchange by streams is only possible in intervals where they are present, subject to thermodynamic heat transfer feasibility. In the first Interval (K = 1), Hot Stream 1 splits into two branches to potentially exchange heat with Cold Streams 1 and 2. The same split and heat exchange pattern occurs in the second Interval for Hot Stream 1. Hot Stream 2 can potentially exchange heat with Cold Streams 1 and 2 in the second Interval. In the third Interval, Hot Stream 2 can potentially exchange heat only with Cold Stream 1. It should be observed that in Figure 3.2, the first, second and third intervals can have a maximum of two, four and two exchangers respectively.

The successive temperatures of the hot and cold streams at temperature locations different from those which they define (i.e. intermediate temperatures) are variables to be optimised. This means that the SBS does not adhere strictly to the vertical heat transfer concept of pinch technology. It is also important to mention that the utility flows are treated as process streams with variable flow rates in SBS.

3.2.2. Construction of the MENS Supply-Based Superstructure

The application/adaptation of the SBS to MENS is illustrated in Figure 3.3 where a typical MENS problem with two rich streams (R1 and R2) and two lean streams (S1 and S2) is represented. Figure 3.3 is simply the MENS analogue of Figure 3.2 with the superstructure partitioned using the supply compositions of all the streams in the MEN.

In the MENS SBS illustrated in Figure 3.3, the composition interval boundaries are defined by the supply compositions of all streams arranged in descending order. In the illustration, the supply composition of rich stream R1 is higher than the supply composition of rich stream R2. The supply composition of lean stream S2 is higher than the supply composition of lean stream S1 but lower than the supply compositions of R1 and R2. Every other characteristic of the MEN superstructure in Figure 3.3 is identical to those discussed for Figure 3.2 for HENS, with the appropriate terminology modifications. The process and external lean streams are equally represented for mass exchange in the MEN superstructure. This is different from pinch technology where external lean streams are only placed below the pinch.

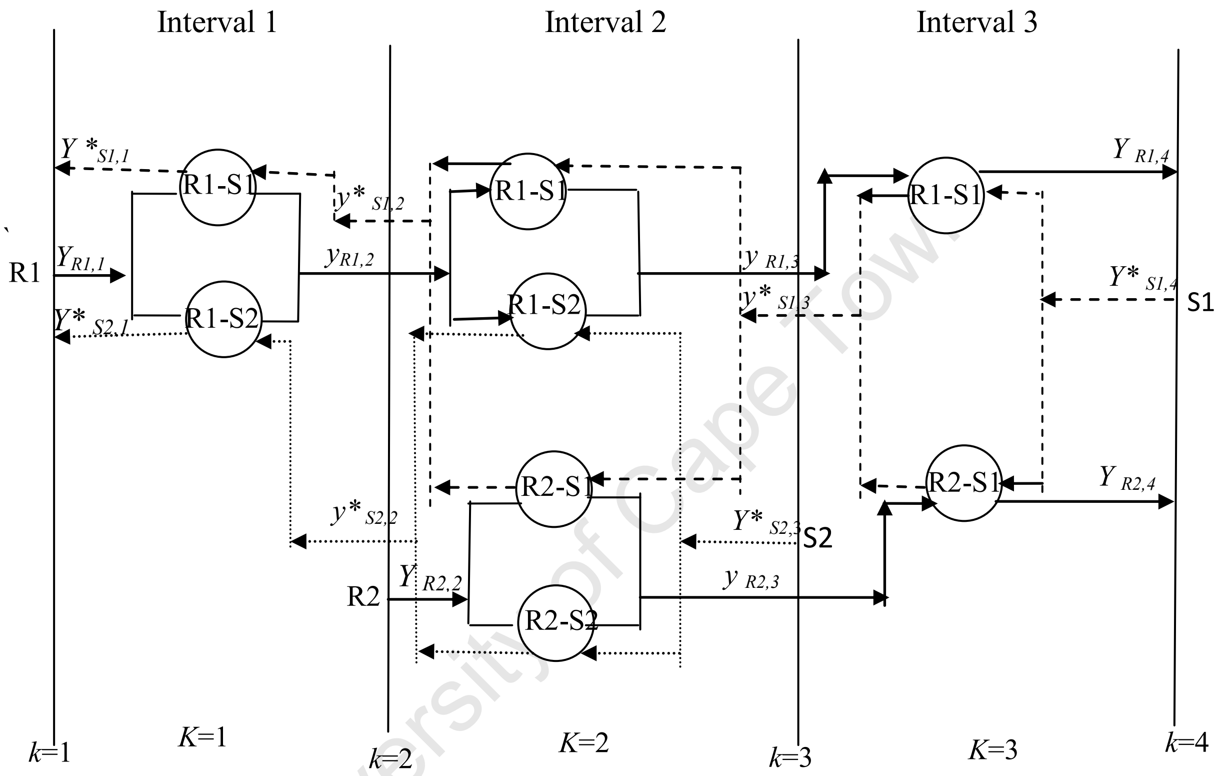


Figure 3.3: SBS for MENS with two rich streams and two lean streams

3.2.2.1 *Mass Exchange and regeneration Networks*

In cases where regenerants have to be used for regeneration of external MSAs, either for economic or environmental reasons, the synthesis of the regeneration network has to be done simultaneously with that of the regular MEN. In such a situation, the regular MEN is regarded as the primary network while the regeneration network is called the secondary network. The interaction of the primary network and the secondary network can be achieved in a number of ways but the method of interaction that will be adopted in this study is through the regenerable MSA. The regeneration process in MEN always leads to an increase in the dimensionality in the networks because the supply and target compositions of the MSA that is to be regenerated are not always given, and are usually determined in the optimization process. The regenerating agent, which is an additional MSA is also present to remove the mass load from the regenerable lean stream(s). This always leads to more difficulties in tackling the mass exchange and regeneration networks, even though the supply and target compositions of the regenerating agents along with the upper limits on its flow rate are always given in the problem. The illustrative Figure 3.4 shown below is the SBS approach to the simultaneous synthesis plus optimisation of mass exchange and regeneration networks.

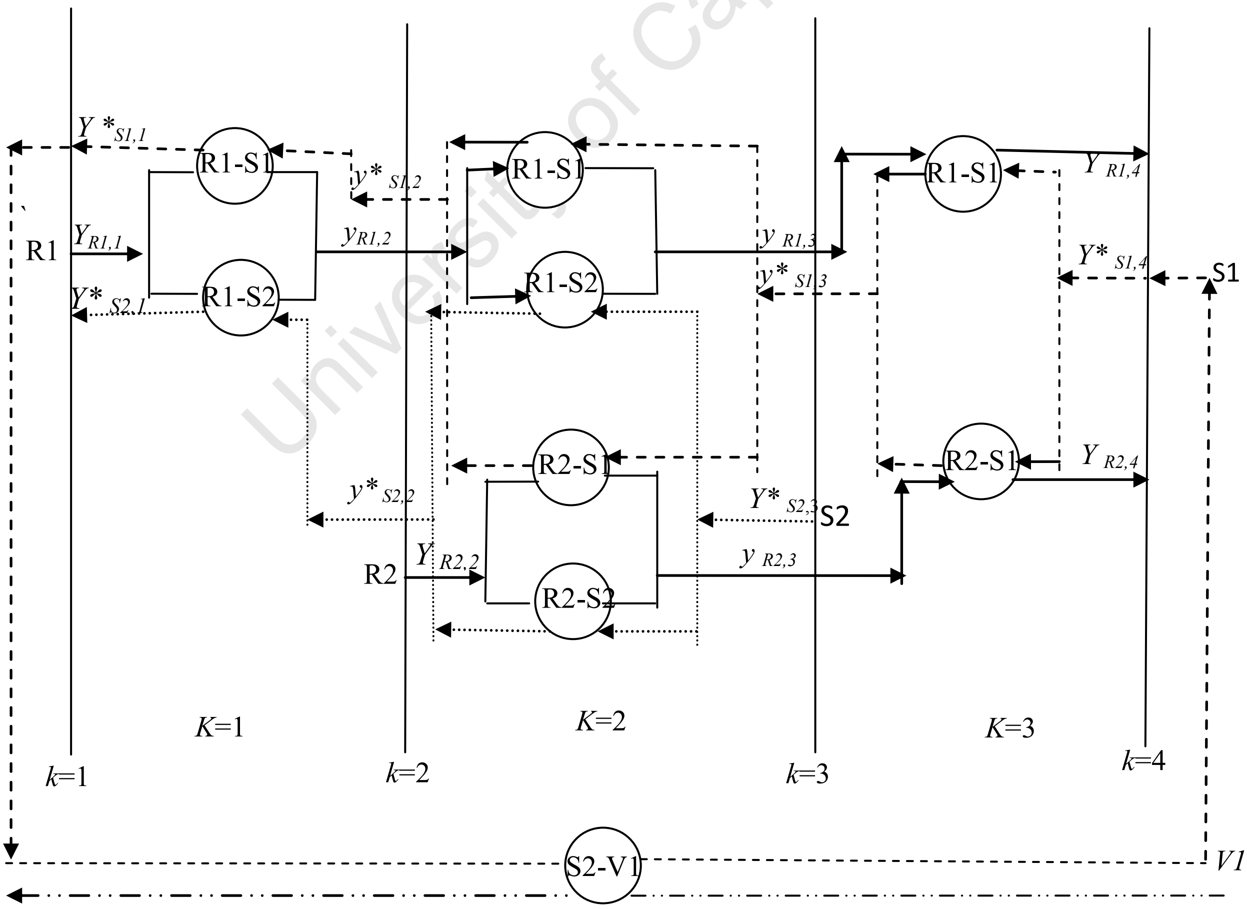


Figure 3.4: SBS for MENS with a regeneration network

3.2.3 Construction of the Supply and Target-Based Superstructure (S&TBS)

In this approach, the supply temperatures of the hot streams and the target temperatures of the cold streams are combined and sorted in descending order, with only one value taken for any values that are repeated. The listing defines the temperature interval boundaries in the HEN superstructure shown in Figure 3.5. In the figure, the supply temperature of Hot Stream 1, is higher than the supply temperature of Hot Stream 2, , while the target temperature of Cold Stream 1, is higher than the target temperature of Cold Stream 2, , and the supply temperature of Hot Stream 2 is higher than the target temperature of Cold Stream 1 (i.e. . Contrary to the SBS, where all the streams in the synthesis task automatically fall within the superstructure, it is necessary in the S&TBS to use the lowest supply temperature of the cold streams (usually the supply temperature of the cold utility) to define the last interval boundary in the superstructure. Thus, temperature boundary k = 5 is the additional interval boundary , and is the supply temperature of the cold stream with the lowest supply temperature . This ensures that all the streams in the synthesis task fall within the superstructure. In the superstructure, each hot stream begins at the interval boundary that corresponds to its supply value and ends at the additional interval boundary, while each cold stream begins at the additional interval boundary and ends at the interval boundary that corresponds to its target value.

The grid diagram in Figure 3.5 represents two hot streams and two cold streams with the hot streams (H1 and H2) situated between the interval boundaries that correspond to their respective supply temperatures (,) and the last (added) interval boundary in the superstructure. Similarly, the cold streams (C1 and C2) are situated between the last (added) interval boundary and the interval boundaries that correspond to their respective target temperatures (,).

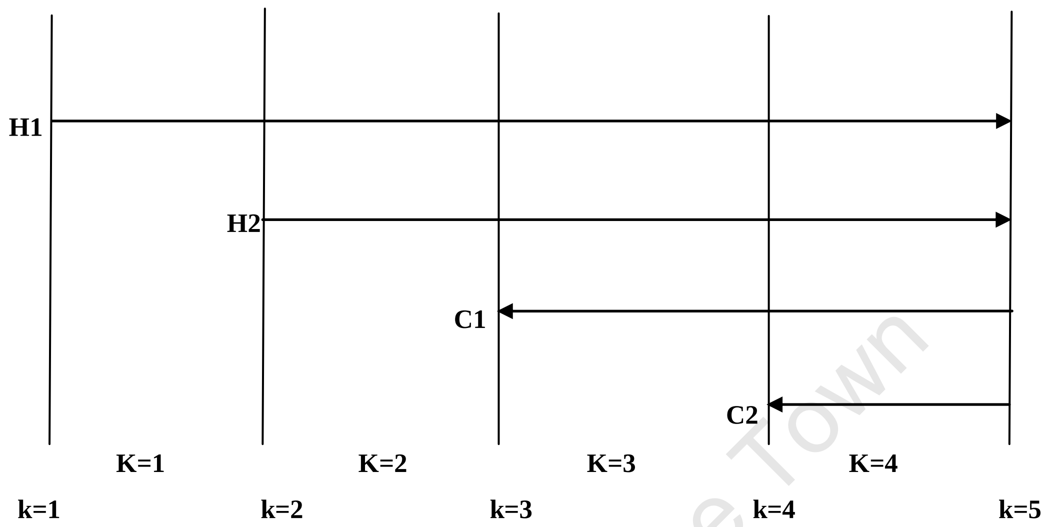


Figure 3.5: Grid diagram of S&TBS for two hot and two cold streams.

The heat exchange between hot streams and cold streams in an interval within the superstructure is subject to the presence of such streams in that interval and to thermodynamic feasibility. An analogous structure to Figure 3.5 represents the MENS superstructure.

Hot Stream 1 can exchange heat in all intervals while Hot Stream 2 can also exchange heat in all intervals except Interval 1 (although in fact neither of them can exchange heat in either Interval 1 or Interval 2 because there are no cold streams in these two intervals). Cold Stream 1 cannot exchange heat in Intervals 1 and 2 while Cold Stream 2 can only exchange heat in the last interval.

3.2.4 Construction of the Target and Supply-Based Superstructure (T&SBS)

In this approach, the target temperatures/compositions of hot/rich streams and the supply temperatures/compositions of cold/lean streams are used to define the interval boundaries of superstructures. Figure 3.6 shows the grid diagram for two hot streams and two cold streams as a typical T&SBS for HENS. In the superstructure, the hot streams (H1, H2) extend between the first (added) temperature interval boundary and the interval boundaries that correspond to their respective target temperatures (and) whereas the cold streams extend between the interval boundaries that correspond to their supply temperatures ( ) and the first (added) interval boundary in the superstructure. The analogue of Figure 3.6 represents the MENS T&SBS counterpart.

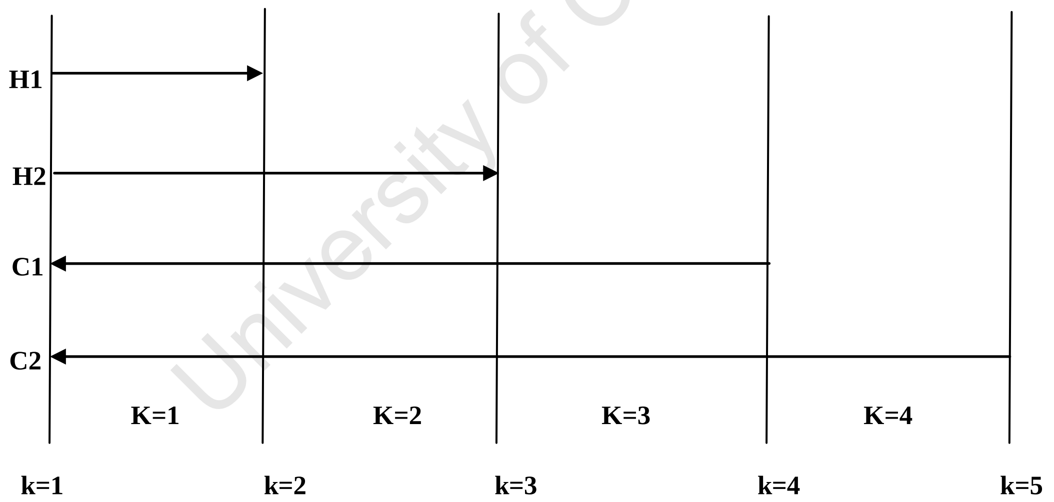


Figure 3.6: Grid diagram of T&SBS for two hot and two cold streams

The combined target temperatures/compositions of hot/rich streams and supply temperatures/compositions of cold/lean streams are sorted in descending order, with only one value used for any that are repeated. The resulting list defines the temperature/composition boundaries in the superstructure shown in Figure 3.6 for a HENS problem. Unlike in the SBS where all the temperatures/compositions of the task fall within the superstructure, there is a need to use the highest supply temperature of the hot stream (usually the supply temperature of the hot utility in HENS) to define the first interval boundary as shown in Figure 3.6 above. This is to ensure that all temperatures/compositions in the synthesis task fall within the superstructure. Thus, the first temperature boundary in this superstructure is where each of the hot streams begins and where each of the cold streams ends.

3.2.5 Target Based Superstructure (TBS)

Efforts have been made by the present author to use the target temperatures/compositions of the hot/cold streams and the target temperatures/compositions of the cold/lean streams to define the interval boundaries of a superstructure for HEN for the minimization of TAC. This section presents the difficulties in the use of such a superstructure.

The use of the target temperatures/compositions of the hot/rich streams and the target temperatures/compositions of the cold/lean streams to partition a HENS superstructure is presented in Figure 3.7 shown below where the attempt appears not to be feasible. This is due to the restriction imposed by the intervals defined by target values of all streams even when two additional interval boundaries are introduced to ensure that all the hot/rich and cold/lean stream conditions in the HEN fall within the superstructure.

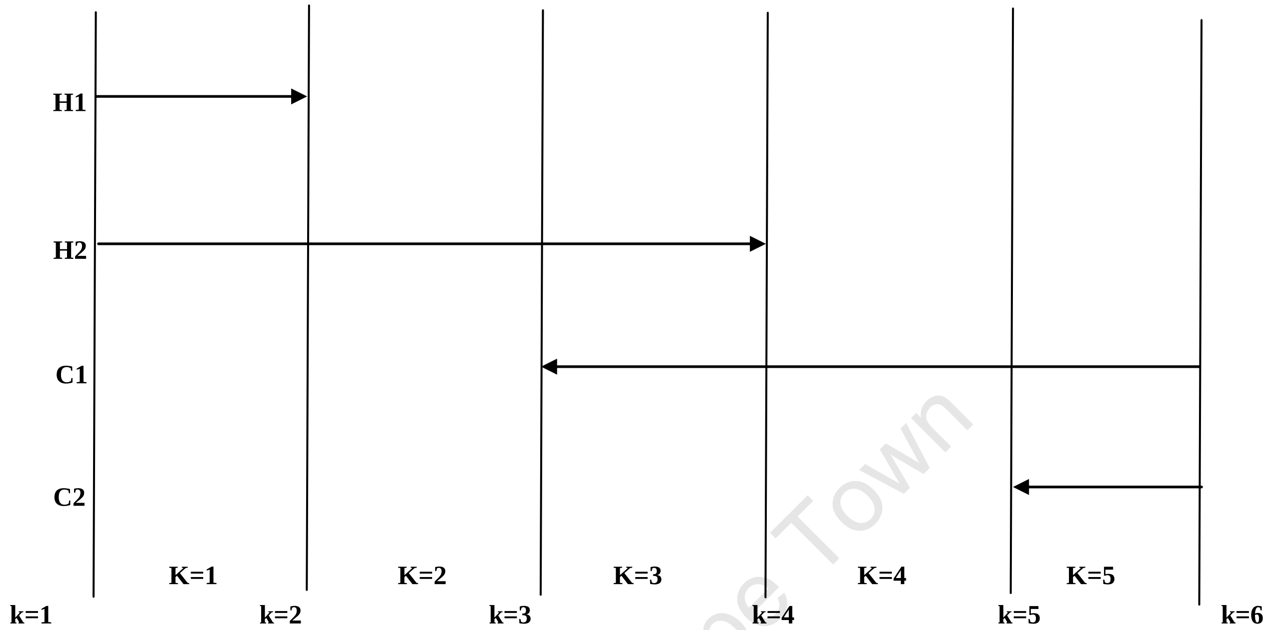


Figure 3.7: Grid diagram of TBS for two hot and two cold streams

The grid diagram in Figure 3.7 shows two hot streams, H1 and H2, and two cold streams, C1 and C2. The hot streams begin at the first (additional) interval created by the supply temperature of the hot stream with the highest supply temperature and end at the interval boundaries that correspond to their target values. The cold streams begin at the last (additional) interval (i.e. the interval boundary created by the supply temperature of the cold stream with the lowest supply temperature) and end at the interval boundaries that correspond to their target values. In the superstructure represented above,

. Thus the hot stream with the highest target temperature (usually the hot utility) is restricted to the first interval, while the cold stream with the highest target temperature (C1) is restricted by temperature interval boundary k = 3. This makes the heat exchange between hot stream H1 (usually hot utility) and the cold streams that do not end in the first interval impossible. The same trend is observed for the cold stream with the lowest target temperature (usually cold utility) which is restricted by the interval boundary that corresponds to its target value, This situation makes it impossible for heat exchange between cold stream C2 (usually cold utility) and all hot streams that do not end in the last interval. The implication of this is that no utility can be used at the extreme ends of a TBS; as it could only possibly work for networks where there are hot and cold streams that can be used to achieve the highest and lowest target temperatures.

This thesis will therefore consider the application of the SBS, S&TBS and T&SBS superstructures to the solutions of HENS and MENS problems. The TBS will not be applied to any HEN/MEN problem; therefore, no results will be presented for this superstructure. The next section will compare all the previous superstructures formulated (the SWS and its MEN analogue, the IBMS) and the SBS, S&TBS and the T&SBS presented in this thesis, as well as Commeaux's superstructure for MENS.

3.3 CHARACTERISTICS OF HEN AND MEN SUPERSTRUCTURES

The characteristics of different HENS and MENS superstructures as presented by various workers and of those of SBS, S&TBS and the T&SBS presented in this thesis are highlighted in Table 3.1 and Table 3.2 respectively as shown below. The TBS is not included because the formulation and the implementation are not feasible as explained above. These characteristics (Tables) show the differences and the similarities that exist between the various superstructures in terms of their formulation and implementation. The major difference in the formulation of the superstructures is the manner of interval definition. This results in different ways in which the boundaries of the various superstructures are fixed. It also informs the intervals where the HEN/MEN streams will be present for heat/mass exchanged in the various superstructures. The MINLP formulation is commonly adopted in the various superstructure modelling.

Table 3.1: Characteristics of the HENS superstructures

SWS of Yee and Grossman (1990)	IBMS of Isafiade and Fraser (2008a)	SBS	S&TBS	T&SBS
Maximum of the number of hot streams or the number of cold stream determines the number of stages (intervals) in the superstructure.	The values of supply and target temperatures of either the hot streams or the cold streams determine the number of intervals in the superstructure (this normally gives more intervals than SWS).	The values of the supply temperatures of both the hot streams and the cold streams determine the number of intervals in the superstructure (this also normally gives more intervals than SWS).	The values of the supply temperatures of hot streams and target temperatures of cold streams determine the number of intervals in the superstructure (this also normally gives more intervals than SWS).	The values of the target temperatures of hot streams and supply temperatures of cold streams determine the number of intervals in the superstructure (this also normally gives more intervals than SWS).
The fixed boundaries are the first and last: the first one being where the hot streams start and the cold streams end, while the last one is the hot stream end and cold streams start.	Interval boundaries are chosen based on the supply and target temperatures of either the hot streams or the cold streams.	Interval boundaries are chosen based on the supply temperatures of the hot streams and the cold streams.	Interval boundaries are chosen based on the supply temperatures of the hot streams and the target temperatures of the cold streams.	Interval boundaries are chosen based on the target temperatures of the hot streams and the supply temperatures of the cold streams.
Heat exchange between each hot stream and each cold stream is possible in all the stages of the superstructure.	Heat exchange by each hot stream is possible only in those intervals created by the supply and target values of that hot stream in a hot-based superstructure; the same goes for each cold stream in a cold-based superstructure (reduced opportunity for thermal exchange within intervals than SWS).	Heat exchange by each hot stream is possible in all intervals except those intervals with higher temperature values than the supply temperature of such stream; thermal exchange by each cold stream is possible in all intervals except intervals with lower temperature values than the supply temperature of such stream (additional opportunity for thermal exchange within intervals	Heat exchange by each hot stream is same as in SBS; exchange of heat by each cold stream is possible in all intervals except those intervals with higher temperature values than the target temperature of that stream.	Heat exchange by each hot stream is possible in all intervals except those intervals with lower temperature values than the target temperature of that stream; exchange of heat by each cold stream is as in SBS.

		than IBMS).		
All streams exist in all the superstructure intervals.	The hot streams exist in all the intervals between their supply and target temperatures in a hot based superstructure, while the cold streams exist in all the intervals. Converse applies in a cold-based superstructure.	The hot streams exist in all intervals defined by temperatures lower than their supply temperatures. The cold streams exist in all intervals defined by temperatures higher than their supply temperature.	Hot streams existence in the intervals are as in SBS. Cold streams exist in all intervals at temperatures lower than their target values.	Hot streams exist across the intervals at temperature higher than the target values. Cold streams existence across intervals as in SBS.
MINLP model formulation but NLP sub optimisation step usually needed.	MINLP model formulation, NLP not required.	Same as IBMS.	Same as IBMS.	Same as IBMS.
Splitting and (isothermal) mixing of stream is possible in every stage of the superstructure.	Splitting and (isothermal) mixing of streams is possible in every interval created in the superstructure.	Same as IBMS.	Same as IBMS.	Same as IBMS.
Utilities are placed at the ends of the superstructure	Utilities are treated as process streams in the superstructure	Same as IBMS	Same as IBMS	Same as IBMS

Table 3.2: Characteristics of MENS superstructures

SWS of Szitkai *et al*. (2006)	NLP of Comeaux (2000)	IBMS of Isafiade and Fraser (2008)	SBS	S&TBS	T&SBS
The sum of the number of rich streams and the number of lean streams determine the number of stages in the superstructure though this can be chosen arbitrarily sometimes.	The values of the supply and target compositions of the rich streams and equilibrium equivalent of the lean streams determine the number of superstructure intervals.	The values of supply and target compositions of either the rich streams or the lean streams determines the number of superstructure intervals (this normally gives more intervals than SWS).	The values of supply compositions of both the rich streams and the lean streams determine the number of superstructure intervals (this also normally gives more intervals than SWS).	The values of supply compositions of the rich streams and the target composition of the lean streams determine the number of superstructure intervals.	The values of the target compositions of rich streams and the supply composition of lean streams determine the number of superstructure intervals.
The fixed boundaries are the first and the last: the first being where the rich streams begin and the lean streams end, while the last is where the rich streams end and the lean streams begin.	Interval boundaries are chosen based on the supply and target compositions though the target is extended for the lean streams.	Interval boundaries are chosen based on the supply and compositions of either the rich streams or the lean streams.	Interval boundaries are chosen based on the supply compositions of the rich streams and the lean streams.	Interval boundaries are chosen based on the supply compositions of the rich streams and the target compositions of the lean streams.	Interval boundaries are chosen based on the target compositions of the rich streams and the supply compositions of the lean streams.
Mass exchange between rich and lean streams is possible in all the superstructure stages.	Extension of lean stream is adopted to ensure a match at least with each rich stream in the superstructure stages.	Mass exchange by a rich stream is possible only between the intervals defined by the supply and target values of such stream in a rich based superstructure. The converse applies for a lean in a lean based superstructure	Mass exchange with a stream is possible in all intervals except those intervals with lower composition values than the supply composition of such stream, (more opportunity for mass exchange within intervals than IBMS).	Exchange of mass by a rich stream is as in SBS but for a lean stream, it is possible in all intervals except those intervals with higher composition values than its target composition value.	Exchange of mass by a stream is possible in all intervals except those intervals with lower composition values than the target composition of such stream. Exchange of mass by a lean stream is as in SBS.

		(reducing opportunity for mass exchange within intervals than SWS)			
Every stream exists across all the intervals.	Every stream exists between the supply and extended target composition values of rich and lean stream respectively in the superstructure	The rich streams exist in the intervals between their supply and target compositions values In a rich-based superstructure, while the lean streams exist across all the intervals. Converse is the case in a lean-based superstructure.	Rich streams existence is across all intervals at compositions lower than their supply composition. Lean streams existence is across all intervals at compositions higher than their supply composition.	Rich streams exist across all intervals as in the SBS. Lean streams exist across all intervals at compositions lower than their target compositions.	Rich streams exist across all intervals at compositions higher than their target composition. Lean streams exist across all intervals as in SBS.
The target compositions of rich streams are fixed at the last interval location while those of lean streams are fixed at the first interval locations in the superstructure.	The target composition of each rich stream is set at the interval defined by its target value while the target of each lean is extended to match at least once with each rich stream.	The supply and target compositions of rich streams are as in SWS in a lean based superstructure and likewise for lean streams in a rich based superstructure.	The target compositions of all the rich and the lean streams are as in SWS.	The target compositions of the rich and the lean streams are as in SWS.	The target compositions of the rich and the lean streams are as in SWS.
The existence or otherwise of matches in the superstructure model are checked using binary variables.	Branch flow rates are used to determine existence of matches rather than binary variables.	Same as SWS.	Same as SWS.	Same as SWS.	Same as SWS.
MINLP model formulation but NLP sub optimisation step usually required	NLP model formulation	MINLP model formulation	Same as IBMS	Same as IBMS	Same as IBMS

Splitting and iso-composition mixing of streams is possible in every stage in the superstructure	Splitting and mixing of a rich stream is possible only between the intervals created by supply and target of such stream. The converse goes for the lean stream.	Splitting and iso-composition mixing of stream is possible in any interval where a stream exists.	Same as IBMS.	Same as IBMS.	Same as IBMS.
Process and External lean streams are equally treated in the superstructure	Same as in SWS	Same as in SWS	Same as in SWS	Same as in SWS	Same as in SWS

3.4 CONCLUSION AND SUMMARY

This chapter presented four superstructures for the synthesis of HENs/MENs. The first presented is the SBS where supply temperatures/compositions are used to define the superstructure intervals. The second and third are the S&TBS and T&SBS where combinations of supply and target temperatures/compositions are used for superstructure interval partitioning. The fourth superstructure uses the target temperatures/compositions to define intervals of TBS superstructures. These techniques are similar to the SWS of Yee and Grossmann (1990), the IBMS of Isafiade and Fraser (2008a; 2008b) and Szitkai *et al*. (2006) differing mainly in how the interval boundaries are defined.

The conception of superstructure definition in this manner i.e. SBS, S&TBS, and T&SBS for the minimization of TAC is being presented for the first time. The superstructures presented have the tendency to produce more intervals as conceived when compared with other superstructures that have been presented earlier. The difficulty encountered in the restrictions of target temperatures/compositions of streams in TBS is also presented in this chapter. The characteristics and the comparison of various HENS and MENS superstructures including the ones presented in this thesis have been highlighted.

CHAPTER 4

MODEL VARIABLES AND EQUATIONS FOR SBS, S&TBS AND T&SBS OF THE SYNTHESIS OF HEAT AND MASS EXCHANGE NETWORKS

CHAPTER FOUR: MODEL VARIABLES AND EQUATIONS FOR SBS, S&TBS AND T&SBS FOR THE SYNTHESIS OF HEAT AND MASS EXCHANGE NETWORKS.

4.1 INTRODUCTION

This chapter presents the model variables and equations for HENS and MENS SBS, S&TBS and T&SBS. The equations for the SBS superstructure for mass exchange networks involving the regeneration of the MSAs are also presented.

4.2 HENS AND MENS SBS, S&TBS AND T&SBS MODEL VARIABLES

The indices, sets, parameters and variables which are used to describe and model the SBS for HENS and MENS are shown next.

Sets

C	cold process and utility streams
H	hot process and utility streams
R	rich process streams
S	lean streams (process and external mass separating agents)
K	temperature/composition intervals in the superstructure

Indices

i	hot process or utility stream
j	cold process or utility stream

k index for temperature/composition boundary (k = 1, ...NOK + 1)

l lean stream (process or external mass separating agent)

r rich process stream

Parameters

AC_l annual cost per unit of lean stream l

ACH_{rl} annual cost per height for continuous contact columns involving rich stream r and lean stream l

ACT_{rl} annual cost per stage for staged columns involving rich stream r and lean stream l

AFC area cost coefficient for heat exchangers

b equilibrium line intercept

is the existence of cold stream in interval K (between temperature interval boundaries and

CB_{ij} fixed charge for heat exchangers

CB_{rl} fixed charge for mass exchanger columns involving rich stream r and lean stream l

cold start in the superstructure.

CU cost per unit of cold utility

D area cost index for heat/mass exchangers is the existence of hot stream in interval K (between temperature interval boundaries and),

hot start in the superstructure.

HU cost per unit of hot utility

K_w lumped mass transfer coefficient

m equilibrium constant for the transfer of component from rich stream *r* to lean stream *l*

NOK number of temperature/composition intervals

existence of rich stream *r* in interval *K (*between composition interval boundary *k* and *k+1)*

rich stream r start at composition interval boundary *k*

existence of lean stream *l* in interval K (between composition interval boundary k and k+1)

lean stream *l* starts at composition interval boundary k

supply temperature of hot stream *i*

target temperature of hot stream *i*

supply temperature of cold stream *j*

target temperature of cold stream *j*

T_k temperature of interval boundary *k* supply composition of lean stream l

target composition of lean stream l

supply composition of rich stream r

target composition of rich stream r

equilibrium supply composition of lean stream l

equilibrium target composition of lean stream l

composition of interval boundary k

Γ_H upper bound for driving force in match i, j

upper bound for driving force in match r, l

ε_{min} minimum composition difference in the lean phase

Ω_H upper bound for heat exchanged in match i, j

Ω_Z upper bound for mass exchanged in match r, l

conditional operator

Binary variables

variable showing the existence of match ij in interval K in the network

variable showing the existence of match rl in interval K in the network

Positive variables

heat exchanger driving force for match ij in temperature interval K

mass exchanger driving force for match *rl* in composition interval *K*

F_i flow rate of hot stream *i*

F_j flow rate of cold stream *j*

G_r flow rate of rich stream *r*

L_l flow rate of lean stream *l*

mass exchanged between stream *r* and stream *l* in composition interval *K*

number of stages in staged column *rlk*

heat exchanged between stream *i* and stream *j* in temperature interval *K*

temperature of hot stream *i* at temperature boundary *k*

temperature of cold stream *j* at temperature boundary *k*

composition of rich stream *r* at composition boundary *k*

equilibrium composition of lean stream at composition boundary *k*

4.3 SBS MODEL EQUATIONS FOR HENS

The SBS model consists of the temperature values used to define the interval boundaries, stream existence conditionals, the constraints equations/inequalities and the objective function as are stated below with their functions in the model.

Assignment of Superstructure Interval Boundary Temperatures

With reference to Figure 3.2, the temperature interval boundaries are specified as follows (note that lower case symbols represent variables to be optimized):

In the illustrative diagram, $T_{C1,1}$ and $T_{C2,2}$ are the target temperatures of the two cold streams, while $T_{H1,4}$ and $T_{H2,4}$ are the target temperatures of the two hot streams

First Set of Stream Existence Conditionals

Since in HEN SBS, a hot stream cannot exchange heat in any interval whose temperature is higher than or equal to its supply value and a cold stream cannot exchange heat in any interval where the temperature is lower than or equal to its supply value, two stream existence conditionals are employed in the superstructure to ensure the aforementioned, one for the hot streams and one for the cold streams. The mathematical representations for these conditionals are as follows:

Second Set of Stream Existence Conditionals

The second set of stream existence conditionals is the stream supply temperature recognition conditionals which recognise the supply temperatures of the set of streams which define the SBS interval boundaries. These are stated in Equations 4.7 and 4.8:

Overall Stream Heat Balance Equations

The total heat exchanged by each stream over all intervals equals the total enthalpy change of that stream. These are shown in Equations 4.9 and 4.10 for hot stream i and cold stream j respectively.

The stream heat capacity flowrate, F, is modelled as a parameter for the process streams and as a variable for the utility streams in Equations 4.9 and 4.10.

Interval Heat Balance Equations

The heat exchanged by each stream in each interval defines the temperature of that stream for the next interval. The heat exchanged between hot stream and cold stream in interval is calculated using the interval heat balance equations for hot and cold streams respectively:

Temperature Feasibility along the Superstructure

Temperatures of hot and cold streams need to decrease monotonically from left to right along the superstructure in order for them to get to their target values. This is ensured by the feasibility constraints shown in Equations 4.13 for hot streams and 4.14 for cold streams:

Logical Constraints

Binary variables $Z_{i,j,k}$, are used in logical constraint equations to model the existence or otherwise of match *i,j* in interval *K*. $Z_{i,j,k}$ takes on a value of '1' if match *i,j* exists in interval *k* and a value of '0' if not. The amount of heat that can be exchanged between streams *i* and *j* is restricted to the smaller of the heat duties of the two streams involved in the match using the parameter

Heat Exchanger Driving Force Calculation

Approach temperatures are used together with the binary variable and the parameter in logical constraint equations in order to calculate heat exchanger driving forces which are further used to calculate heat exchanger areas as done by Yee and

Grossmann, (1990). This is to avoid the inclusion of negative approach temperature for any match. These are described by Equations 4.16 and 4.17.

The value can be the maximum of zero and the temperature differences between the hot and cold streams participating in the match concerned (Shenoy, 1995). This helps to avoid numerical errors due to negative temperature differences for matches which do not exist.

In order to avoid including exchangers of infinite areas in the calculations, an exchanger minimum approach temperature (EMAT) is included in the model. This is represented as:

where is a small positive number.

Objective Function

The objective function that is minimized for HENs is the TAC of the network as done by Yee and Grossmann (1990); this is to enable comparison of results with other simultaneous approaches. The TAC expression is given in Equation 4.19 below where the capital cost of each exchanger is given as the sum of a fixed cost and an area cost.

Chen's first approximation (Chen, 1987) as given in Equation 4.20 is used when calculating the logarithmic mean temperature difference (LMTD). This is to avoid the singularity problem if the driving forces are equal. This was done for comparison with other results since most workers based their results on it, instead of using Chen's second approximation which gives more accurate LMTD. The detail of this has been discussed in the last part of section 2.4.2 in Chapter 2 where the log-mean approximations as presented by various researchers were compared.

Application

Equation 4.19 (the objective function) is minimised in the SBS subject to the feasible space defined by Equations 4.7 to 4.18. This feasible space is due to the fact that Equations 4.7 to 4.18 are all linear except for Equations 4.11 and 4.12. The non linearity in Equations 4.11 and 4.12 is due to the utility stream flows which are some of the optimisation variables. The SBS produce good solutions despite treating the utility flow rates as optimisation variable. In the SBS, matches can easily be preferred or forbidden in the network. This can be achieved by fixing the binary variables concerned in the match.

4.4 SBS MODEL EQUATIONS FOR MENS

The Equations which are used to model the MENS SBS are mostly the analogue of those of the HENS SBS.

Assignment of Superstructure Interval Boundary Compositions

The four interval boundaries are assigned composition as shown below:

First Set of Stream Existence Conditionals for MENS

Similar to HENS SBS, stream existence conditionals are employed to ensure that a rich stream cannot exchange mass in those intervals where compositions are higher than or equal to its supply value while a lean stream cannot exchange mass in those intervals where the compositions are lower than or equal to its supply value:

Second Set of Stream Existence Conditionals

The second set of stream existence conditionals is the stream supply composition recognition conditionals that enable the model to recognise the stream whose supply composition define the composition interval boundary:

Overall Stream Mass Balance Equations

The total mass exchanged by each stream over all intervals must equal the total component mass change of such stream as shown in Equations 4.28 and 4.29 for rich stream *i* and lean stream *j* respectively.

The rich stream flowrate G_r is modeled as a parameter in Equation 4.29, whereas the lean stream flowrate L_l in Equation 4.30 is modelled as a variable in SBS. Note that the stream flowrates are assumed to be constant throughout the network, which is true if mass ratios are used (provided there is minimal evaporation, if a liquid stream is involved), and a good assumption for low concentrations when mass fractions are used.

Interval Mass Balances

The mass exchanged by each stream in each interval defines the composition of that stream for the next interval. The interval mass balance equations for rich and lean streams which are presented in equations 4.31 and 4.21 are used to calculate those interval boundary compositions.

Composition Feasibility along the Superstructure.

Monotonic reductions of composition from the first composition boundary to the last composition boundary in the superstructure are ensured using constraints in Equations 4.33

and 4.34. This translates to a decrease in composition from supply to target and target to supply for rich and lean streams respectively.

Logical Constraints

Similar to HEN SBS, a binary variable Z_{rlk} is used to model the existence of a match *r,l* in interval *K*, if a match exists, Z_{rlk} takes on a value of '1' and '0' if otherwise. An upper bound, Ω, is included to restrict the quantity of mass which can be exchanged in each match to the smaller of the mass loads of the rich and lean streams involved in the match as described in Equation 4.35.

Calculation of Exchanger Driving Forces

The exchanger rich and lean end composition differences which are continuous variable denoted as and , respectively, are used together with the logical constraint Z_{rlk} in the equations to calculate exchanger driving forces Equations (Equations 4.36 to 4.39). These equations also include the parameter Γ_M which is set as the maximum of '0' and the composition differences between rich stream *r* and lean stream *l* in interval *K* (Shenoy, 1995), to ensure that no negative approach compositions are included for any match.

Similar to HENS SBS, an exchanger minimum approach composition (EMAC) is incorporated in the model to avoid exchangers of infinite sizes in the optimal network:

where is a small positive value.

The integer infeasible path MINLP (IIP-MINLP) formulation by Sorsak and Kravanja (2002) as used by Szitkai *et al*. (2006) is also used in SBS model. This is to enable the solver to search for feasible solution through infeasible solutions (Szitkai *et al*., 2006). The equation is shown in Equation 4.40:

where is the relaxed versiuon of the real variable while are positive and negative tolerances respectively, these tolerances equal zero eventually.

<u>*Objective Function*</u>

The objective function of the MEN SBS is the minimization of network TAC, as shown in Equations 4.41 and 4.43 below. The exchanger mass -based capital cost calculation method of Hallale (1998) is used in this study for continuous contact columns, while the per stage costing method of Papalexandri *et al*. (1994) is adopted for costing stage-wise columns.

The expression for the continuous contact columns based objective function is as follows:

where

while for stage-wise columns, the expression is:

where N_{rlk} is the number of stages for match i,j in interval k.

Chen's first approximation (1987) is used for the calculations of LMCD in MENS SBS, as was done for LMTD in HENS. A detailed comparison of the various log-mean approximations and the errors associated with them is given in section 2.4.3 in Chapter 2.

4.4.1 SBS Model Equations for Simultaneous Mass Exchange and Regeneration Networks

The increase in dimensionality of the regeneration problem leads to the following additional equations.

The overall mass balance for the regenerating agent is as given in Equation 4.45 below:

Logical Constraints

The existence or otherwise of a match between the lean stream l and regenerating stream v in the network is denoted using the logical constraint with a binary variable z_{lv} taking on a value of '1' if a match exists and '0' if otherwise. An upper bound, Ω, is used to constrain the amount of mass which can be exchanged in the match between lean stream and regenerating stream as done in Equation 4.34.

Exchanger driving forces Calculation

Approach composition difference, are used for the calculation of the driving forces for the matches between the regenerable lean stream *l* and the regenerating agent, *v*.

The composition in the lean phase is used for the calculations of the driving forces in the matches between the regenerating agent and the regenerable lean stream. Similar to Equations 4.36 to 4.39, an upper bound to either activate or deactivate equations 4.47 to 4.50 is included in the equations.

Logarithmic mean composition difference (LMCD)

Chen's first approximation (1987) is used for the calculation of LMCD in continuous contact column to avoid the problem of singularities in the model as was done for LMCD in the primary network.

Objective Function

The objective function minimizes the TAC of the primary and secondary network simultaneously. This comprises of the annual operating cost of regenerable MSA and the regenerating agent (MSA) and the annual capital cost of the primary and secondary mass exchanger networks.

(4.51)

Where is the expression of number of stages defined by Shenoy and Fraser (2004).

4.5 S&TBS MODEL EQUATIONS FOR HENS

The overall energy balances to ensure that streams get to their target temperatures and interval energy balances which refer to heat exchanged by hot stream and cold stream in S&TBS are similar to those of the SBS.

Moreover, in the S&TBS model equations, the temperature feasibilities along the superstructure, the use of binary variables $Z_{i,j,k}$, in logical constraint equations to ensure the existence or otherwise of match *i,j* in interval *k*, the approach temperatures to calculate the heat exchanger driving force at the interval boundaries, and the objective functions in the HEN superstructure are as in the HEN SBS. Those equations in S&TBS that are different from those of SBS are stated below.

Assignment of Superstructure Interval Boundary Temperatures in S&TBS

With reference to Figure 3.5, the interval boundary temperatures in S&TBS are specified as follows (the lower case symbols represent optimization variables):

First Set of Stream Existence Conditionals in S&TBS

In order to achieve the situation where a hot stream will not be able to exchange heat in any interval whose temperature is higher than or equal to its supply value, and a cold stream will not exchange heat in any interval where the temperature is lower than or equal to its supply value, the S&TBS functions with the first set of stream existence conditionals stated for the SBS in Equations 4.5 and 4.6. The S&TBS with such conditionals are labelled S&TBS Type 1.

In S&TBS Type 2, however, the first conditional for hot streams is the same as in Type 1, that is Equation 4.5, but the second conditional is that a cold stream cannot exchange heat in those intervals where the temperature is greater than or equal to its target value, it is as shown in equation 4.58 below.

Second Set of Stream Existence Conditionals in S&TBS

The second set are the stream existence recognition conditionals that consists of the stream supply and target temperature conditionals that recognises the supply or target temperatures of the set of streams which define the interval boundaries in the S&TBS. The first two are the same as Equation 4.7 and 4.8 in SBS while the remaining two are given in Equations 4.59 and 4.60 below as follows:

The next section presents the model equations for the MEN S&TBS.

4.6 S&TBS MODEL EQUATIONS FOR MENS

The analogue of Figure 3.5 is the S&TBS adaptation for MENS. The overall mass balances to ensure that streams reach their target compositions and interval mass balances which refer to mass exchanged by rich stream and lean stream are also similar to those of the MEN SBS.

In the MEN model equations of S&TBS, the composition feasibilities along the superstructure, the use of binary variables $Z_{i,j,k}$, in logical constraint equations to ensure the existence or otherwise of match r,l in interval k, the approach compositions to calculate the mass exchanger driving force at the interval boundaries, and the objective functions are as in the MEN SBS. Those equations in S&TBS that are different from those of SBS are stated below.

Assignment of Superstructure Interval Boundary Compositions for S&TBS

The model equations are presented below.

First Set of Stream Existence Conditionals for MENS

Similar to the HENS SBS, the Type 1 of S&TBS uses stream existence conditionals that ensure that a rich stream cannot exchange mass in those intervals whose composition is higher than or equal to its supply value while a lean stream cannot exchange mass in those intervals where the composition is lower than or equal to its supply value: The equations employed to achieve the aforementioned conditions are the same as those of MEN SBS in Equations 4.25 and 4.26 for Type 1 of S&TBS. In Type 2, the first conditional is the same as Equation 4.25 but the second conditional is that a lean stream cannot exchange mass in those intervals where the composition is greater than or equal to its target value, it is as shown in equation 4.70 below.

Second Set of Stream Existence Conditionals

The S&TBS also uses a set of stream existence conditionals which are the stream supply and target composition recognition conditionals. The first two are the same as Equations 4.27 and 4.28 in MEN SBS while the remaining two are given in Equations 4.71 and 4.72 below:

The Model equations of the HEN T&SBS is presented next.

4.7 T&SBS MODEL EQUATIONS FOR HENS

The overall energy balances to ensure that streams reach their target temperatures and interval energy balances (which refer to heat exchanged by hot stream and cold stream) are similar to those of the SBS and the S&TBS.

In the T&SBS HEN model equations, the feasibilities of temperature along the superstructure, the use of binary variables $Z_{i,j,k}$, in logical constraint equations that ensure the existence or otherwise of match i,j in interval k, the approach temperature for the heat exchanger driving force calculation at the boundaries, and the objective functions are as in the SBS and the S&TBS.

The second set of stream existence conditionals which are the stream supply and target recognition conditionals to recognize the hot and cold streams that define the interval boundaries in the superstructure are the same as those use for the HENS S&TBS. The differences that exist in the models will, however, be presented as follows.

Assignment of Superstructure Interval Boundary Compositions for T&SBS

In Figure 3.5, the interval boundary temperatures in T&SBS are specified as follows:

First Set of Stream Existence Conditionals in T&SBS

Similar to the SBS and the S&TBS, the T&SBS works with stream existence conditionals stated in Equations 4.78 and 4.79 which respectively imply the following: a hot stream should be considered for matching in an interval *K* (which lies between boundaries and) if the target temperature of such a stream is less than or equal to the interval boundary that begins that interval (i.e. boundary *k*), while a cold stream is to be considered for matching in an interval K (which lies between boundaries and if the supply temperature of such stream is less than or equal to the temperature interval boundary *k* that starts the interval.

4.8 T&SBS MODEL EQUATIONS FOR MENS

In the same vein as HENS T&SBS, the equations used to model the MEN T&SBS are similar to those presented for MEN SBS and S&TBS. The overall mass balances and the interval mass balances which refer to mass exchanged by rich stream and lean stream are the same as stated for the MEN SBS.

The feasibilities of composition along the superstructure, the use of binary variables $Z_{r,l,,k}$, in logical constraint equations that ensure the existence or otherwise of match *r,l* in interval *k*, the approach composition for the mass exchanger driving force calculation at the boundaries, and the objective functions are as in the MEN SBS.

The second set of stream existence conditionals are the stream supply and target recognition conditionals that recognize the rich and lean streams that define the interval boundaries in the superstructure that are as stated for the MENS S&TBS. The differences from S&TBS are set out below.

Assignment of Superstructure Interval Boundary Compositions for T&SBS

In the MEN analogue of Figure 3.6, the interval boundary composition in MEN T&SBS are specified as follows:

First Set of Stream Existence Conditionals in T&SBS

Similar to the MEN SBS and the MEN S&TBS, the MEN T&SBS also works with stream existence conditionals stated in Equations 4.85 and 4.86 below. The conditionals imply that a rich stream should be considered for matching in an interval *K* (which lies between boundaries and) if the target composition of such stream is less than or equal to the interval boundary that starts that interval, while a lean stream is to be considered for matching in an interval K (which lies between boundaries and if the supply composition of such stream is less than or equal to the composition interval boundary that starts the interval.

4.9 SOLUTION AND INITIALISATION

The SBS, S&TBS and T&SBS models presented in this thesis have been solved in the General Algebraic Modeling Systems (GAMS) environment (Rosenthal, 2007) with the solver DICOPT++, which uses CPLEX for the MILP and CONOPT for the NLP sub-problems. The solutions obtained with the use of these superstructures gave results which compare favourably with those reported in the literature. This will be shown in Chapter 6 where all the results obtained by various researchers are compared with the results obtained in this thesis. The initialization approach that was adopted is the one that was used by Isafiade and Fraser (2008a). This initialization was based on a similar approach by Shenoy (1995); using exchanger minimum approach temperature (EMAT) in HENS and the exchanger minimum approach composition (EMAC) in MENS. Upper bounds are set for heat capacity flowrates of the utilities in HEN and external MSAs in MENS, by determining the maximum possible requirements for all utility streams (for example, the maximum hot utility required would satisfy all the cold stream heating demands).

4.10 CONCLUSION AND SUMMARY

The mathematical equations and variables for the modelling of HEN and MEN SBS, S&TBS and the T&SBS were presented in this chapter. The various conditionals that enable the different models to function as conceived were presented along with the equations. Similar to the SWS of Yee and Grossmann (1990) and SWS of Szitkai *et al*. (2006), isothermal and isocompostion assumptions were made respectively in HENS and MENS SBS, S&TBS and T&SBS models. This is to reduce non linearity in the HENS and MENS models.

CHAPTER FIVE

APPLICATIONS OF SBS, S&TBS AND T&SBS TO HENS AND MENS EXAMPLE PROBLEMS

CHAPTER FIVE: APPLICATIONS OF SBS, S&TBS AND T&SBS TO HENS AND MENS EXAMPLE PROBLEMS

This chapter presents the applications of the superstructures presented in Chapters 3 and 4 to different literature problems. The superstructures will be compared with the previous interval/stage based methods where the solutions exist. In this chapter, the term 'interval' will be adopted for the stage based SWS and its derivatives. This will be done throughout in the examples presented to prevent confusion with stage-wise mass exchangers. The detailed comparison of all the solutions including those that are not interval based will be presented in the next chapter.

5.1 HENS EXAMPLES

Example 1: (Lee *et al*., 1970)

This example is the 4SP1 problem from Lee *et al*. (1970). It involves two hot and two cold streams, one hot utility (steam) and one cold utility (water). The problem specifications are given in Table A1 of Appendix A. The solution to this problem has been presented by different sets of workers including Lee *et al*. (1970), Grossmann and Sargent (1978), Papoulias and Grossmann (1983), Linnhoff and Flower (1978), Bagajewicz *et al*. (1998) and Krishna and Murty (2007). It has also been solved for a scenario where the match between H1 and C1 is forbidden (termed match restriction) (Papoulias & Grossmann, 1983; Dolan *et al*., 1987; Yee & Grossmann, 1990; Krishna & Murty, 2007).

Case with no match restriction

The SBS, S&TBS and T&SBS of this study have been applied to this problem; the SBS has five intervals and the network TAC obtained is \$10,794/yr with the network structure featuring five units with a split of Hot Stream 2, as shown in Figure 5.1. The network structure obtained for the S&TBS Type 1 is shown in Figure 5.2 with TAC of \$10,786/yr. Type 2 of S&TBS has identical structure with the SBS and has a TAC of \$10,795 /yr. The two S&TBS networks, in a manner similar to SBS, have five intervals each with a split of one of the hot streams (H1 for Type 1 and H2 for Type 2). The network structures obtained for the T&SBS with TAC of \$11,204/yr is shown in Figure 5.3 with six intervals and splits of both hot streams. The Type 1 of S&TBS only reduced the total annualised investment cost by a marginal value of 0.07 % when compared with the SBS; while the TAC of Type 2 is about the same as the SBS network TAC and the two structures are identical. Of all the techniques presented in this thesis, the T&SBS produced the highest TAC for this Example. All solutions have similar AOC and ACC and neither dominates. The SBS and S&TBS have one redundant interval (interval not used for matching) each at one extreme end while the T&SBS has two unused intervals for matching at one end.

Case with match restriction

This is a case where any match between H1 and C1 is forbidden, (this can be required industrially to avoid streams mixing if there is an exchanger leak, i.e for safety). Yee and Grossman (1990) used cold-to-cold matching in the SWS networks to obtain a TAC of \$13,800/yr, although this option does not appear to be used in industry. The application of SBS of this study results in a TAC of \$20,019/yr. Type 1 and Type 2 of S&TBS with five intervals each produce networks with TACs \$33,136/yr and \$18,710 /yr respectively.

T&SBS produces a network with six intervals and a TAC of \$33,243/yr. Type 2 of S&TBS features five units as shown in Figure 5.4 while Type 1 and T&SBS feature four units each.

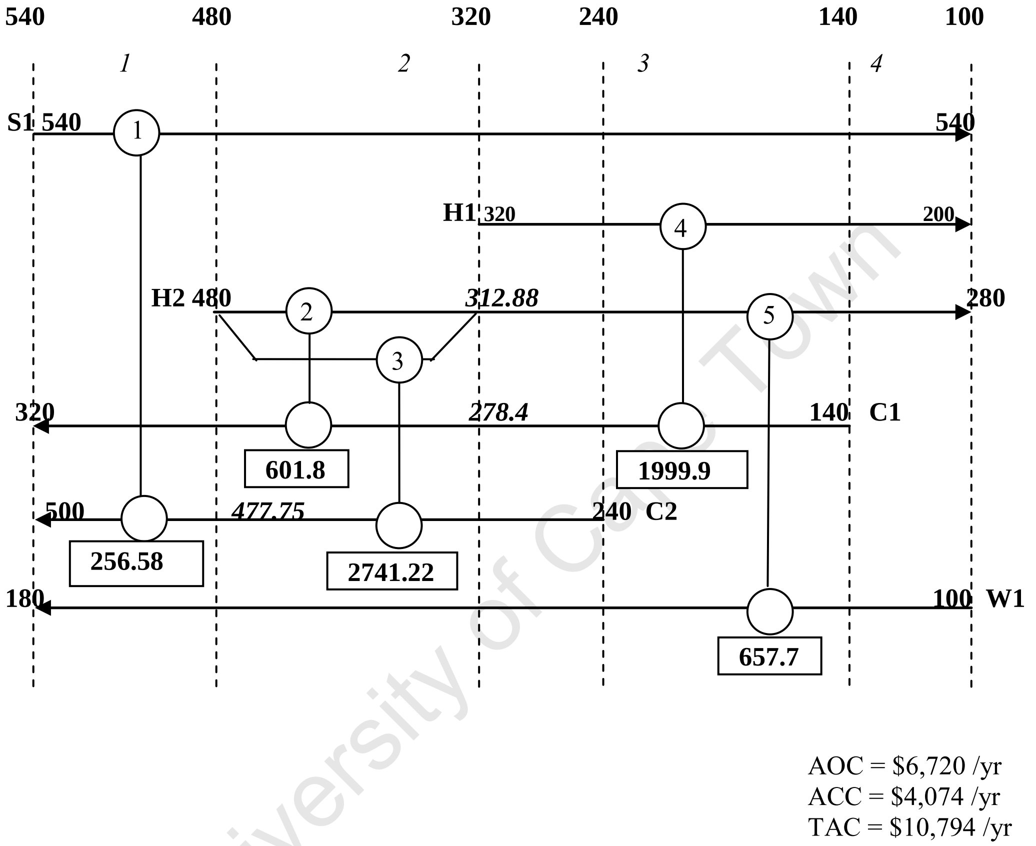
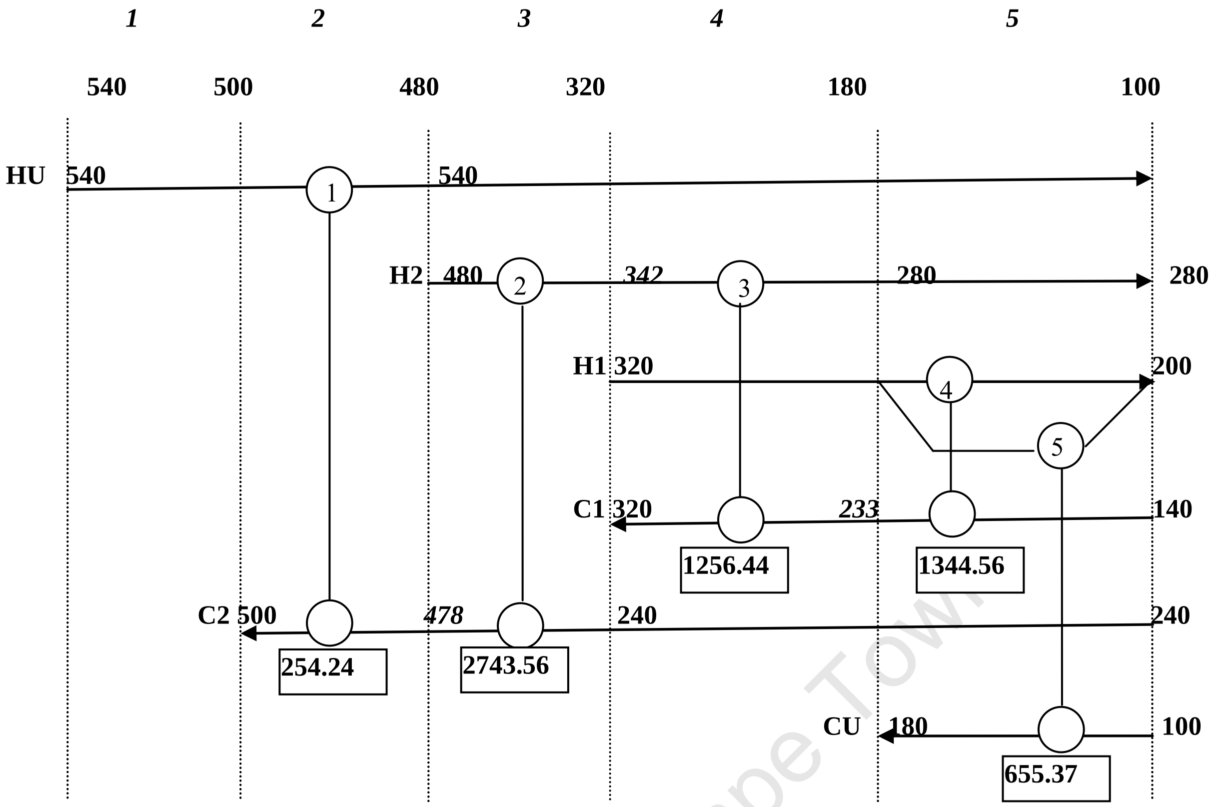
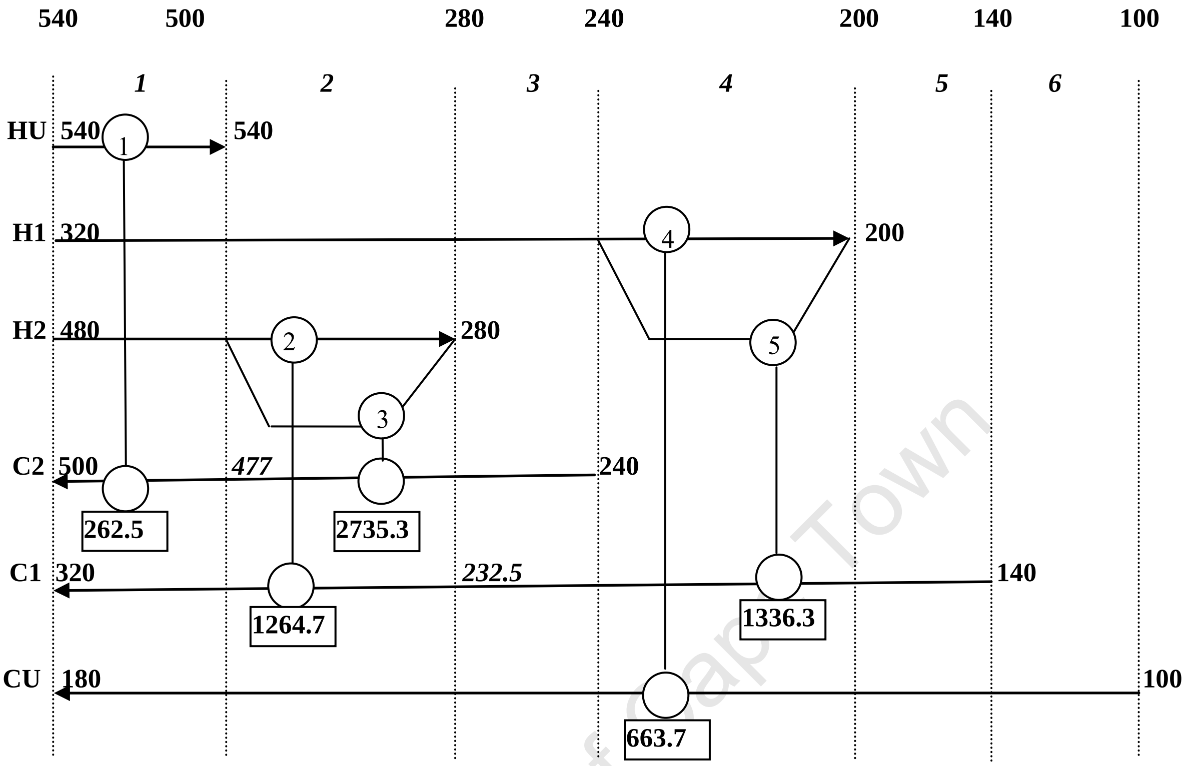


Figure 5.1: The SBS network structure for Example 1 featuring five units with a TAC of \$10,794



AOC = $6,678 /yr
ACC = $4,108 /yr
TAC = $10,786 /yr

Figure 5.2: The S&TBS (Type 1) network structure for Example 1 featuring five units with a TAC of $10,786/yr



AOC = $6,827 /yr
ACC = $4,377 /yr
TAC = $11,204/yr

Figure 5.3: The T&SBS network structure for Example 1 featuring five units with a TAC of $11,204/yr

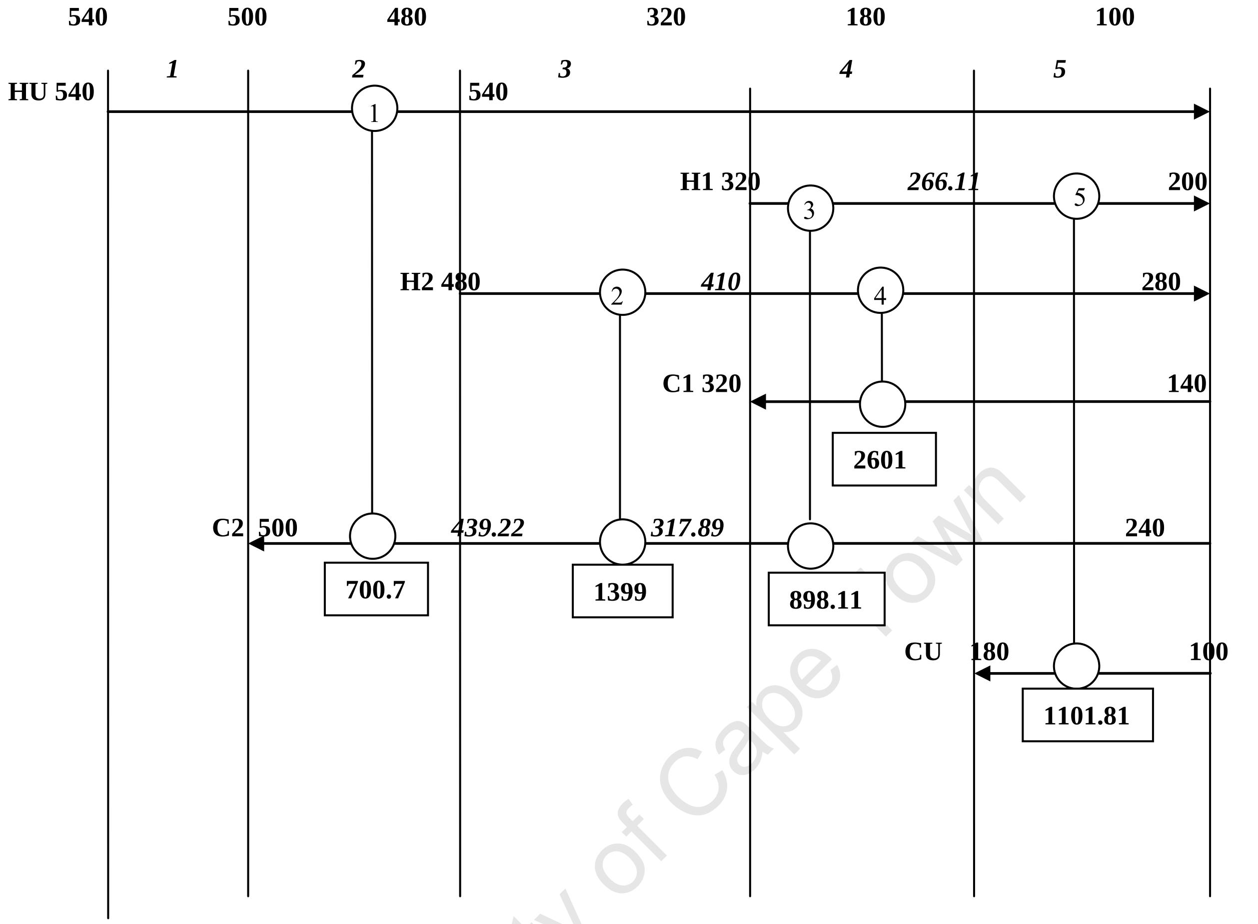


Figure 5.4: Network structure of Type 2 S&TBS with H1,C1 forbidden featuring TAC of $18,710/yr

Example 2: 4S1 (Shenoy, 1995)

Shenoy's (1995) 4S1 problem also involves two hot streams, two cold streams and one hot and one cold utility. It has also been solved by Isafiade and Fraser (2008a) and the problem specifications are in Table A2 of Appendix A. This example features equal heat transfer coefficients for all streams. Shenoy (1995) solved this problem using the SWS of Yee and Grossmann (1990) with the Paterson (1984) approximation for LMTD to obtain a TAC of $235,400/yr while Isafiade and Fraser used the IBMS with Chen's first approximation. The hot stream based IBMS gave a TAC of $237,800/yr while the cold stream based IBMS gave a TAC of $239,332/yr. The network structures of Shenoy (1995), hot based and cold based

IBMS of Isafiade and Fraser (2008a) are shown in Figure 5.5, 5.6 and 5.7 respectively where each structure features six units. Two intervals were used for the SWS while the IBMS has five in its network. Solutions of some examples using different approximations for LMTD are presented in Table C1 of Appendix C.

The TAC obtained with the SBS is \$235, 931, that of S&TBS is \$235,781/yr while T&SBS features \$240,253/yr and the network structures with six units each are shown in Figures 5.8, 5.9 and 5.10 respectively. The SBS network has five intervals while the S&TBS and the T&SBS have six intervals each in their networks. All the solutions presented including those of this study involve six units each and at least two splits with H2 always being one of the splits because of its large heat capacity flowrate. Type A and B of S&TBS give TAC of 235,382 \$/yr when Paterson (1984) approximation was used as shown in Table C1 of appendix C.

The splits occur in H2 and C2 in SWS, SBS and S&TBS as shown in Figures 5.5, 5.8 and 5.9 respectively. However, it occurs in H2 and C1 in the hot based IBMS and in H2, C1 and C2 in the cold based IBMS as shown in Figures 5.6 and 5.7 respectively. The split in T&SBS network structure as shown in Figure 5.10 is as in the cold based IBMS but the duties are different. The stream matches of the S&TBS and T&SBS take place over six intervals each, giving opportunity for more intervals than in any other technique presented earlier. The Type 1 and Type 2 of S&TBS have similar structures resulting in a TAC which is just 0.16% higher than the best solution (the SWS), but lower than all other solutions. All solutions have similar AOC and ACC with ACC dominating. Type 1 and Type 2 of S&TBS have one and two unused intervals for matching respectively at their extreme ends while the T&SBS have three unused intervals at its extreme end.

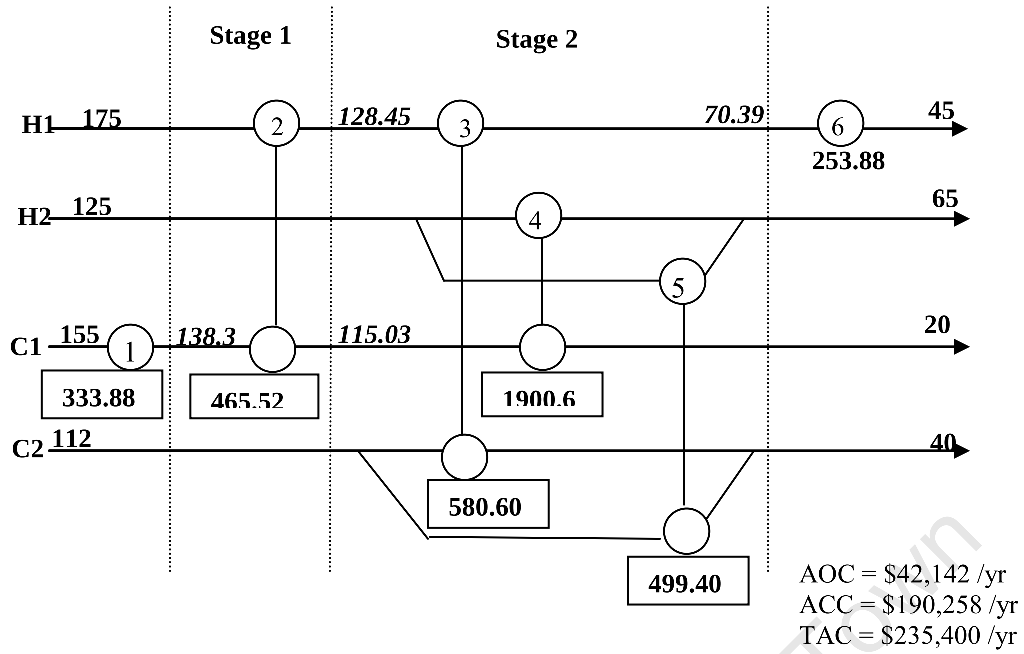


Figure 5.5: Network structure generated by Shenoy (1995) for Example 2 using the SWS of Yee and Grossman (1990)

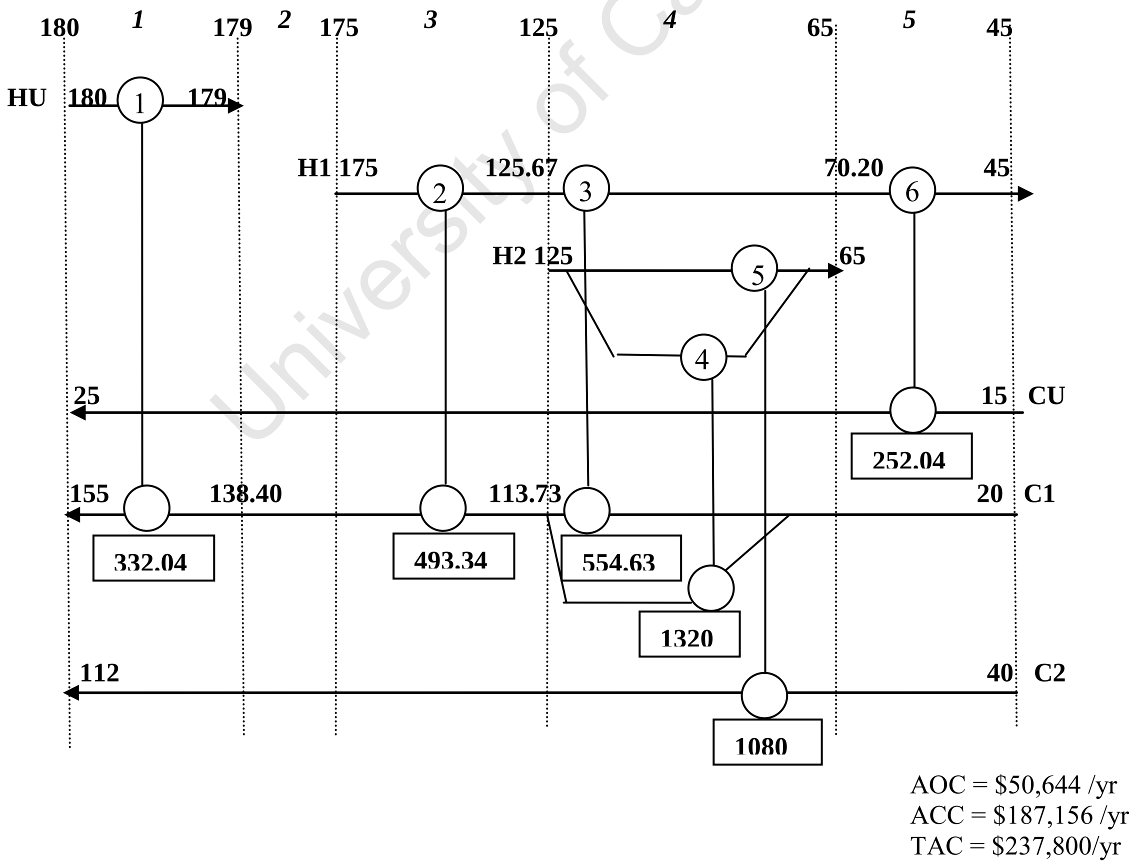
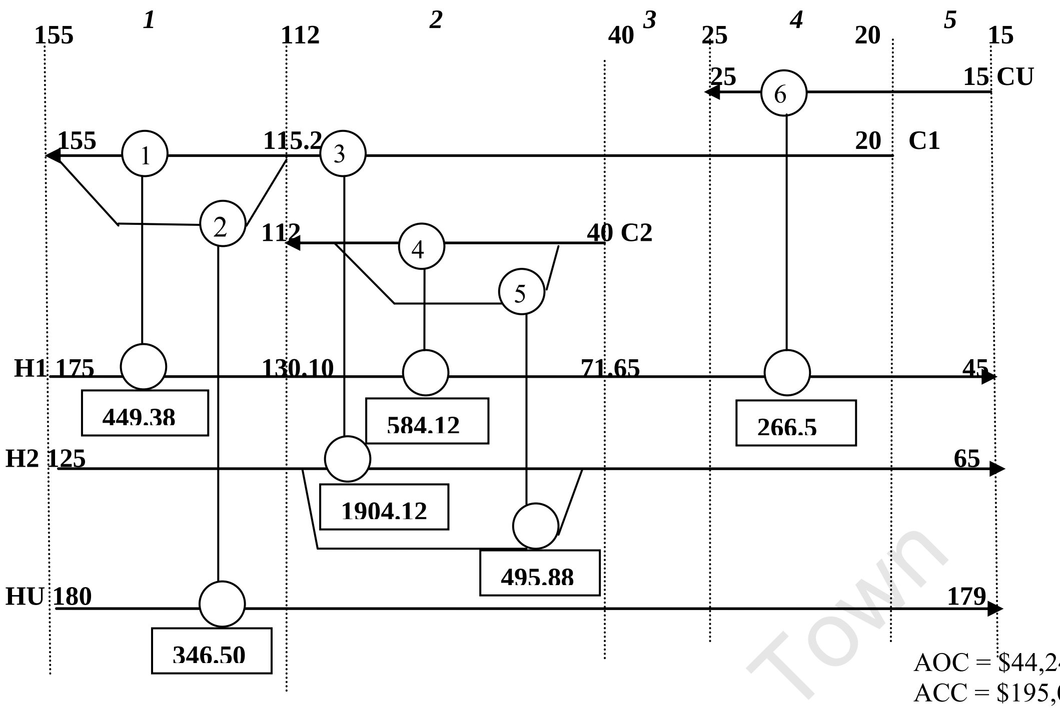
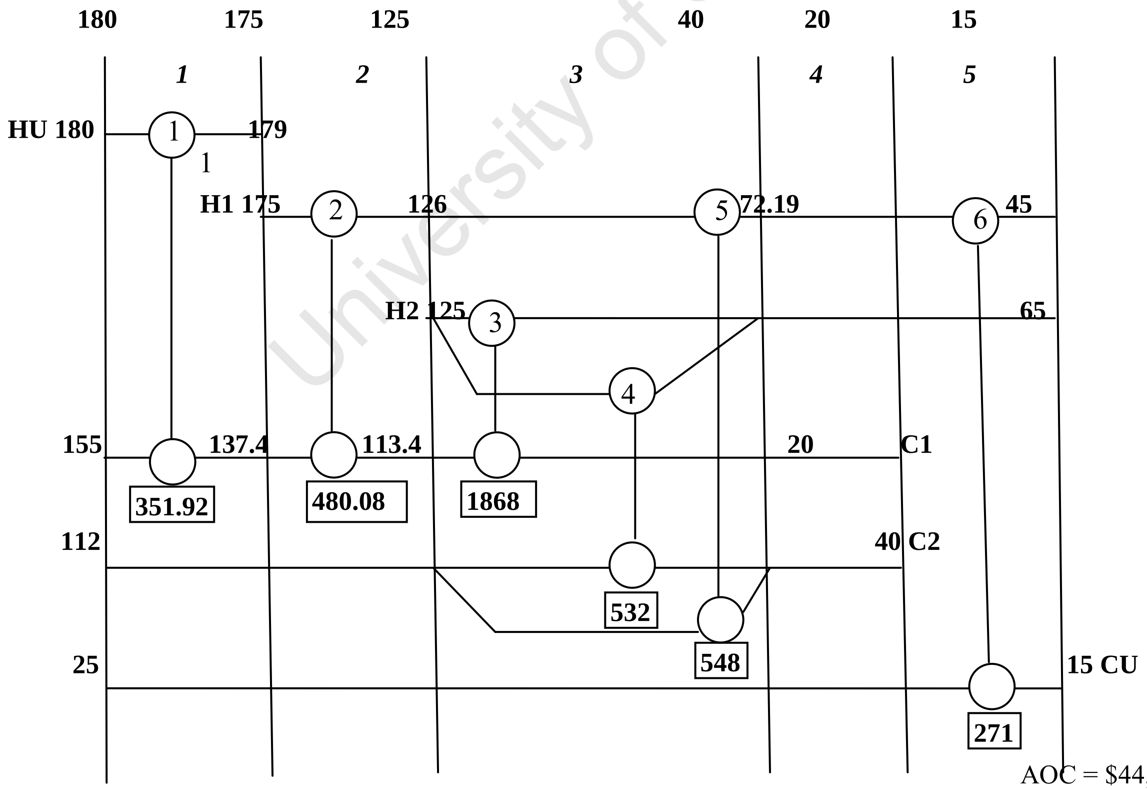


Figure 5.6: The Hot based IBMS network structure for Example 2 featuring a TAC of $237,800/yr



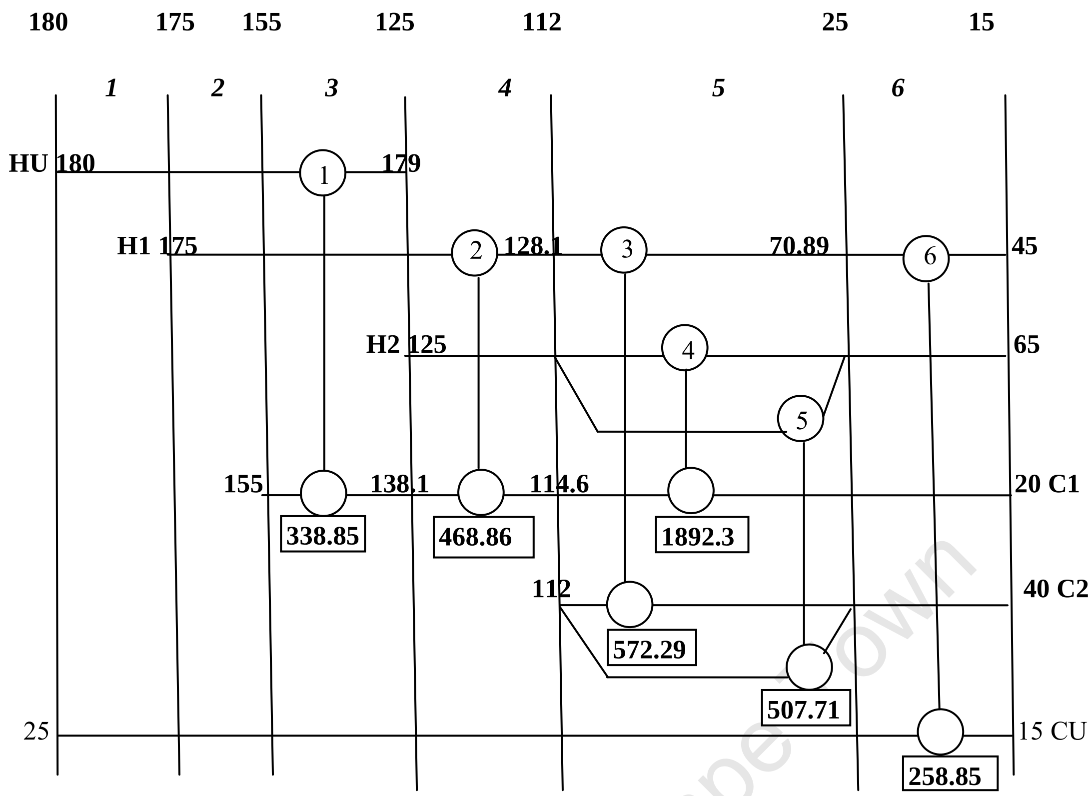
AOC = $44,245 /yr
ACC = $195,087 /yr
TAC = $239,332 /yr

Figure 5.7: The Cold based IBMS network structure for Example 2 featuring a TAC of $239,332/yr



AOC = $44,940 /yr
ACC = $190,991 /yr
TAC = $235,931/yr

Figure 5.8: SBS network structure for Example 2 featuring six units with a TAC of $235,931/yr



AOC = $43,250 /yr
ACC = $192,531 /yr
TAC = $235,781 /yr

Figure 5.9: Network Structure of S&TBS (Type 1 and 2) for Example 2 featuring six units with a TAC of $235,781/yr

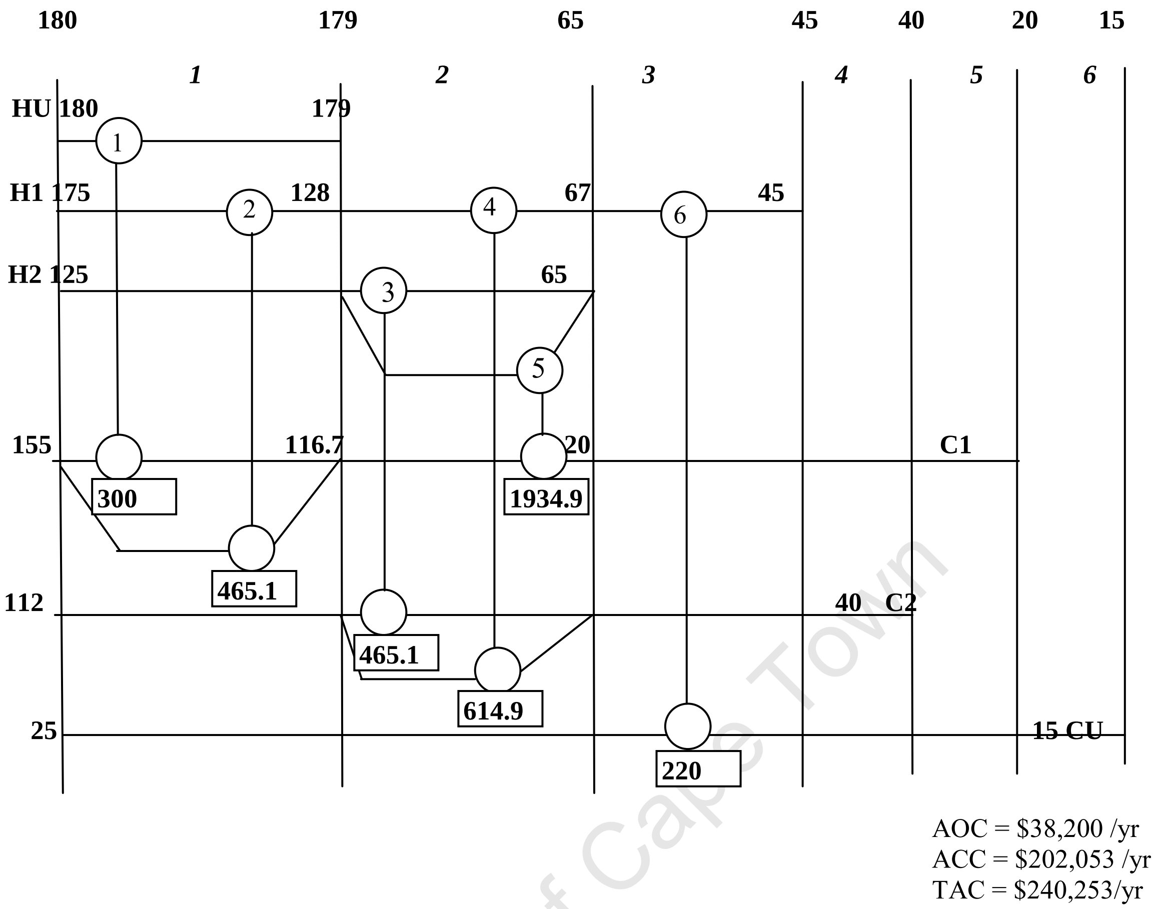
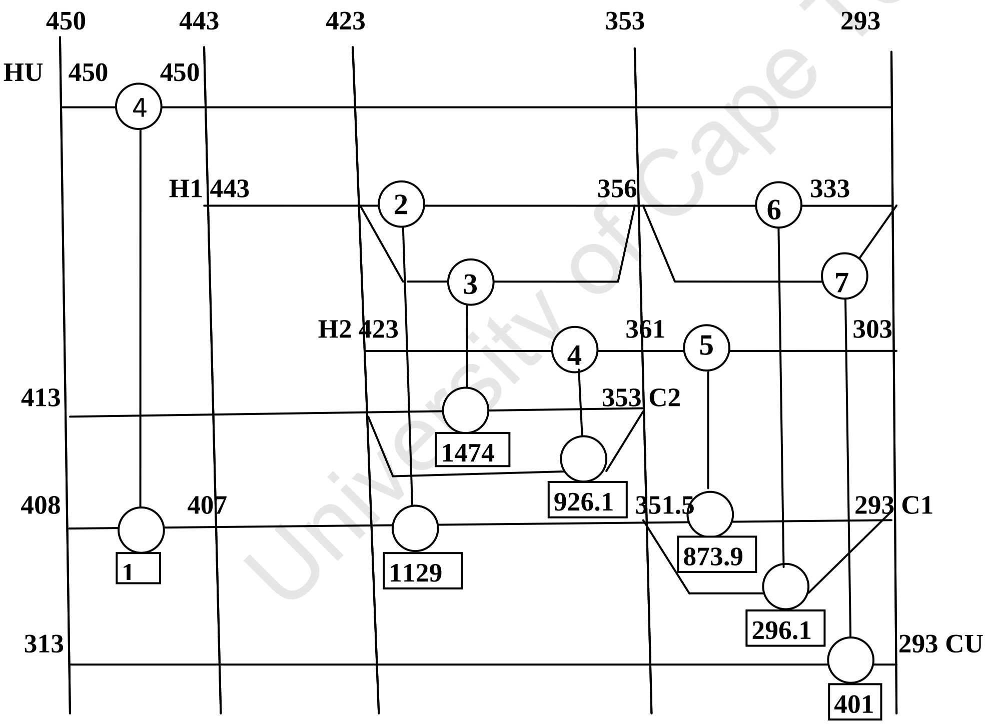


Figure 5.10: Network Structure of T&SBS for Example 2 featuring six units with a TAC of $240,253/yr

<u>Example 3: (Linnhoff *et al*., 1982)</u>

This is another example involving two hot streams and two cold streams, together with steam and cooling water as utilities taken from Linnhoff *et al*. (1982). The problem specifications are presented in Table A3 of Appendix A.

The SWS of Yee and Grossman (1990) used two intervals i. e. maximum of number of hot stream or cold stream to obtain a network with five units and TAC of $80,274/yr. The SBS of this study obtained a TAC of $90,521/yr for this problem with four intervals and seven units as shown in Figure 5.11. The network structures for Type 1 and Type 2 of S&TBS are shown in Figures 5.12 and 5.13 with TACs of $93,391/yr and $90,672/yr respectively, with six intervals each. The S&TBS though gave the same number of heat exchanger units as SWS but with higher costs. The T&SBS gives a network structure having aTAC of $87,611/yr as shown in Figure 5.14 with five units. This cost is the lowest for this example of all the techniques presented in this thesis. The SBS has a lower AOC and a higher ACC than the S&TBS and the T&SBS. The S&TBS and the T&SBS have similar AOC and ACC with ACC dominant in all the solutions. The S&TBS has three redundant intervals at the extreme ends while the T&SBS has one.



AOC = $8,100 /yr
ACC = $82,421 /yr
TAC = $90,521 /yr

Figure 5.11: SBS Network Structure for Example 3 featuring seven units with a TAC of $90,521/yr

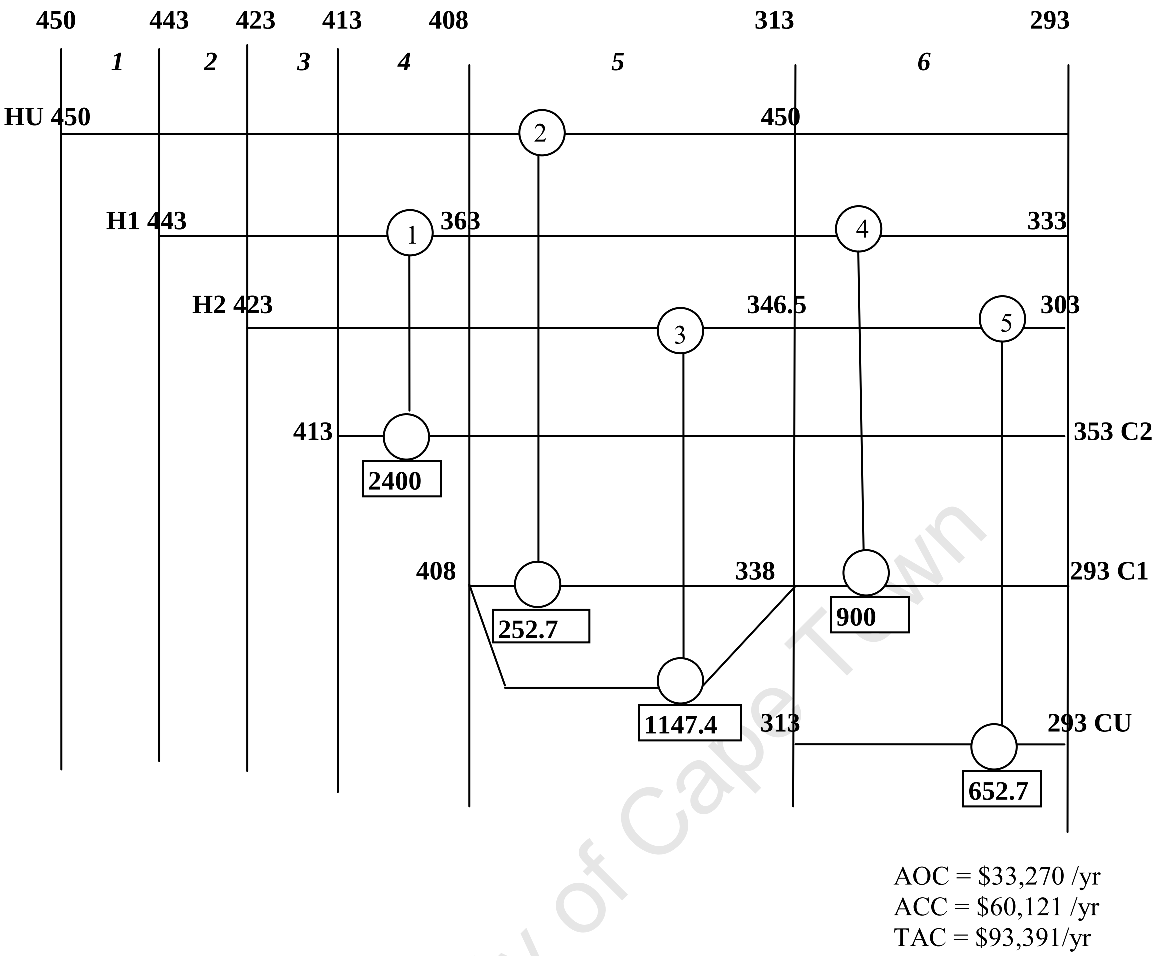


Figure 5.12: S&TBS (Type 1) Network Structure for Example 3 featuring five units with a TAC of $93,391/yr

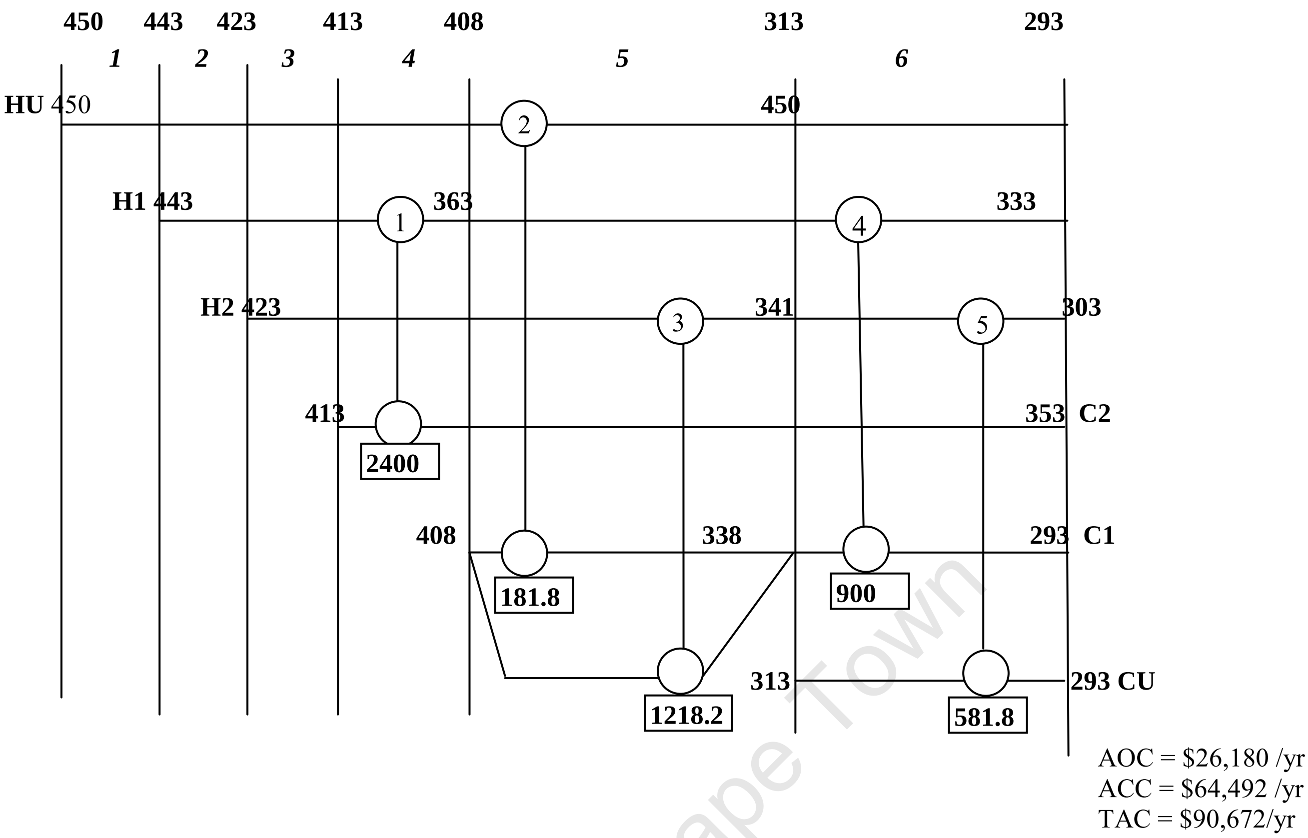


Figure 5.13: S&TBS (Type 2) Network Structure for Example 3 featuring five units with a TAC of $90,672/yr

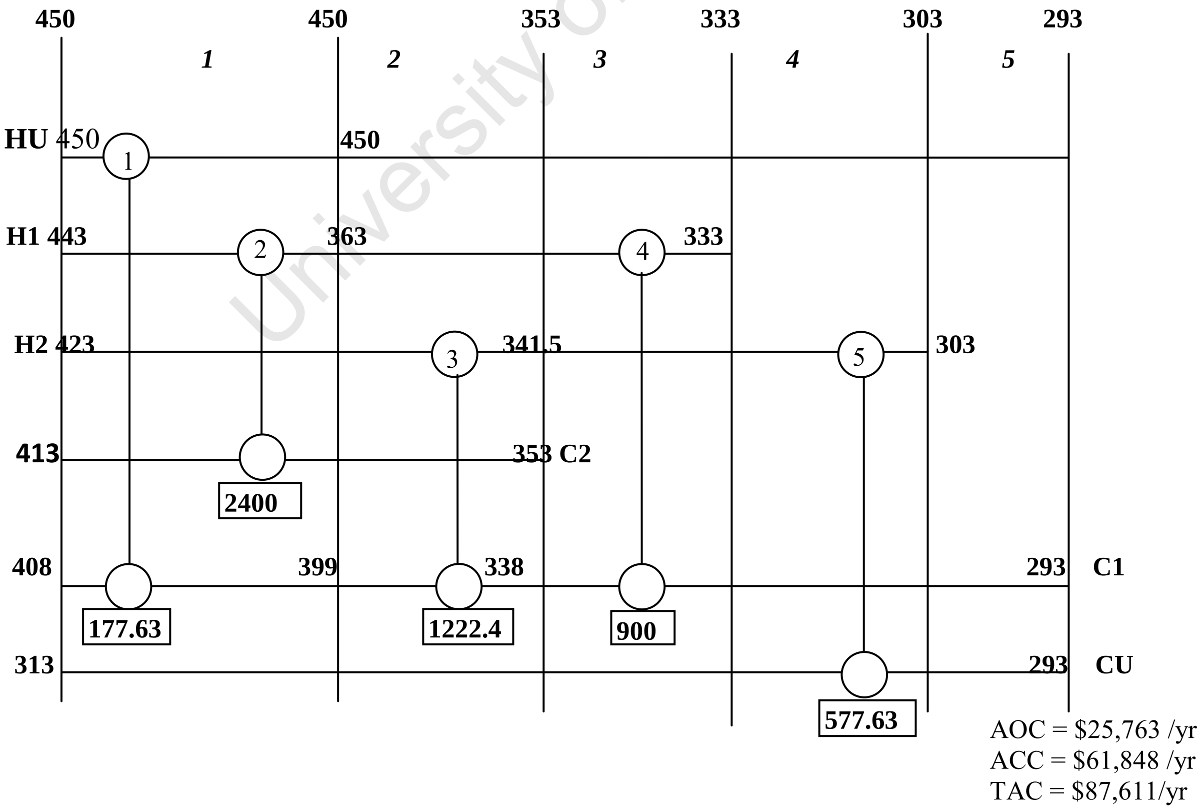


Figure 5.14: T&SBS Network Structure for Example 3 featuring five units with a TAC of $87,611/yr

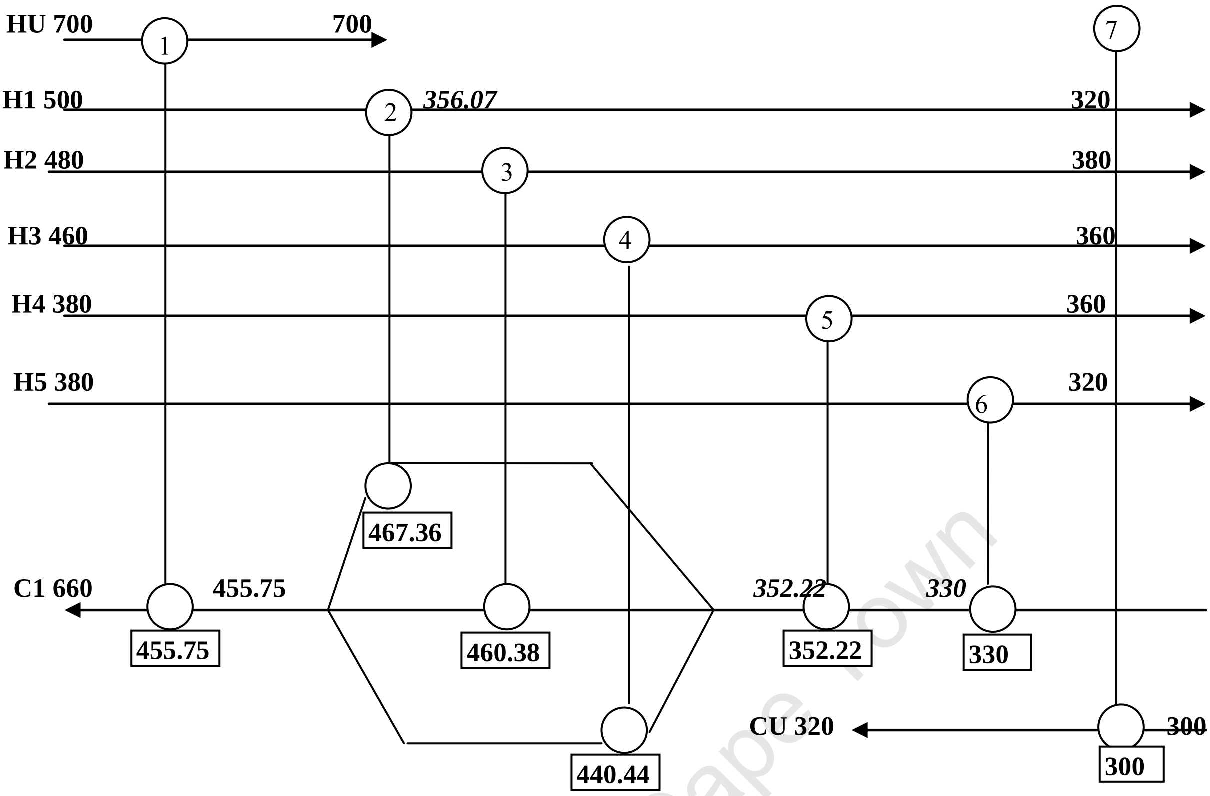
Example 4: (MAGNETS problem)

This problem was taken from the MAGNETS User Manual for the investigation of the SWS by Yee and Grossmann (1990), and has also been solved by Isafiade and Fraser (2008a) to verify the IBMS. The problem data is shown in Table A4 of Appendix A. The problem involves five hot streams and one cold stream along with steam and cooling water as utilities. The SWS has five intervals while the IBMS has seven intervals in the hot basis and three in the cold basis for this problem.

The network structures of the SWS and the hot based IBMS are shown in Figure 5.15 and 5.16 where each structure features seven units with TAC $576,640/yr and $581,942/yr respectively. The cold based IBMS features seven units in its network with TAC $595,064/yr. The superstructures presented in this study have been applied to this problem; the SBS network structure is presented in Figure 5.17 with six intervals, it features eight units with TAC of $580,023/yr. The Type 1 and Type 2 of the S&TBS have seven intervals each for this problem and feature seven and ten units respectively. The network structure of Type 2 of S&TBS is shown in Figure 5.18. The T&SBS has six interval and seven units with TAC of $581,954/yr. Type 1 of S&TBS and the T&SBS have network structures that are similar to the IBMS structure, even though the interval boundaries are different. The TAC of Type 1 is $581,942 while Type 2 has a TAC of $577,602/yr. The TAC of Type 2 of S&TBS is just about 0.1% higher than the network cost of the SWS, but lower than the TACs obtained by the IBMS and the SBS. The T&SBS features six intervals and seven units with a TAC of $581,954/yr.

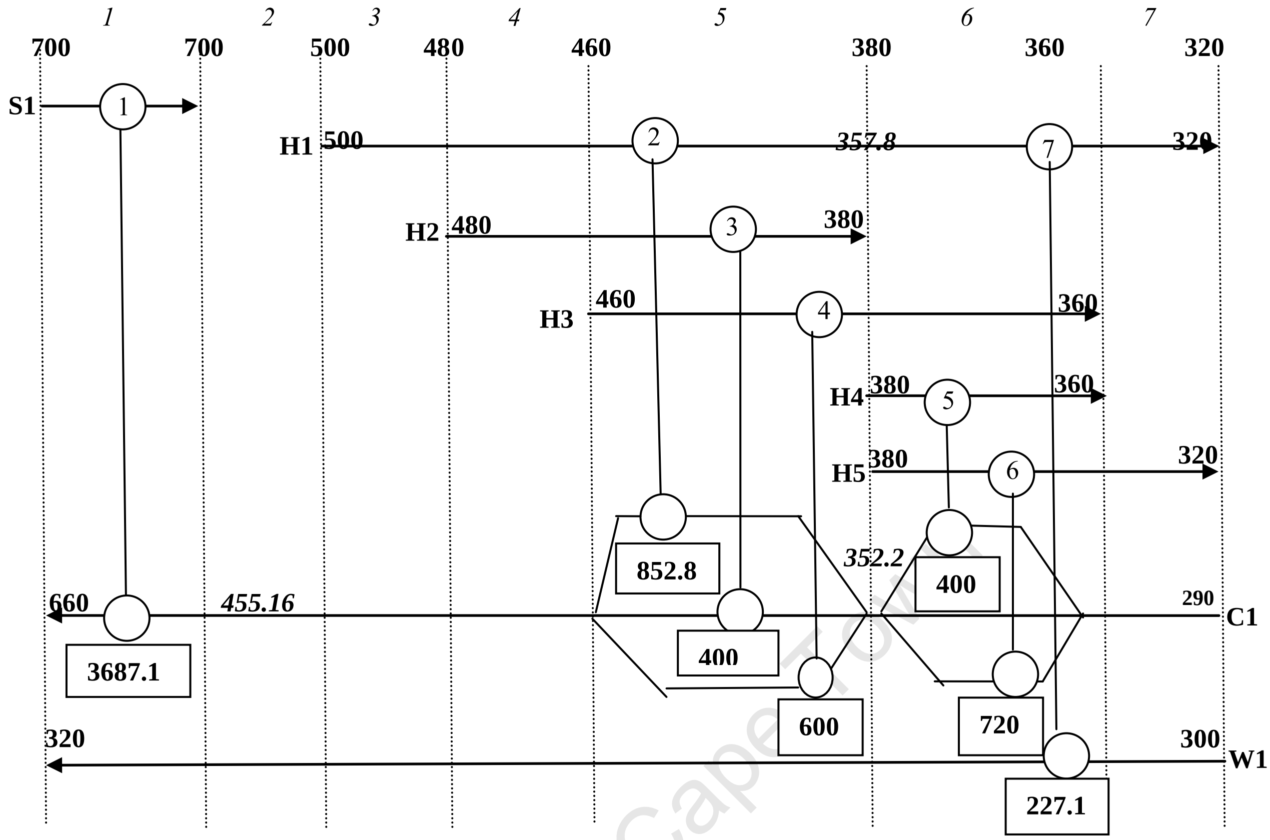
The splits in all the networks as anticipated by Yee and Grossmann (1990) are due to the presence of a single cold stream of fairly large size that matches with many hot streams. Note that the SWS has five intervals defined by the number of hot streams, the IBMS features seven intervals defined by the supply and target temperatures of the hot streams, and cold stream C1 splitting and mixing in the intervals created like this, while the SBS has six intervals and the cold stream C1 splitting and mixing in intervals created by the supply temperatures of streams where that of C1 is involved.

In the IBMS, all the hot streams are constrained at both their supply and target temperatures while the SBS gives more freedom to both the hot and cold streams concerning the intervals where they could exchange heat. The S&TBS and the T&SBS also give more freedom to the hot and cold streams regarding the intervals where these streams can exchange heat. This is because each of the streams exists in at least two of their intervals in their respective networks. The TAC of T&SBS, though higher than that of the hot based IBMS, it is much lower than that of the cold based IBMS. The Type 1 of S&TBS structure is identical to that of the IBMS. All the solutions have similar AOC and ACC with dominant AOC. The IBMS, SBS and Type 1 of S&TBS have one unused interval each at their extreme ends while Type 2 of S&TBS and the T&SBS have two unused intervals each at their extreme ends. Compared with the SBS, Type 2 of S&TBS has extra splits for H1 and C1 in the lowest temperature interval. The comparison for all the structures and their TACs will be presented in Chapter 6 of this thesis.



AOC = $516,874 /yr
ACC = $59,766 /yr
TAC = $576,640 /yr

Figure 5.15: The network structure generated by SWS of Yee and Grossmann (1990) for Example 4 with TAC $576,640/yr



AOC = \$518,471 /yr
ACC = \$63,471 /yr
TAC = \$581,942 /yr

Figure 5.16: IBMS network structure for Example 4 featuring seven units with multiple splits of the cold stream, with a TAC of \$581,900/yr

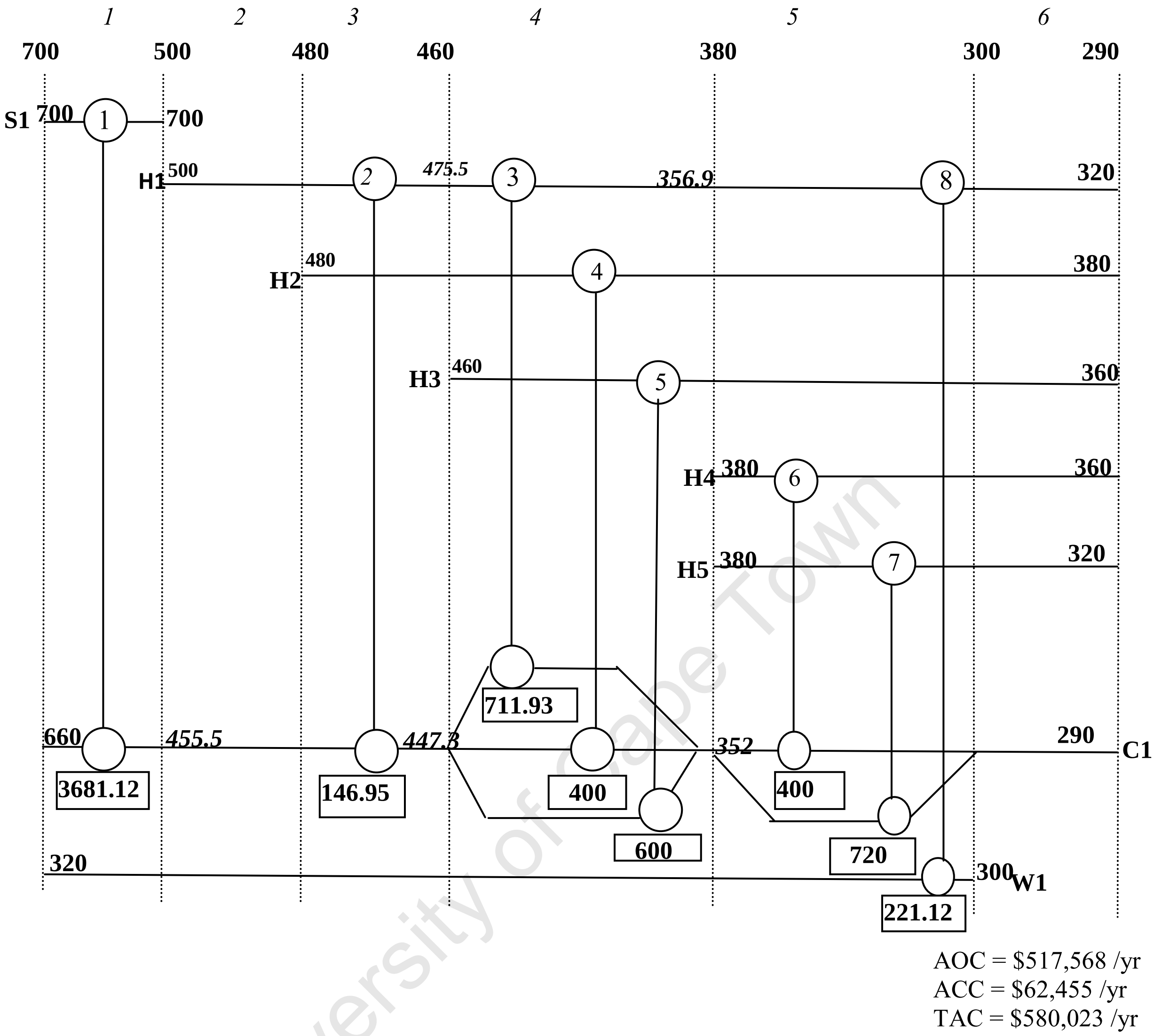


Figure 5.17: The network structure for Example 4 of the SBS featuring eight units and one 3 way split and one 2 way split of the cold stream with, a TAC of $580,023/yr

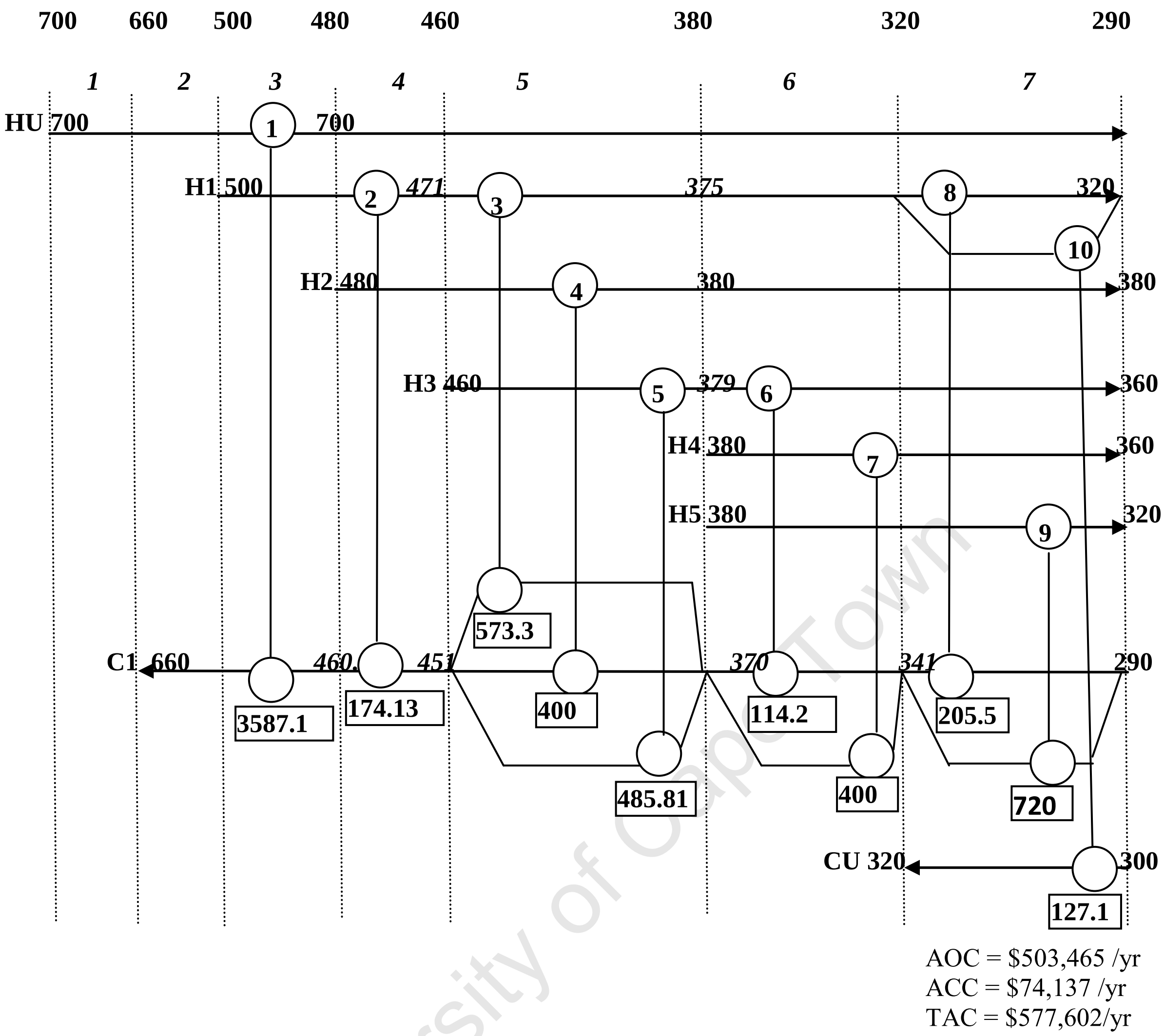


Figure 5.18: The S&TBS (Type 2) network structure for Example 4 featuring ten units with multiple split of the cold stream with a TAC of $577,602/yr

Example 5: (Aromatic plant)

The aromatic plant problem requires the determination of the optimal network of heat exchangers for four hot streams and five cold streams having significantly different heat transfer coefficients (Linnhoff & Ahmad, 1990; Zhu *et al.*, 1995; Lewin, 1998; Petersen, 2005; Krishna & Murty, 2007). The stream and cost data for this problem are shown in Table A5 of Appendix A. The application of the SBS to this problem produced a network with a TAC of M$2.976 /yr with 14 units as shown in Figure 5.19. Type 1 and Type 2 of the

S&TBS network structures are shown in Figures 5.20 and 5.21 with 13 and 11 units with a respective TAC of M$2.979/yr and M$2.940/yr. The T&SBS network structure for this problem with TAC M$2.922/yr with 17 units is shown in Figure 5.22.

This shows that the new SBS, S&TBS and the T&SBS are able to solve problems with different heat transfer coefficients. All the solutions have similar AOC and ACC and neither is dominant. The SBS has three redundant intervals at the extreme ends while the Type 1 of the S&TBS and the T&SBS have four redundant intervals at their extreme ends. Type 2 of S&TBS has two redundant intervals at its exteme end.

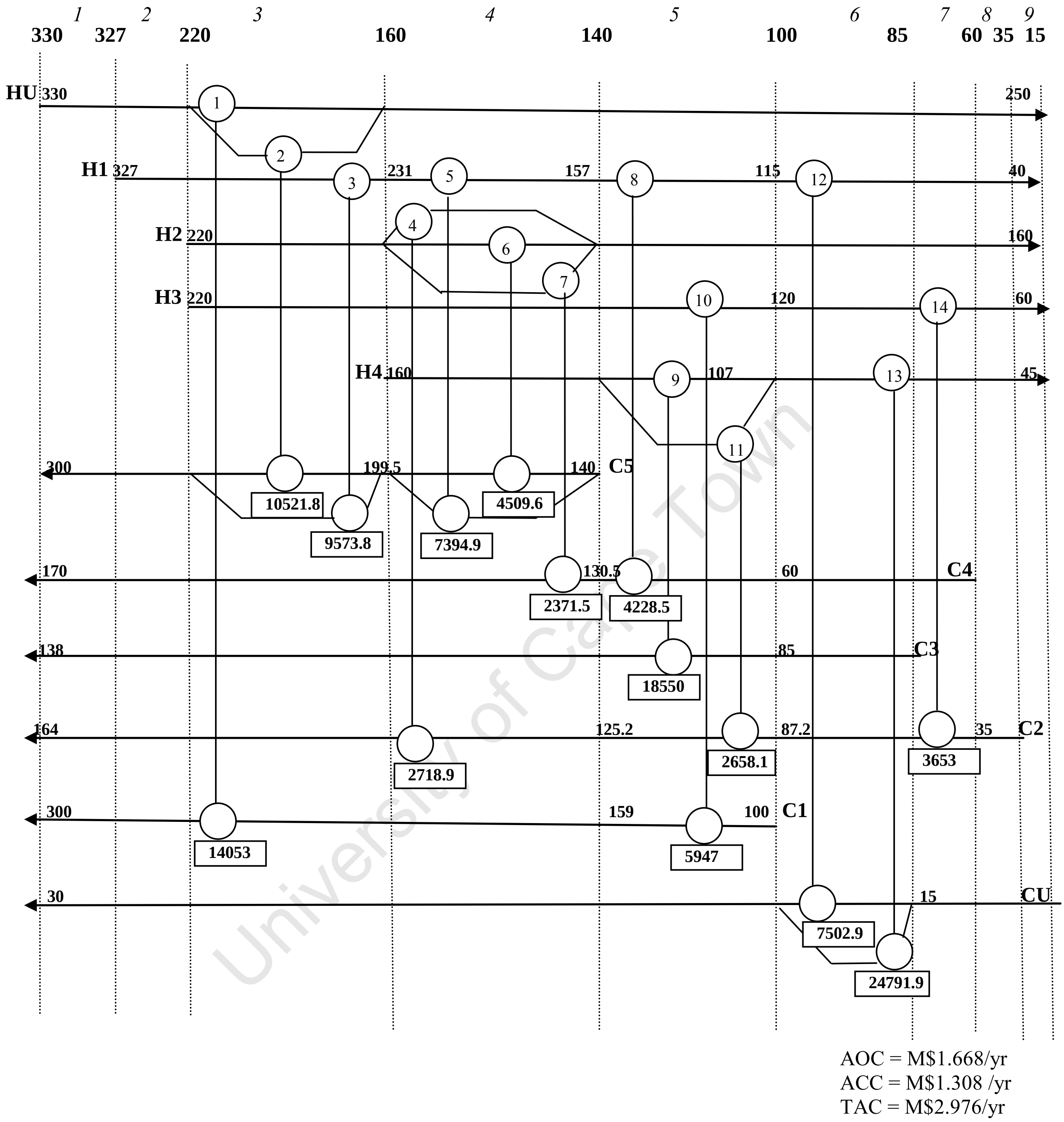


Figure 5.19: SBS network structure for Example 5 featuring 14 units with six stream splits with TAC of M$2.976/yr.

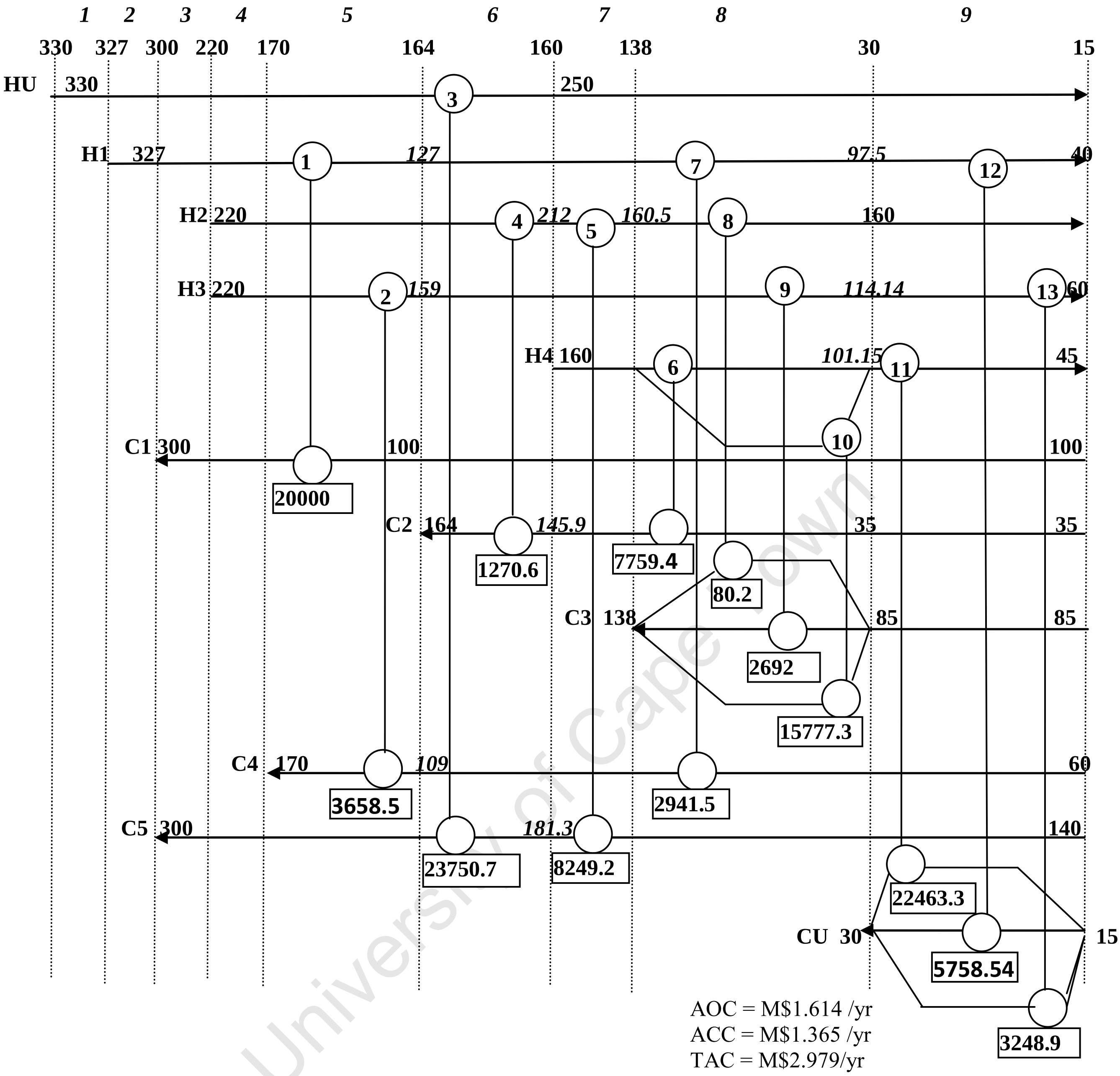


Figure 5.20: The S&TBS (Type 1) of Example 5 network structure featuring thirteen units with a TAC of M$2.979/yr

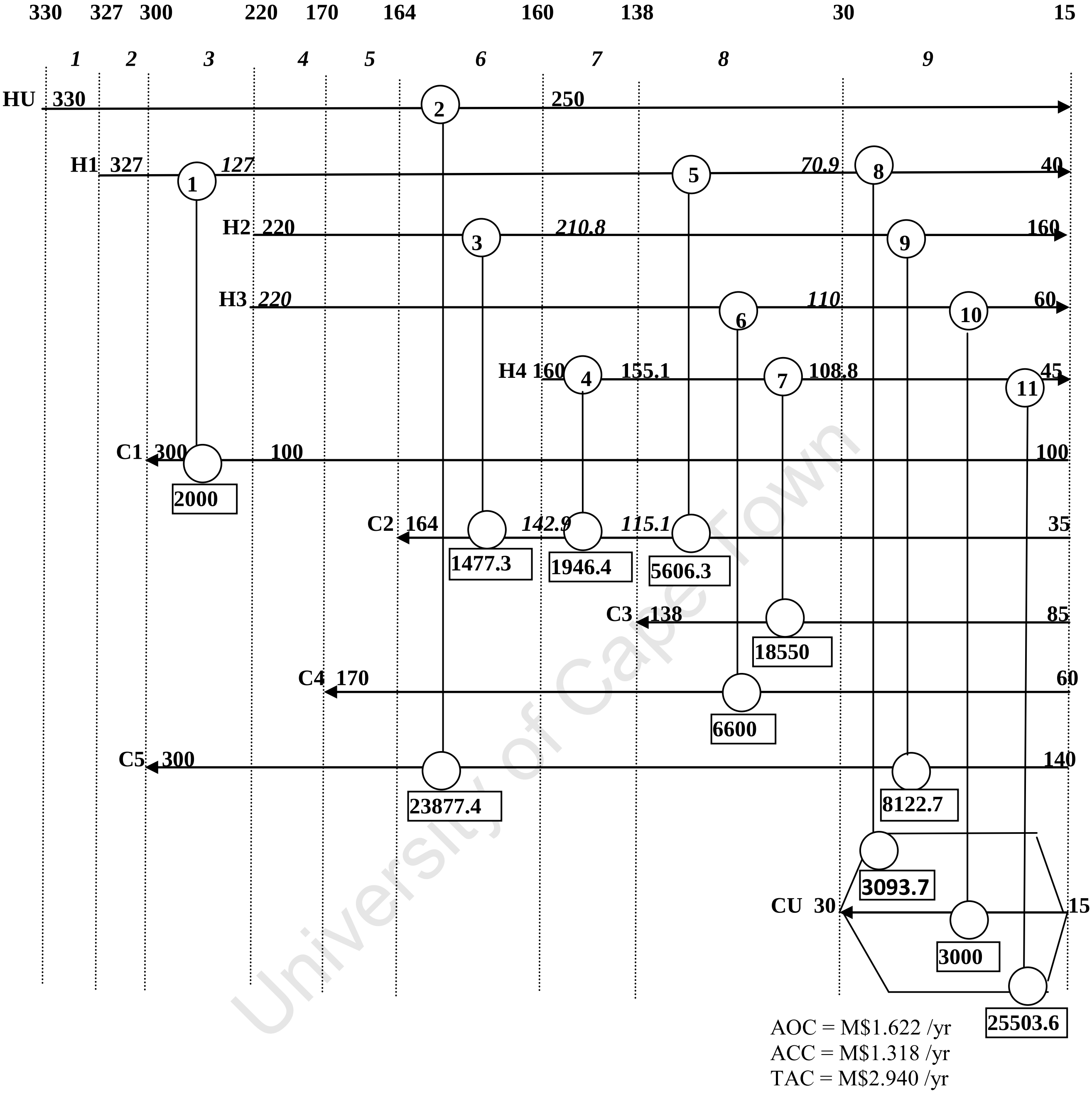
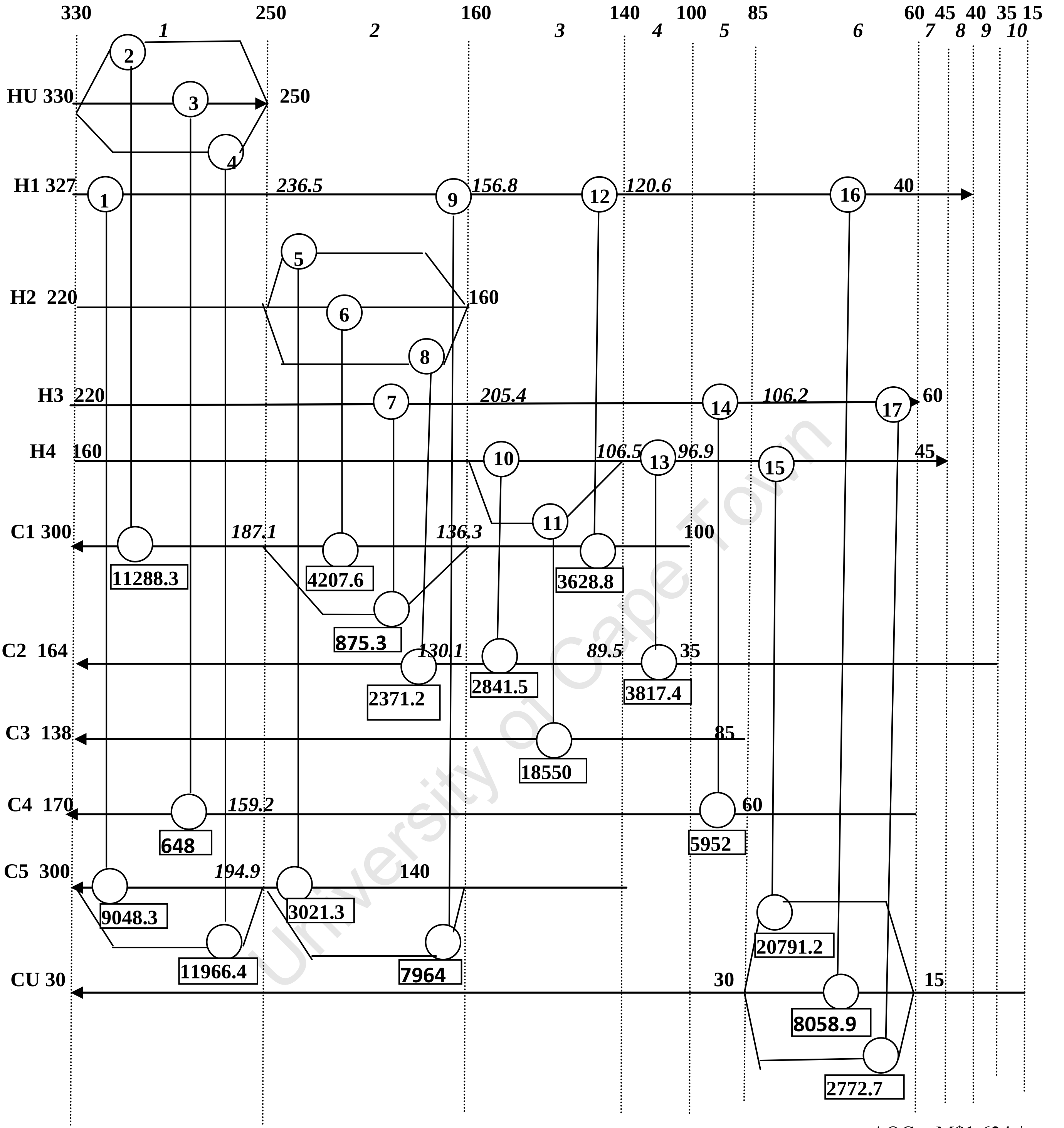


Figure 5.21: The S&TBS (Type 2) of Example 5 network structure featuring eleven units with a TAC of M$2.940/yr



AOC = M$1.624 /yr
ACC = M$1.298 /yr
TAC = M$2.922/yr

Figure 5.22: The T&SBS network structure of Example 5 featuring seventeen units with a TAC of M$2.922/yr

5.1.1 Application of the SBS, S&TBS and the T&SBS to Multiple Utility Problems in HENS.

The problems associated with the use of multiple utilities (i.e. more than one hot utility and more than one cold utility) in HENS have compelled researchers as mentioned in the review (Chapter 2), to evolve different techniques for the efficient use of such utilities when the need for their use arises. The superstructures presented in this thesis can be of great benefit when determining the placement of these utilities for optimum use in HENS since all the competing costs in multiple utility problems can be optimized in a single step. Two examples will be presented to demonstrate the application of the superstructures presented in this thesis to the optimum use of multiple utilities. The network structure of the newly developed superstructures with the lowest TAC will be shown in the two multiple utilities examples being presented.

5.1.2 Multiple Utility Examples

Example 6. (Shenoy *et al*., 1998)

This problem was presented by Shenoy *et al*. (1998) to demonstrate the concept of the cheapest utility principle (CUP). It involves a system that comprises two hot streams and one cold stream. The process uses three hot utilities (steam) at different levels namely: low pressure, medium pressure and high pressure steam (LP, MP and HP) and cooling water (CW). Shenoy *et al*. applied the CUP technique, which is essentially a targeting (pinch) methodology using a fixed ΔTmin to determine the optimum load for multiple utilities with cost traded off through the energy and capital requirements in a typical HEN. In the solution, Shenoy *et al*. started with the hottest hot utility (HP) which is the most expensive utility and gradually replaced it with MP and LP for the minimisation of the total annual cost (TAC). The stream and cost data for the problem are presented in Table A6 of Appendix A while their CUP optimisation solutions are presented in Table 5.1. This problem has been solved by Isafiade and Fraser (2008) using the IBMS technique, and by Jose *et al.* (2010) using a stagewise superstructure (SWS) MINLP based approach through a disjunctive formulation. The IBMS solution is presented in Table 5.2 while the SWS based approach of Jose *et al.* (2010) is presented in Table 5.3. The SBS, S&TBS and T&SBS techniques have been applied to this problem and the results are presented in Table 5.4, 5.5 and 5.6 respectively. The SBS optimal network structure (the lowest for Example 6) presented in Figure 5.23 is about 3.7 % and 4.8% higher than the network structure of Shenoy *et al*. (1998) and Isafiade and Fraser (2008a) respectively. The combinations of the three hot utilities together with the one cold utility produced the minimum TAC in the CUP technique of Shenoy *et al*. (1998). If the load of 1 kW is eliminated in the solutions of interval based techniques, then, the combinations of two hot utilities together with the one cold utility produced the minimum TAC in all the interval based techniques (IBMS, SWS, SBS, S&TBS and T&SBS) that were applied to this problem.

Table 5.1: Utility Load Distribution for Example 6 for different combinations of hot utilities using CUP, as presented by Shenoy *et al*. (1998)

Options	Cold utility load (KW)	HPS Load (KW)	MPS Load (KW)	LPS Load (KW)	N	TAC target (£/yr)	TAC design (£/yr)
1 (3 HU)	725.5	203	53	119.5	9	96,412	98,263
2 (2 HU)	725.5	240	-	135.5	7	96,839	98,699
3 (1 HU)	664	314	-	-	5	100,965	105,027

Table 5.2: Utility Load Distribution for Example 6 for different combinations of hot utilities using IBMS, as presented by Isafiade and Fraser (2008)

Options	Cold Utility Load (KW)	HPS Load (KW)	MPS Load (KW)	LPS Load (KW)	N	TAC design (£/yr)
1 (3 HU)	694.27	256.56	86.71	1	7	100,954
2 (3 HU)	739.34	244.61	1	143.72	9	97,211
3 (2 HU)	693.65	256.55	87.10	-	6	100,942
4 (2 HU)	743.70	252.71	-	140.99	7	98,845
5 (1 HU)	675.45	325.45	-		5	102,396

Table 5.3: Utility Load Distribution for Example 6 for different combinations of hot utilities as presented by Jose *et al.* (2010)

Option	Cold Utility Load (KW)	HPS Load (KW)	MPS Load (KW)	LPS Load (KW)	N	TAC design (£/yr)
1(2 HU)	740	238.7	0	151.3	7	97,079

Table 5.4: Utility Load Distribution for Example 6 for different combinations of hot utilities using SBS

Options	Cold Utility Load (KW)	HPS Load (KW)	MPS Load (KW)	LPS Load (KW)	N	TAC design (£/yr)
1 (3HU)	690.76	267.96	71.79	1	7	101,897
2 (2HU)	676.20	325.10	-	1	6	102,403
3 (2HU)	690.15	268.06	72.09	-	6	101,889
4 (1HU)	675.50	325.50	-	-	5	102,403

Table 5.5: Utility Load Distribution for Example 6 for different combinations of hot utilities using S&TBS

Options	Cold Utility Load (KW)	HPS Load (KW)	MPS Load (KW)	LPS Load (KW)	N	TAC design (£/yr)
1 (3HU)	676.79	324.79	1	1	7	102,462
2 (2HU)	690.15	268.06	72.1	-	6	101,889
3 (2HU)	676.34	325.34	-	1	6	102,431
4 (1HU)	675.49	325.49	-	-	5	102,402

Table 5.6: Utility Load Distribution for Example 6 for different combinations of hot utilities using the T&SBS

Options	Cold Utility Load (KW)	HPS Load (KW)	MPS Load (KW)	LPS Load (KW)	N	TAC design (£/yr)
1 (3HU)	690.71	267.93	71.78	1	7	101,893
2 (2HU)	710.98	240.29	120.61	-	6	110,451
3 (2HU)	800	429.67	-	20.33	5	119,557
4 (1HU)	800	450	-	-	3	120,078

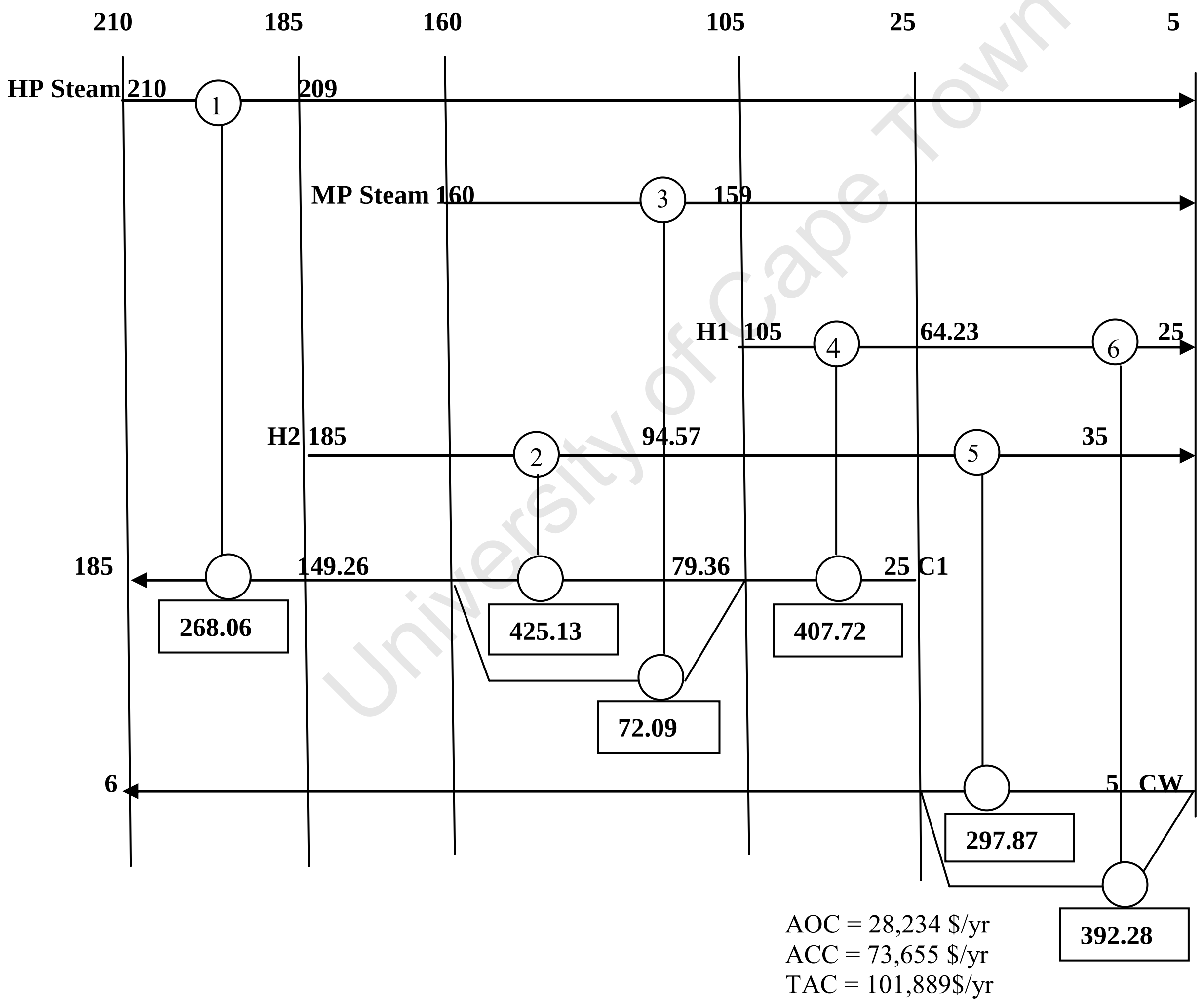


Figure 5.23: SBS Optimal structure for Example 6 featuring TAC of £101,889 /yr

<u>Example 7. (Shenoy *et al*., 1998)</u>

Another problem from Shenoy *et al.* (1998), involves two hot streams and three cold streams along with three hot utilities: steam levels low pressure, medium pressure and high pressure steam (LP, MP and HP) and two cold utilities, cooling water (CW) and air cooling (AC). Shenoy *et al*. used the CUP technique in a manner similar to Example 6 above to determine the optimal use of utility for this system. The stream and cost data for this problem are shown in Table A7 of Appendix A while the CUP optimisation results of Shenoy *et al.* are shown in Table 5.7. This problem was also solved with the IBMS technique of Isafiade and Fraser (2008a) and the SWS based model of Jose *et al.,* (2010). The solutions of the IBMS and the SWS are presented in Tables 5.8 and 5.9 respectively. The SBS, S&TBS and the T&SBS have also been applied to this problem and the results are shown in Tables 5.10, 5.11 and 5.12 respectively. The SBS optimal network structure is shown in Figure 5.24 which is just about 0.3% higher than the network structure of Jose *et al.,* but lower than the CUP of Shenoy *et al*. and the IBMS of Isafiade (2008) by about 3% and 2.2% respectively. All the techniques use combinations of two hot utilities (HPS and MPS) to obtain their lowest TACs except the IBMS that used 1kW of LPS along with the HPS and MPS. The technique of Jose *et al*. works well for multiple utility problems but it is yet to be applied to those involving single utility. The techniques presented in this thesis can, however, serve as alternatives.

Table 5.7: Utility Load Distribution for Example 7 for different combinations of hot utilities as presented by Shenoy *et al*. (1998)

Options	HPS load (KW)	MPS Load (KW)	LPS Load (KW)	CW Load (KW)	Air C Load (KW)	N	TAC target ($/yr)	TAC design ($/yr)
1(3HU,1CU)	1600	6860	-	7760	-	11	1130.34	1182.94
2 (2HU,1CU)	1600	6860	-	7760	-	11	1130.34	1212.69
3 (2HU,2CU)	4885	3575	-	3600	4160	9	1130.34	1158.50
4(2HU,2CU)	2730	5730	-	3600	4160	9	1130.34	1163.14

Table 5.8: Utility Load Distribution for Example 7 for different combinations of hot utilities as presented by Isafiade and Fraser (2008)

Options	HPS Load (KW)	MPS Load (KW)	LPS Load (KW)	CW Load (KW)	AC Load (KW)	N	TAC design ($/yr)
1(3HU,2CU)	4298.5	4033.4	1	714.85	19.38	10	1135.89
2(3HU,2CU)	6096.74	2089.1	1	707.87	16.32	9	1153.11
3(2HU,2CU)	6027.75	1977.6	-	707.33	9.28	8	1154.63
4(2HU,1CU)	5928.5	1852	-	708.7	-	7	1150.46

Table 5.9: Utility Load Distribution for Example 7 for different combinations of hot utilities as presented by Jose *et al*. (2010)

Option	HPS Load (KW)	MPS Load (KW)	LPS Load (KW)	CW Load (KW)	AC Load	N	TAC design ($/yr)
1(2 HU)	4290	4075.3	-	7665.3	-	8	1,121,175

Table 5.10: Utility Load Distribution for Example 7 for different combinations of hot utilities using SBS

Options	HPS Load (KW)	MPS Load (KW)	LPS Load (KW)	CW Load (KW)	AC Load (KW)	N	TAC design ($/yr)
1(3HU,2CU)	9302	75.96	1	2177	6503	8	1260315
2(3HU,2CU)	7787.3	-	1	7063.3	25	9	1191188
3(2HU,2CU)	4228.71	4098	-	7078.7	548.03	8	1125417
4(2HU,1CU)	6007.77	1770.9	-	7078.7	-	7	1150303

Table 5.11: Utility Load Distribution for Example 7 for different combinations of hot utilities using S&TBS

Options	HPS Load (KW)	MPS Load (KW)	LPS Load (KW)	CW Load (KW)	AC Load (KW)	N	TAC design ($/yr)
1(3HU,2CU)	4566.35	4098.21	1	7416.35	549.21	9	1193256
2(3HU,2CU)	1	11319.57	-	5427.6	5192.96	8	1215323
3(2HU,2CU)	9327.72	-	3972	6586.56	6013.44	7	1294549
4(2HU,1CU)	5926.2	1852	-	7078.65	-	7	1150436

Table 5.12: Utility Load Distribution for Example 7 for different combinations of hot utilities using the T&SBS

Options	HPS Load (KW)	MPS Load (KW)	LPS Load (KW)	CW Load (KW)	AC Load (KW)	N	TAC design ($/yr)
1(3HU,2CU)	2547.7	9167.5	1	5709	5306.68	9	1248063
2(2HU,2CU)	6264.35	1852	-	7391.83	25	8	1226806
3(2HU,2CU)	9302.6	-	284	2384	6502	7	1259939
4(2HU,1CU)	3300	10000	-	12600	-	6	1341815

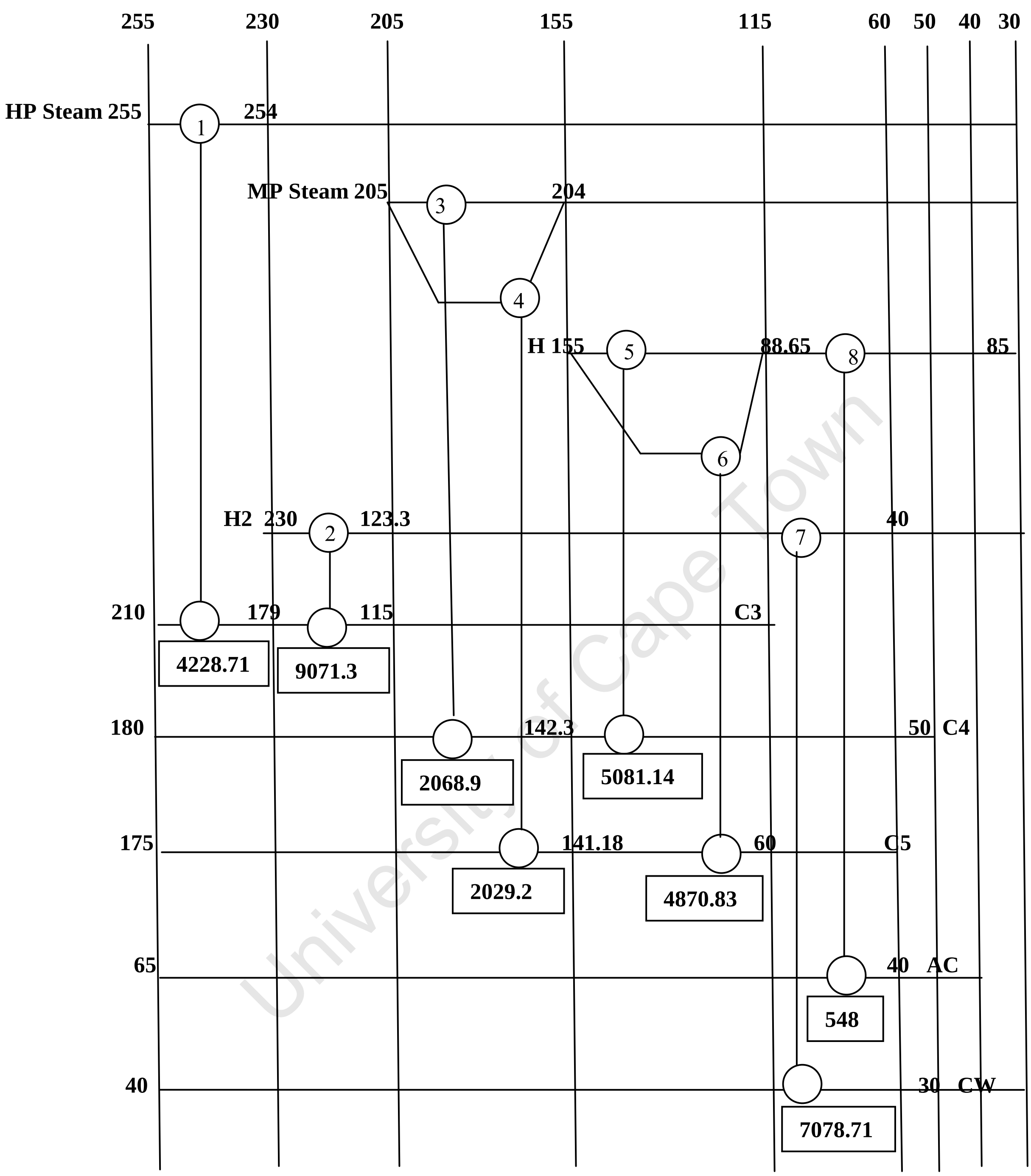


Figure 5.24: The Optimal SBS Network structure for Example 7 featuring TAC of $1,125,417/yr

AOC = $574,441 /yr
ACC = $550,976 /yr
TAC = $1,125,417/yr

5.2 MENS EXAMPLES

Example 8: (Ammonia removal Hallale, 1998)

This example would be used to demonstrate the capability of SBS, S&TBS and T&SBS to solve MEN problems involving continuous contact exchangers. It is taken from Hallale (1998), andit has been solved by other researchers (Emhamed *et al*., 2007; Szitkai *et al*, 2006; Isafiade & Fraser, 2008). Hallale did not present an optimal TAC solution for this problem unlike Szitkai *et al*.). It is a problem where ammonia is to be removed from five gaseous streams (composed mainly of air). Two process MSAs, S1 and S2, along with an external MSA, S3, are available for the removal. The exchangers for this removal are all packed column mass exchangers. The problem data are given in Table B1 of Appendix B. The capital costing method based on exchanger mass presented by Hallale (1998) is adopted for the column costing to enable comparison with previous workers.

The network structures of Szitkai *et al*. (2006) and Isafiade and Fraser (2008b) are shown in Figures 5.25 and 5.26 with TACs of \$134,000/yr and \$133,323/yr respectively. The solution of Szitkai *et al*. (2006) has eight units but did not specify the number of intervals used for this problem, the IBMS features seven units with five intervals.

The solution obtained using the SBS has a superstructure with six intervals and a TAC of \$129,901/yr as shown in Figure 5.27. The two types of S&TBS feature six intervals each in their superstructure and the networks structures are shown in Figure 5.28 for Type 1 (TAC of \$132,372/yr) and Figure 5.29 for Type 2 (TAC 132,331\$/yr) respectively. The T&SBS produced a TAC of \$131,524/yr with a superstructure having five intervals (shown in Figure 5.30). Type 1 and Type 2 of S&TBS and T&SBS have nine units each in their networks. The network structures of Szitkai *et al*, (2006) the IBMS and the Type 2 of S&TBS have one 3 way split of S3 while the SBS has two 2 ways splits of S3. The Type 1 of S&TBS has one 4 ways split of S3 while the T&SBS has two 2 ways splits each of S1 and S3. The IBMS has two intervals that are not used for matching at its extreme ends while the SBS and the T&SBS have one redundant interval each. The two S&TBS have three intervals that are not used for matching at their extreme ends.

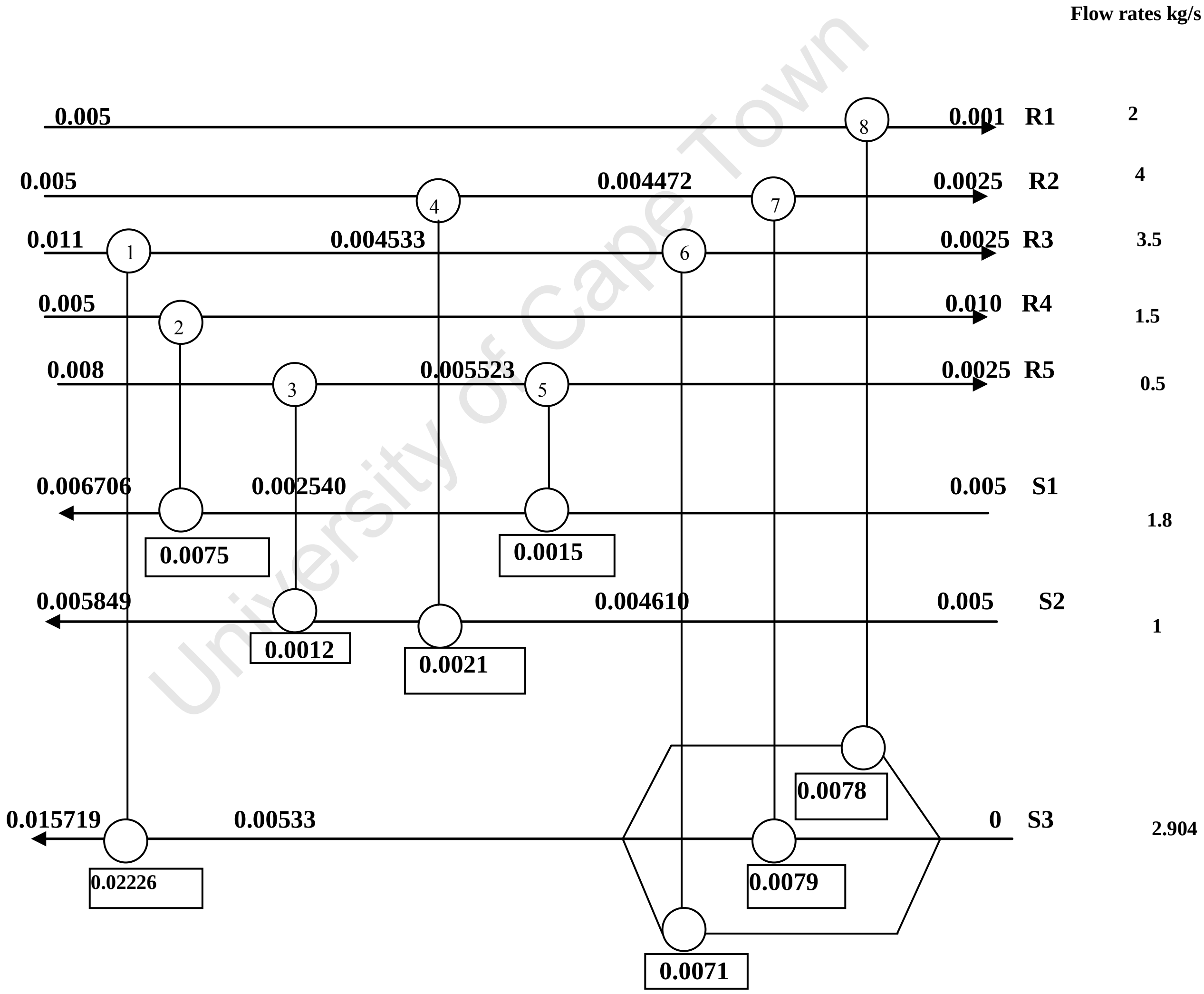
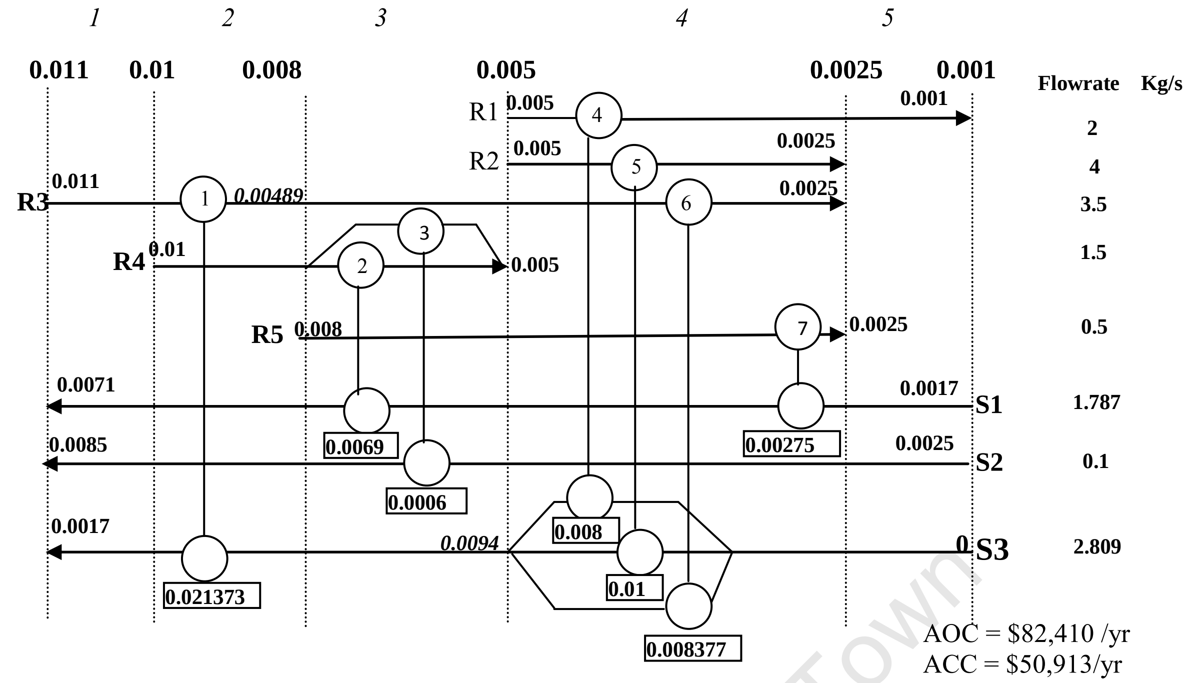
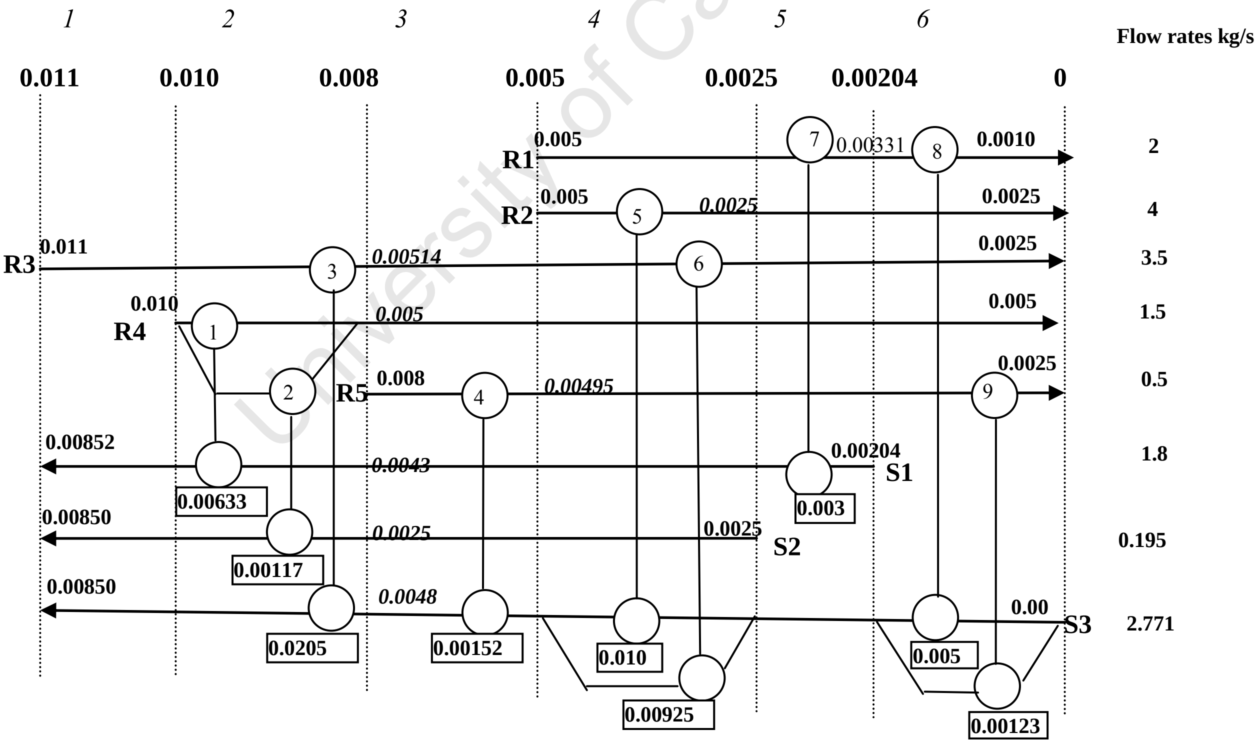


Figure 5.25: Network structure of ‘SWS’ of Szitkai *et al*. (2006) for Example 8 featuring eight units with a TAC = $134,000/year



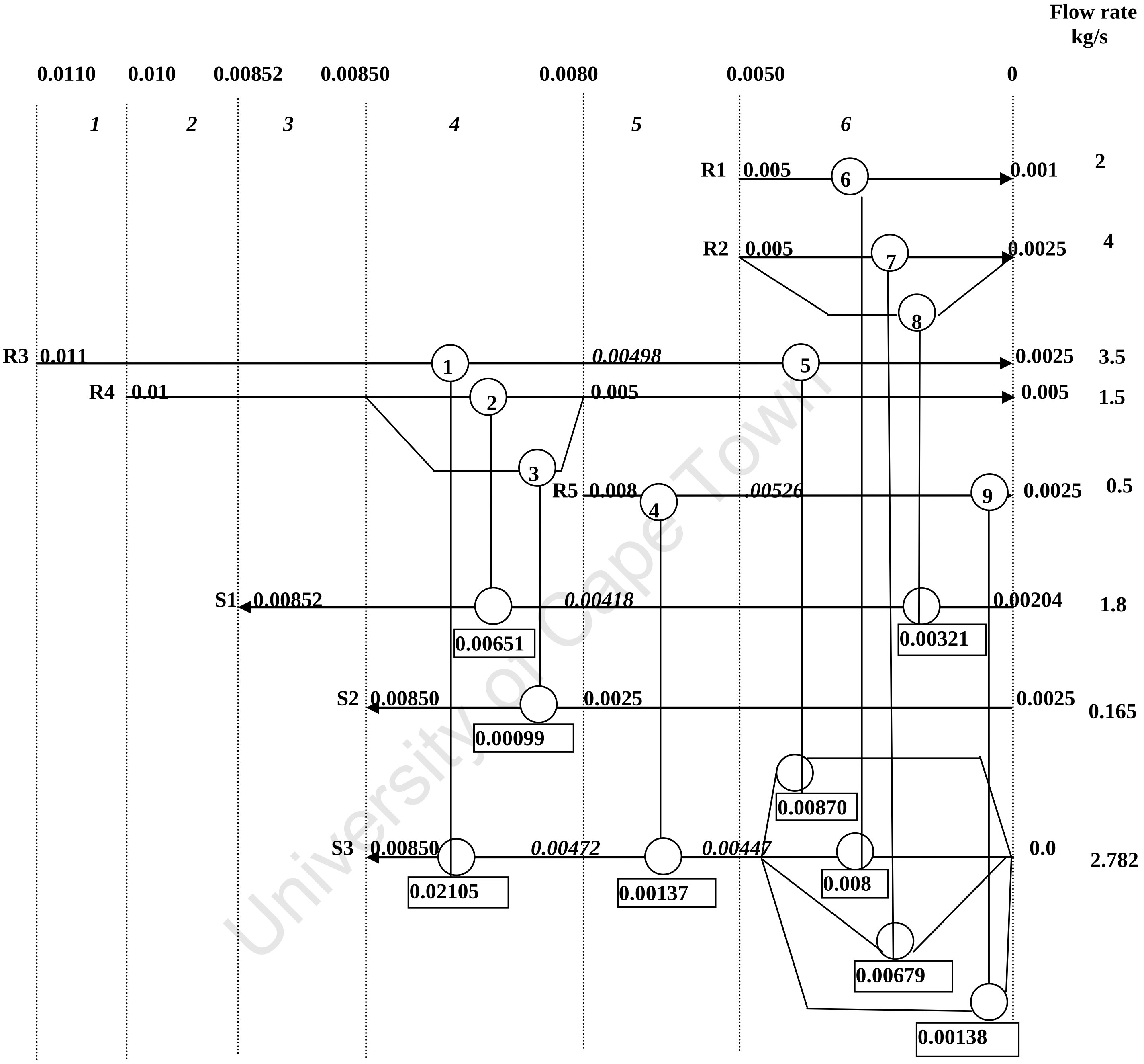
AOC = $82,410 /yr
ACC = $50,913/yr
TAC = $133,323 /yr

Figure 5.26: IBMS network structure for Example 8 featuring seven units with a 2-way split for a rich stream and a 3-way split for a lean stream with TAC of $133,323/yr



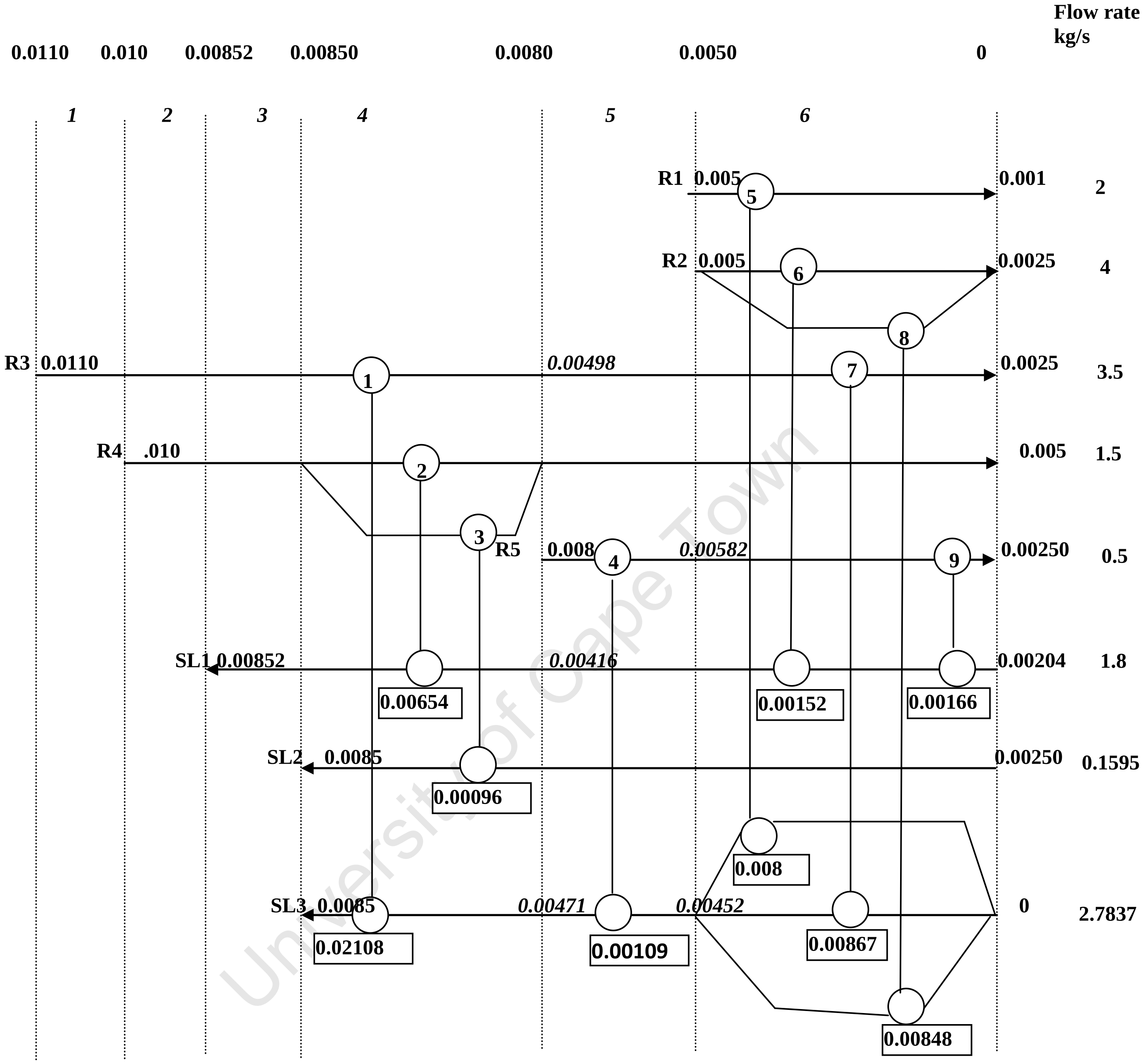
AOC = $81,301 /yr
ACC = $48,600 /yr
TAC = $129,901 /yr

Figure 5.27: Network structure for Example 8 of SBS featuring nine units with a split of a rich stream and two separate 2 way splits of a lean stream with a TAC of $129,901/yr



AOC =$ 81,624 /yr
ACC = $50,748 /yr
TAC = $132,372/yr

Figure 5.28: The S&TBS (Type 1) network structure of Example 8 featuring nine units with a TAC of $132,372/yr



AOC = $81,653 /yr
ACC = $50,678 /yr
TAC = $132,331/yr

Figure 5.29: The S&TBS (Type 2) network structure of Example 8 featuring nine units with a TAC of $132,331/yr

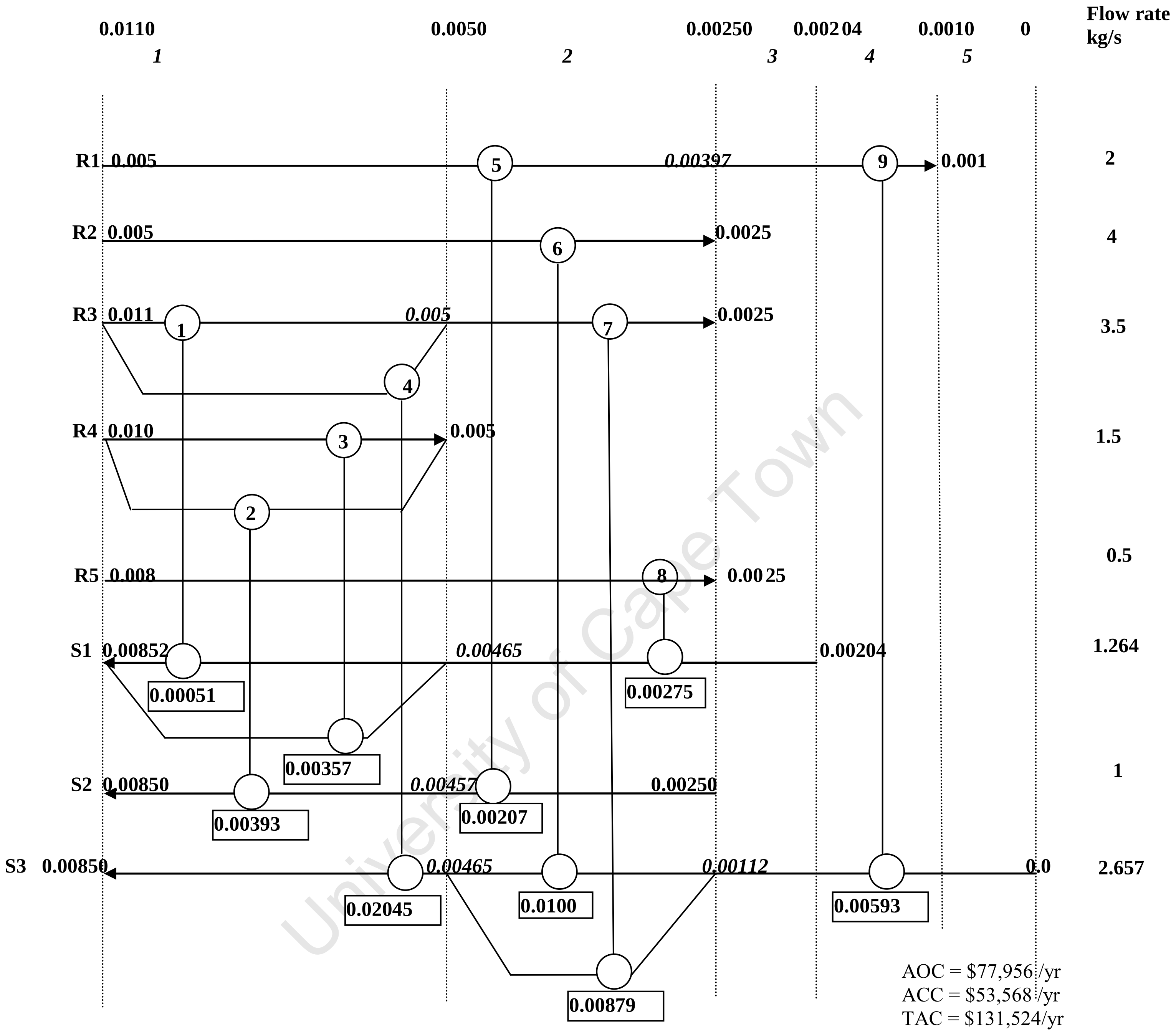


Figure 5.30: The T&SBS network structure of Example 8 featuring nine units with a TAC of $131,524/yr

Example 9: Dephenolisation of aqueous wastes (El-Halwagi, 1997)

This example, where phenols are to be absorbed from two aqueous streams, R1 and R2 using solvent extraction, is taken from El-Halwagi (1997). The process lean streams available (free) for this removal are gas oil (S1) and lube oil (S2) along with an external lean stream (not free), light oil (S3). The whole gas oil stream S1 was specified to be used up. The mass exchangers are sieve tray columns and the capital cost data of Papalexandri *et al*. (1994) which specified $4552 per year per equilibrium stage was used. Problem specifications for the problem can be found in Table B2 of Appendix B.

Workers that have solved this problem for TAC optimisation include Hallale & Fraser, 2000a; Comeaux, 2000; and Isafiade & Fraser, 2008b. The network structures obtained by Comeaux (2000) and first option of the lean based IBMS of Isafiade and Fraser (2008b) with TACs $333,300/yr and $338,168 /yr are shown in Figures 5.31 and 5.32 respectively. The insight based solution of Commeaux (2000) features seven units while the lean based IBMS features six. Note that the IBMS network structure and the SBS network structure are the same, but with different mass loads, and were generated by a different number of intervals.

This problem has been solved using the SBS, S&TBS and T&SBS of this study. The SBS and Type 2 of S&TBS obtained TACs of $339,579/yr and $421,147/yr as shown in their network structures in Figures 5.33 and 5.34 respectively. The SBS has six units while Type 2 of the S&TBS has five. No solution to this problem could be found with the S&TBS (Type 1) and the T&SBS techniques.

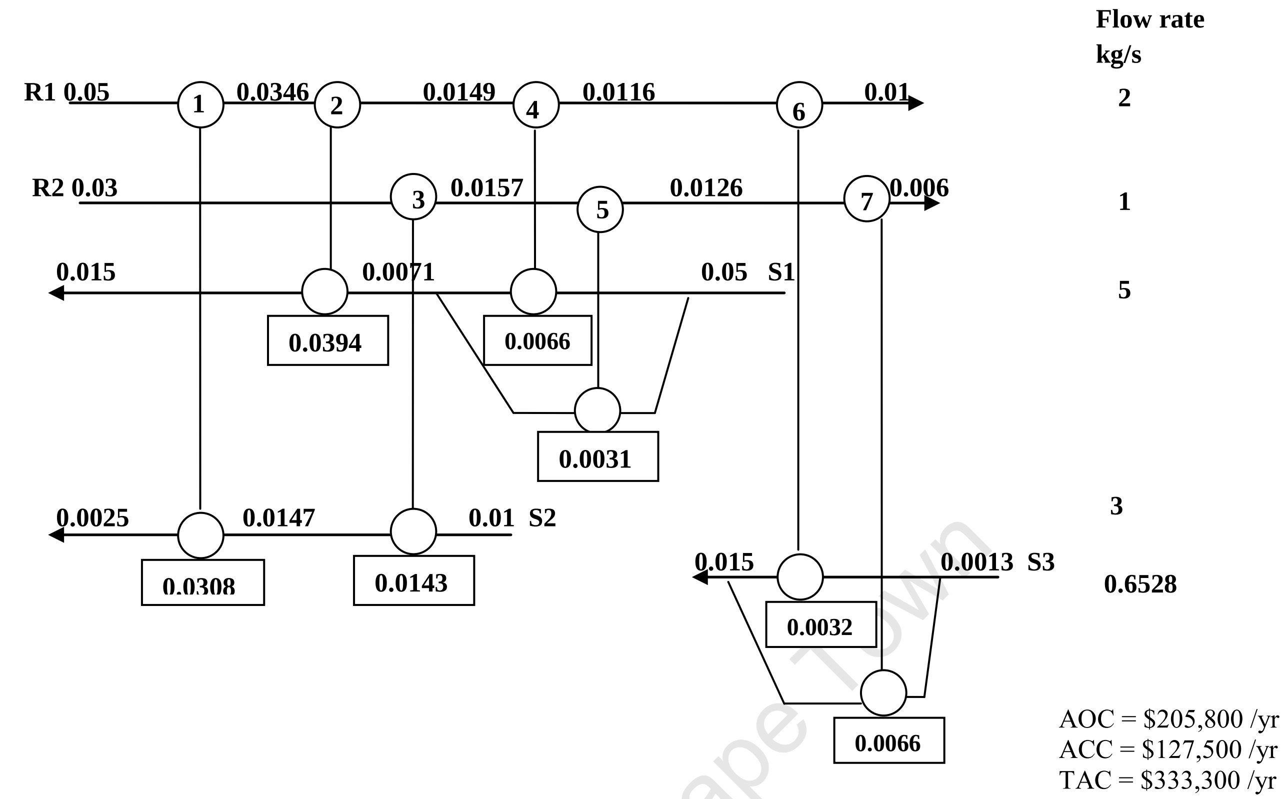


Figure 5.31: Insight based Superstructure of Comeaux (2000) for Example 9 featuring a TAC of $333,300/yr

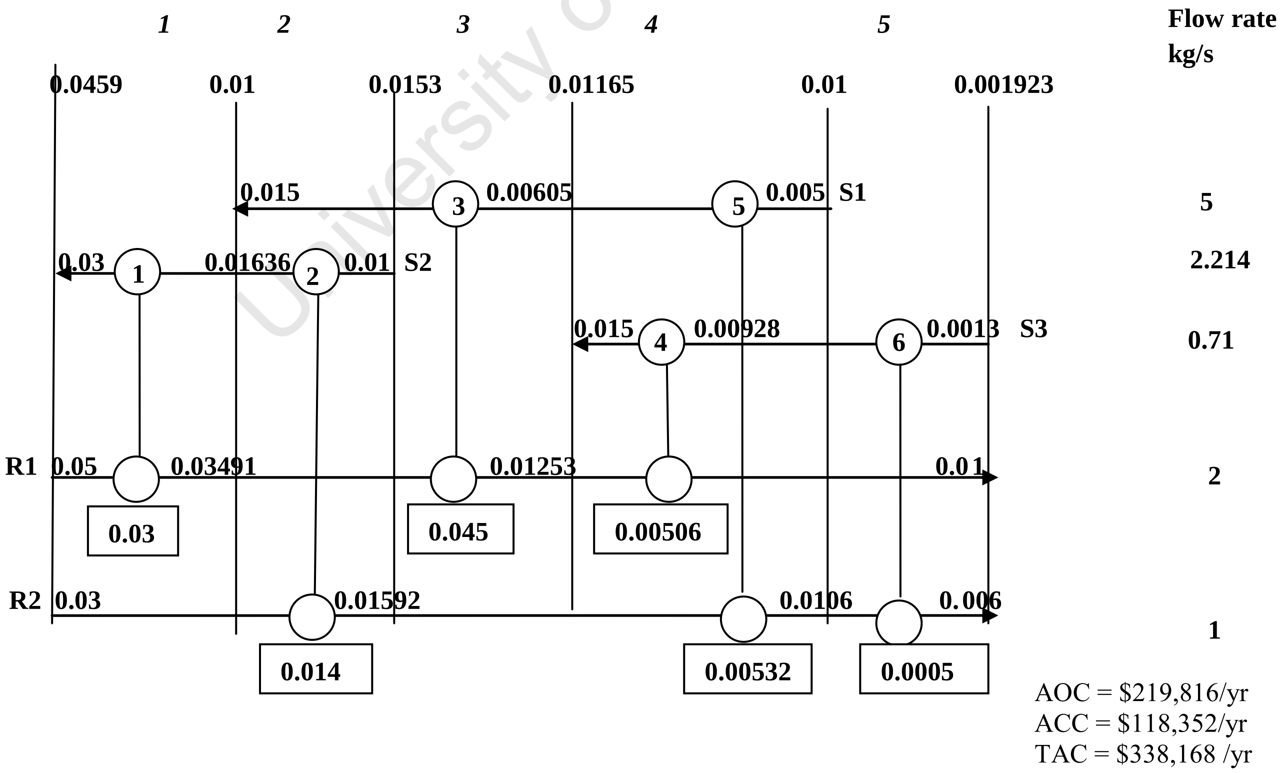


Figure 5.32: Lean based IBMS superstructure of Isafiade and Fraser (2008b) for Example 9 featuring a TAC of $338,168/yr

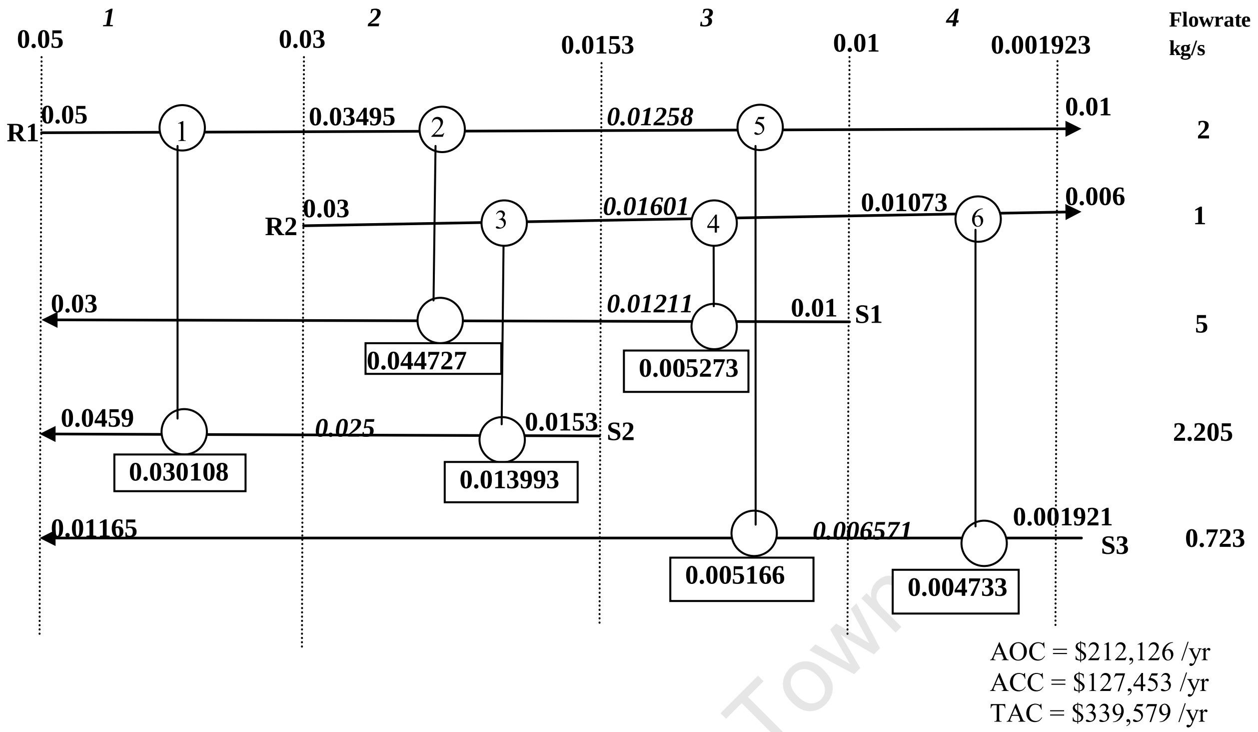


Figure 5.33: SBS network for Example 9 featuring six units with a TAC of $339,579/yr

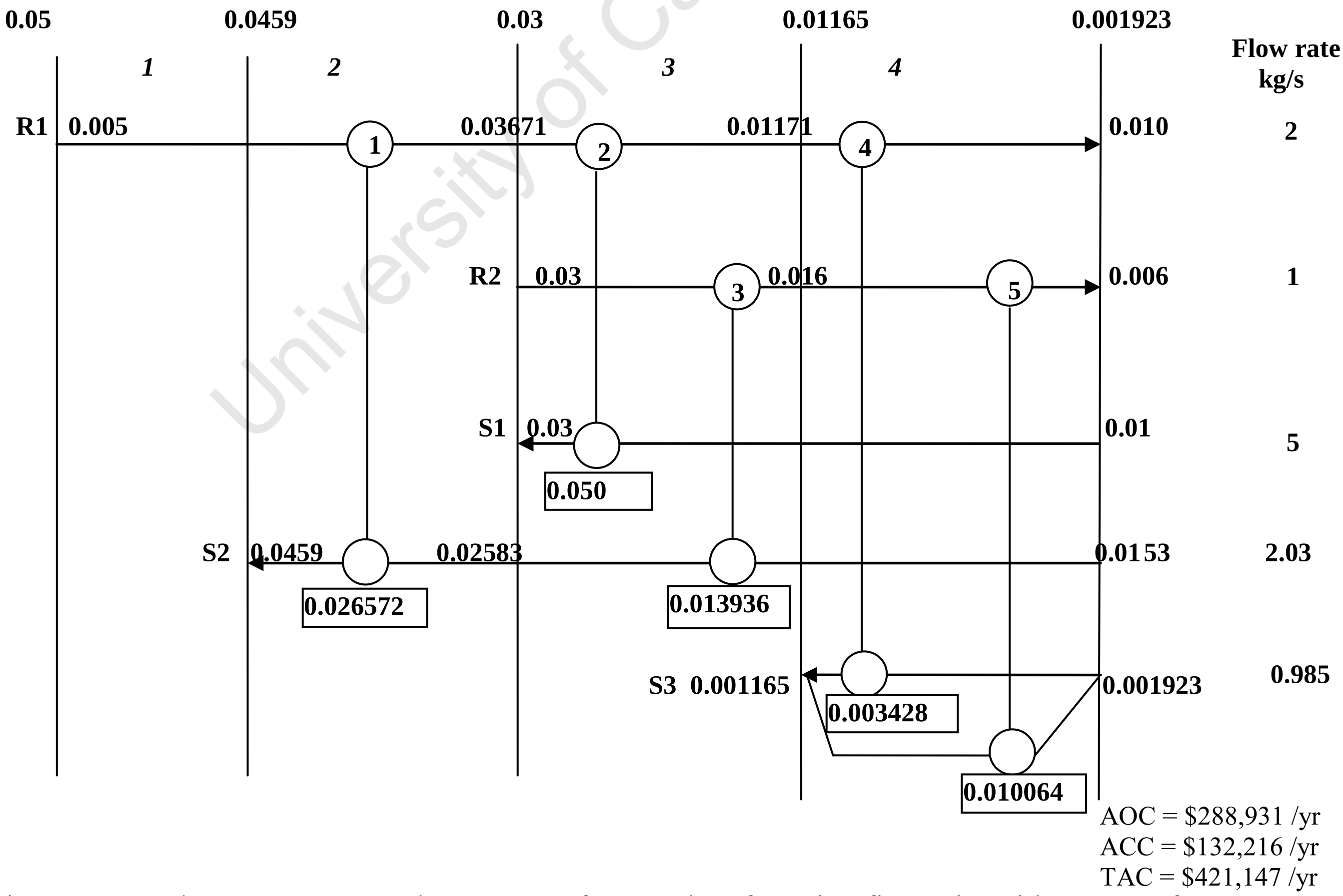


Figure 5.34: The S&TBS network structure of Example 9 featuring five units with a TAC of $421,147/yr

Example 10: Coke oven gas problem (El-Halwagi and Manousiouthakis, 1989)

This MEN problem was taken from El-Halwagi and Manousiouthakis (1989). It involves the removal of hydrogen sulphide and carbon dioxide from two rich streams (coke-oven gas, R1, and tail gas from a Claus unit, R2). One process lean stream (aqueous ammonia), S1, and one external lean stream (chilled methanol), S2, are available for this removal. Compatible targets for this example were established by El-Halwagi and Manousiouthakis (1990) while Hallale and Fraser (2000c) pointed out that H_2S controls the lean stream flow rate and the number of stages in the exchanger, consequently, this problem can be solved as though H_2S were the only transferred component. Others workers who included the CO_2 removal along with H_2S and treated this problem as a multicomponent problem generated the same MEN as that found by El-Halwagi and Manousiouthakis (Papalexandri *et. al*., 1994, Chen and Hung, 2005). The problem specifications are shown in Table B3 of Appendix B.

The SWS of Chen and Hung (2005) obtained a TAC of \$429,700/year with four units. The lean based IBMS of Isafiade (2008) features a TAC of \$446,840/yr with four units while the rich based features a TAC of \$530,471/yr with four units. The application of SBS to this problem produces a TAC of 469,968\$/yr and the network structure with five units is presented in Figure 5.35. The network structures for the two types of S&TBS and T&SBS solutions are basically the same as presented in Figure 5.36 with four units, even though the TAC for T&SBS of \$526,471/yr is slightly higher than those for S&TBS (Type 1 and Type 2) which is \$524,244.

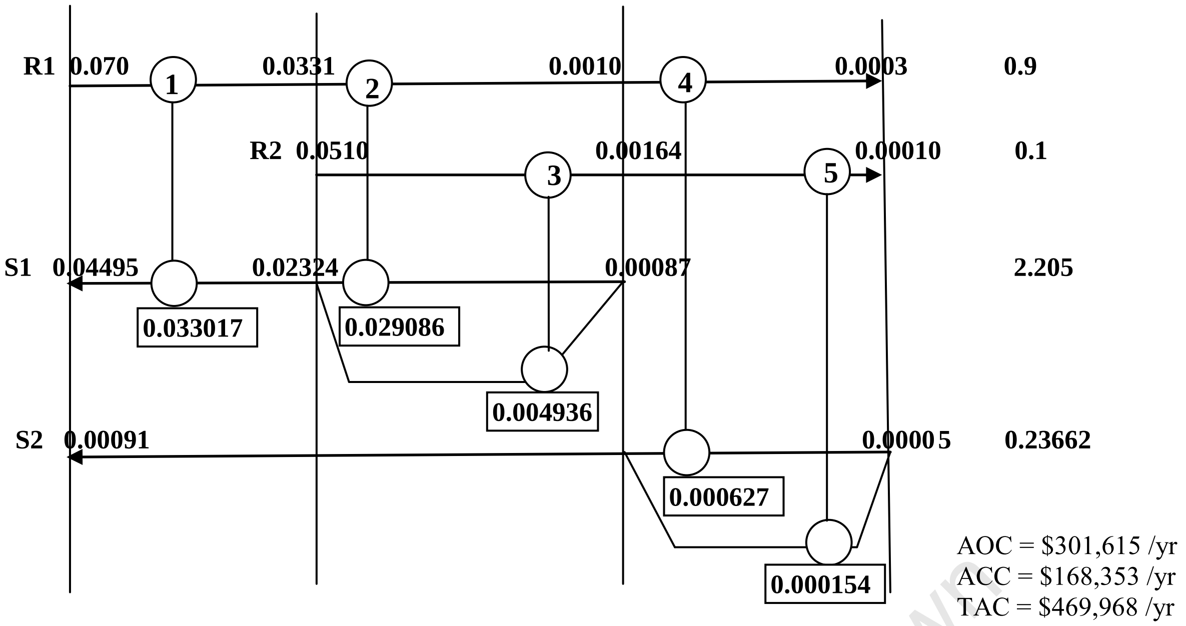


Figure 5.35: The SBS network for Example 10 with TAC of $469,968 /yr

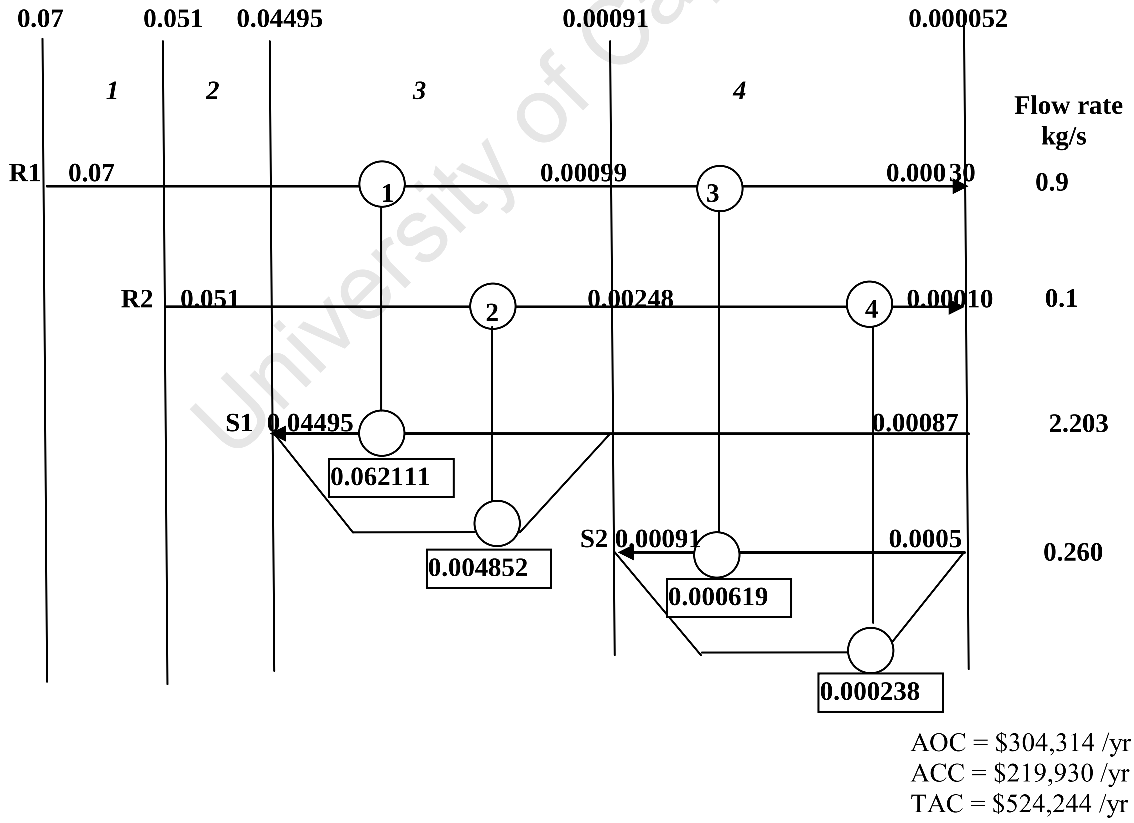


Figure 5.36: The S&TBS (Type 1 and Type 2) network structure for Example 10 featuring four units with TAC of $524,244/yr

Example 11: Dephenolization of coal conversion waste (Papalexandri *et. al*., 1994)

This problem entails simultaneous mass exchange and regeneration of one of the MSAs. In this problem, phenol is to be removed from four aqueous streams, R1 to R4. Two MSAs are available for phenol removal, the first one is light oil, (S1) which is used on a once-through basis, and the second one is activated carbon, (S2), this is regenerated using caustic soda, H1, as the regenerant in a stripping process, and then recycled for re use. The supply and target compositions of the regenerable MSA, and are unknown, and have to be determined in the MENS task, but the supply and target compositions of S1 and the regenerating agent Z are given. The problem specifications are shown in Table B4 of Appendix B. Note that the cost shown in Table B4 for S2 refers to the actual usage of the stream and not the circulating flow, but different workers have not been using this value because a ratio of make-up flow to circulating flow has not been specified.

The SWS of Chen and Huang (2005) obtained a TAC of $694,000/yr with seven units for this problem. The SWS of Szitkai (2003) and the IBMS of Isafiade and Fraser (2008) obtained TACs of $720,000/yr and $689,300/yr respectively for this problem. Szitkai (2004) did not state the number of units while the IBMS features eight units.

The result of the application of SBS to this problem produced a TAC of $693,976/year with eight units. The network structure is shown in Figure 5.38. No solution to this problem could be found using the S&TBS and T&SBS techniques.

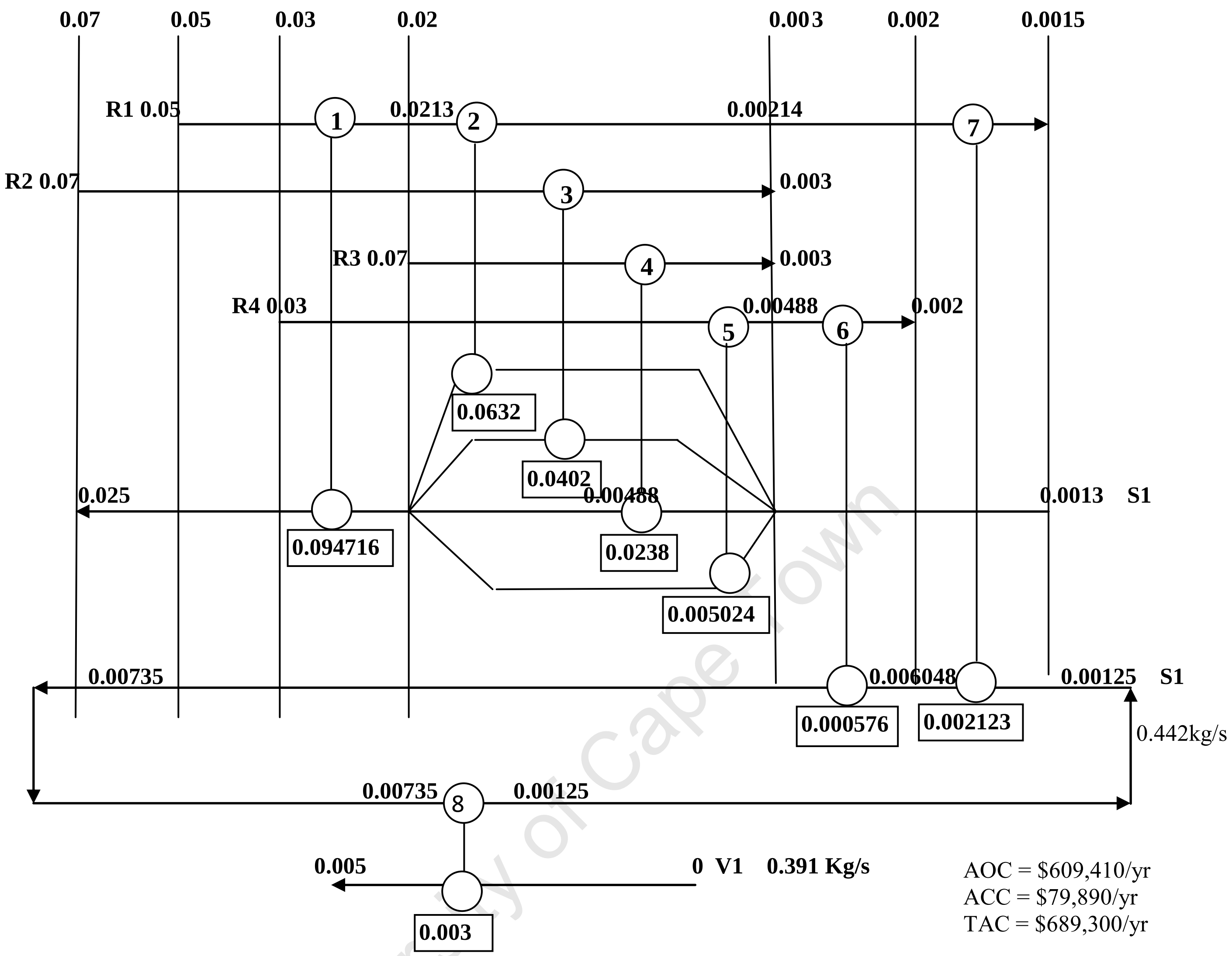


Figure 5.37: IBMS network structure for Example 9 featuring 8 units with a TAC of $698,300/yr

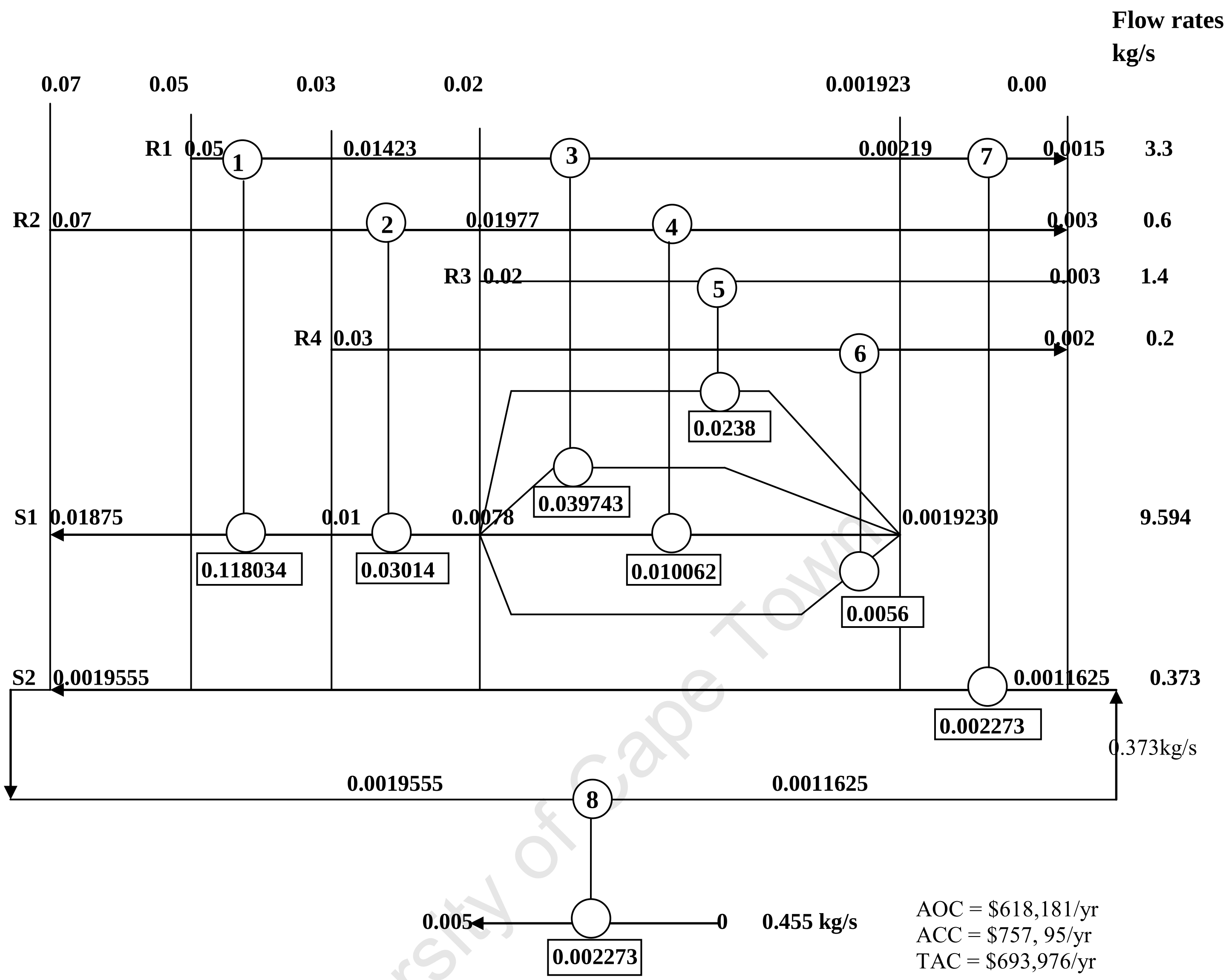


Figure 5.38: SBS network structure for Example 9 featuring 8 units with a TAC of 693,976 $/yr

5.3 FEATURES OF THE NEW SUPERSTRUCTURES

The superstructures presented in this thesis have the following features:

- Since the utilities in HENS are treated as process streams and the external lean streams in MENS are treated as process lean streams in those superstructures, there is the advantage of simultaneous consideration of the process and utility streams in HENS as well as process and external lean streams in MENS.

- The isothermal mixing assumptions at the interval boundary junctions of these superstructures eliminates the need for non linear heat/mass balances in the superstructure models. This is, however, similar to the SWS technique and its derivatives.
- The introduction of additional intervals in those superstructures allows for more combinations of stream matches in the networks, similar to spaghetti design, as pointed out by Shenoy (1995). In spaghetti designs, the numbers of stages are necessarily equal to the number of enthalpy intervals, whereas, in SWS, that was originally conceived to be similar to the spaghetti design, much smaller numbers of intervals were used.
- Different utilities in HENS at different temperature levels and cost as well as different external MSA in MENS at different composition levels and costs are simultaneously considered in the respective HEN and MEN superstructures. This is an advantage over the pinch technique whose original concept did not account for TACs in HENS involving multiple utilities and in MENS involving multiple external MSAs.
- The superstructures are able to achieve simultaneous minimization of TACs in various HENS and MENS tasks.

5.4 CONCLUSION AND SUMMARY

The superstructures presented in this study have been applied to eleven HEN and MEN literature problems as presented by various researchers. This shows that the SBS, S&TBS and T&SBS are able to solve HEN problems including those of forbidden/restricted matches, HEN problems with significantly different heat transfer coefficient and those involving multiple utilities. The superstructures have also been shown to be able to solve MENs problems with continuous contact columns, those involving stagewise columns and MENs problem involving the regeneration of an MSA.

However, solutions to two of the stagewise column MEN problems presented could not be obtained with either the S&TBS or T&SBS. This could be due to an increase in non linearity because of the presence of the modified Kremser equation in the model. The solutions to all MEN problems were, nevertheless, obtained with the SBS technique.

The superstructures presented in this study have the potential to create a relatively larger number of intervals for HENS and MENS. This can be seen in Examples presented where one or more of the newly presented superstructures provided the highest number of intervals in nine out of eleven examples solved. These nine are those examples where solutions can be obtained using all the three techniques presented. Larger numbers of intervals provide more opportunity for matches between streams (Shenoy, 1995), compared to the SWS where the number of stages is determined by the number of hot or cold streams present. The superstructures presented also give more freedom for heat/mass exchange between a stream and its opposite kind in the intervals created. The examples solved with the SBS, S&TBS

and the T&SBS have solutions that are within the range of previous results as obtained by different sets of researchers that have presented interval based superstructures for HENS and MENS, with easy initialization, and solutions that were found quickly.

The features of the new superstructures have also been presented.

CHAPTER SIX

DISCUSSION AND COMPARISON OF RESULTS

CHAPTER SIX: DISCUSSION AND COMPARISON OF RESULTS

This chapter presents the discussion and comparison of results obtained over all the examples solved in this thesis with those of all other researchers that have presented solutions for the problems solved. The first part of the discussion will be the presentations of tables where all the examples solved in Chapter 5 are arranged in descending order of TAC and their percentage differences. These tables will compare some network characteristics peculiar to each example such as number of units, stream splits and TACs obtained in the present study with those of previous researchers. A table that compares the results presented in all these tables will then be presented to see how each technique performs over all the examples solved. Another table that compares the effects of intervals on TAC will be presented. This will then be followed by the general discussion based on these tables and the content of this thesis in the second part.

Example 1: 4SP1 (Lee *et al*., 1970)

Case with no match restriction

Table 6.1 presents the solutions of various researchers to the 4SP1 problem and the network characteristics as obtained by various researchers. The solution of the State Space approach of Bagajewicz *et al*. (1998) obtains the lowest TAC while the two step targeting procedure of Papoulias and Grossmann (1983) obtains the highest TAC for this example. Notice the first three solutions are much higher than the rest while the last four are reasonably close. All other solutions including those presented in this thesis fall in between these two TAC ranges with the S&TBS (Type 1) of the methods presented in this thesis higher than the lowest by 1.95%.

Table 6.1: Comparison of results for Example 1

Method	ΔT_{min}(°F)	Stream Splits	No of units	Cost ($/year)	Percentage Difference (%)
Two step targeting procedure of Papoulias and Grossman (1983)	50	0	5	13,590[1]	28.45
Evolutionary development method of Linnhoff and Flower (1978)	-	0	5	13,587	28.42
Branch and Bound Method of Lee, *et al*. (1970)	18	0	5	13,481	27.42
T&SBS	0.5	2	5	11,204	5.90
S&TBS (Type 2)	1.6	1	5	10,795	2.03
SBS	1.9	1	5	10,794	2.02
S&TBS (Type 1)	0.9	1	5	10,786	1.95
DEM of Krishna and Murty (2007)	2.1	0	5	10,782	1.91
Mathematical Optimization Technique of Grossman and Sargent (1978)	1	0	5	10,592	0.11
State space approach of Bagajewicz *et al*. (1998)	-	0	5	10,580	0.00

Case with match restriction

This case forbids any match between H1 and C1 as stated in Chapter 5 where the solutions were presented. Some workers incorporated cold-cold matching in their networks as shown in Table 6.2, although this option does not appear to be used in industry. Table 6.2 compares the results obtained by various workers: it may be noted that allowing for cold-cold matching yields much better solutions, and there is a large discrepancy without it.

Table 6.2: Comparison of results for Example 1 with match restriction

Method	Cold-cold matching?	TAC ($/year)	Percent Difference (%)
S&TBS (Type1)	No	33,243	140.9
T&SBS	No	31,243	126.4
Two step targeting procedure of Papoulias and Grossman (1983)	No	21,100	52.9
SBS	No	20,019	45.1
S&TBS (Type 2)	No	18,710	35.6
DEM of Krishna and Murty (2007)	No	18,705	35.5
SWS of Yee and Grossman (1990)	Yes	13,800	0.0
Simulated Annealing of Dolan, *et al.* (1987)	Yes	13,800	0.0

<u>Example 2: 4S1 (Shenoy, 1995).</u>

Table 6.2 presents the comparison of this example, where the method of SWS as presented by Shenoy (1995) obtains the lowest TAC, while the T&SBS features the highest. All the methods feature the same number of units, the SWS has two intervals for this problem while all other techniques have five or six intervals. All the TACs obtained by different sets of workers, especially the lowest four, are fairly close to one another. The SWS obtains the lowest TAC. All the solutions produced splits streams but it is possible that solution without split will produce lower overall cost.

Table 6.3: Cost Comparison for Example 2

Method	Stream Splits	No of intervals	No of units	TAC($/year)	Percentage Difference (%)
T&SBS	3	6	6	240,253	2.06
Cold stream based IBMS of Isafiade and Fraser (2008)	3	5	6	239,332	1.67
Hot sream based IBMS of Isafiade and Fraser (2008)	2	5	6	237,800	1.02
SBS	2	5	6	235,931	0.20
S&TBS (Type 1)	2	6	6	235,781	0.16
S&TBS (Type 2)	2	6	6	235,781	0.16
SWS of Yee and Grossman (1990), applied by Shenoy (1995)	2	2	6	235,400	0.00

Example 3: (Linnhoff, et al., 1982)

The SWS of Yee and Grossmann still features the lowest TAC for this example while the S&TBS (Type 1) features the highest cost. The S&TBS (Type 1) though gives five units which is the lowest for the Example. It is not particularly clear the reason why T&SBS gives a much lower TAC than the SBS and S&TBS in this example.

Table 6.4: Cost Comparison for Example 3

Method	Stream Splits	No of units	TAC($/year)	Percentage Difference (%)
S&TBS (Type 1)	1	5	93,391	16.34
S&TBS (Type 2)	1	5	90,672	12.95
SBS	2	7	90,521	12.77
Magnets Solution of Grossman (1985)	-	6	89,832	11.91
Pinch technique of Linnhoff *et al.*(1982)	-	7	89,832	11.91
T&SBS	2	6	87,611	9.13
SWS of Yee and Grossman (1990)	2	5	80,274	0.00

Example 4: (MAGNETS problem)

The Genetic Algorithm of Lewin (1998) obtains the lowest TAC for this problem while the Cold based IBMS of Isafiade and Fraser (2008a) produced the highest TAC. The Genetic Algorithm features a higher number of units than all the interval based techniques, except the S&TBS (Type 2). This shows that a network with lowest number of units does not necessarily translate to the lowest TAC.

Table 6.5: Comparison of results for Example 4

Method	No of intervals	Stream Splits	No of units	Cost ($/year)	Percentage Difference (%)
Cold Stream Based IBMS of Isafiade and Fraser (2008a)	3	1	7	595,064	3.81
T&SBS	6	1	7	581,954	1.53
Hot Stream Based IBMS of Isafiade and Fraser (2008)	7	1	7	581,942	1.52
S&TBS (Type 1)	7	1	7	581,942	1.52
SBS	6	1	8	580,023	1.19
S&TBS (Type 2)	7	1	10	577,602	0.77
SWS of Yee and Grossman (1990)	5	1	7	576,640	0.60
GA of Lewin (1998)	-	2	9	573,205	0.00

Example 5 (Aromatic Plant)

The sequential Match reduction approach of Petersen (2005) produced the lowest TAC for this problem while the DEM of Krishna and Murty (2005), which is a form of GA approach, gave the highest cost. Note that Krishna and Murty's approach provided another solution which falls between the lowest and the highest TAC for this problem. If this is taken into consideration, then the Block Decomposition approach of Zhu *et al*. (1995) will produced the highest TAC for this example. Apart from the network of Petersen (2005), the T&SBS features the lowest TAC for this problem. The networks of Petersen (2005) and the T&SBS that featured the lowest cost for this example have the highest number of units. This again shows that lowest number of exchanger units does not necessarily translate to the lowest TAC in HEN.

Table 6.6: Comparison of results for Example 5

Method	Stream Splits	No of units	Cost (M$/year)	Percentage Difference (%)
DEM of Krishna and Murty, (2007)	2	-	3.146	8.30
Block Decomposition Technique of Zhu *et al*. (1995)	0	10	2.980	2.58
S&TBS (Type 1)	3	13	2.979	2.55
SBS	6	14	2.976	2.44
Linnhoff and Ahmad (1990)	0	13	2.960	1.89
GA of Lewin, (1998)	0	11	2.946	1.41
DEM of Krishna and Murty, (2007)	0	15	2.942	1.27
S&TBS (Type 2)	1	11	2.940	1.21
GA of Lewin (1998)	2	12	2.936	1.07
T&SBS	7	17	2.922	0.59
Sequential Match Reduction approach of Petersen (2005)	7	17	2.905	0.00

Example 6: Multiple Utility 1 (Shenoy, 1998)

The 'SWS' of Jose *et al* (2010) gave the lowest TAC in this example; it is just 0.14% lower than the IBMS of Isafiade and Fraser (2008a) while the T&SBS gives the highest TAC. This shows that the method of Jose et al. (2010) is able to obtain the lowest TAC for multiple utility problems.

Table 6.7: Summary and Comparison of results from Multiple Utility Example 6

Method	Stream Splits	No. of Units	TAC ($/year)	Percentage Difference (%)
T&SBS	1	7	101,893	4.96
S&TBS	2	6	101,889	4.95
SBS	2	6	101,889	4.95
CUP of Shenoy *et al.* (1998)	-	9	98,263	1.22
IBMS of Isafiade and Fraser (2008a)	-	9	97,211	0.14
SWS of Jose *et al.* (2010).	-	7	97,079	0.00

Example 7: Multiple Utility 2 (Shenoy, 1998)

The 'SWS' of Jose *et al.* (2010) still gives the lowest TAC for this example while the SBS comes second. The T&SBS also gives the highest TAC for this example.

Table 6.8: Summary and Comparison of Results for Multiple Utility Example 7

Method	Stream Splits	No. of Units	TAC ($/year)	Percentage Difference (%)
T&SBS	-	8	1,226,806	9.42
CUP of Shenoy et al. (1998)	-	9	1,158,500	3.33
IBMS of Isafiade and Fraser (2008	2	7	1,150,460	2.61
S&TBS	-	7	1,150,303	2.60
SBS	2	8	1,125,417	0.38
SWS of Jose et *al*. (2010).	-	8	1,121,175	0.00

MEN EXAMPLES

Example 8: Ammonia Removal (Hallale, 1995).

The SBS of this study gives the lowest TAC for this problem, followed by the other two techniques presented in this thesis. The hybrid method of Emhammed *et al.* (2007) gave the highest TAC for this example.

Table 6.9: Comparison of results for Example 8

Method	Splits: rich/lean	No of units	TAC ($/yr)	Percentage Difference (%)
Hybrid method of Emhamed *et al*. (2007)	3/2	10	134,399	3.46
SWS of Szitkai *et al*. (2006)	0/1	8	134,000	3.16
IBMS of Isafiade and Fraser (2008b)	1/1	7	133,323	2.65
S&TBS (Type 1)	2/1	9	132,372	1.90
S&TBS (Type 2)	2/1	9	132,331	1.87
T&SBS	2/1	9	131,524	1.25
SBS	1/2	9	129,901	0.00

Example 9: Dephenolisation of Aqueous wastes (El-Halwagi, 1997)

The insight based technique of Commeaux (2000) gave the two lowest TAC for this problem while the S&TBS gives a TAC that is much higher than the rest. The T&SBS produced no solution to this problem.

Table 6.10: Summary and comparison of TAC for Example 9

Method	Splits: rich/lean	No of Units	Total Cost($/yr)	Percentage Difference (%)
S&TBS (Type 2)	0/1	5	421,147	26.85
Lean based IBMS of Isafiade and Fraser (2008b)	0/0	5	358,292	7.92
Pinch technique of Hallale and Fraser (2000)	0/2	7	345,416	4.04
SBS	0/0	6	339,579	2.28
Lean based based IBMS of Isafiade and Fraser (2008b)	0/0	6	338,168	1.86
First option of Insight based technique of Comeaux (2000)	0/2	7	333,300	0.39
Second option of Insight based technique of Comeaux (2000)	0/2	8	332,000	0.00

Example 10: Coke oven gas problem (El-Halwagi and Manousiouthakis, 1989)

The SWS of Chen and Hung (2006) produced the lowest TAC for this problem. The hyperstructure technique of Papalexandri *et al*. (1994) gives a much higher TAC than all others while the rich based IBMS and all superstructures presented in this thesis give TACs that are significantly higher than the lowest TAC.

Table 6.11: Summary and comparison of TAC for Example 10

Method	Splits: rich/lean	No of Units	Total Cost ($/yr)	Percentage Difference (%)
Hyperstructure technique of Papalexandri et al. (1994)	0/1	3	917,880	113.61
Rich based IBMS of Isafiade (2008)	0/0	4	530,471	23.45
T&SBS	0/2	4	526,471	22.52
S&TBS (Type 1)	0/2	4	524,244	22.00
S&TBS (Type 2)	0/2	4	524,244	22.00
SBS	0/0	5	469,968	9.37
Lean Based IBMS of Isafiade (2008)	0/2	4	446,840	3.99
Pinch technique of Hallale and Fraser (2000a)	0/1	5	431,613	0.44
SWS of Chen and Hung (2005)	0/2	4	429,700	0.00

Example 11 Dephenolization of coal conversion waste (Papalexandri, *et al*., 1994)

The insight based of Commeaux (2000) produced the lowest TAC for this problem while the hyperstructure technique of Papalexandri, *et al*. (1994) gives the highest.

Table 6.12: Summary and Comparison of Results for Example 11

Method	Number of units	TAC($/yr)	% error
Hyperstructure technique of Papalexandri, *et al.* (1994)	6	957000	39.10
SWS of Szitkai (2003)	-	720000	4.66
Pinch Technique of Hallale and Fraser (2000)	8	706000	2.62
SWS of Chen and Hung (2005)	7	694000	0.87
SBS	8	693976	0.86
Rich based IBMS of Isafiade and Fraser (2008b)	8	689300	0.19
Insight based technique of Comeaux (2000)	6	688000	0.00

Table 6.13 below shows the best technique for each of the eleven problems investigated in terms of TAC and the difference between the best solution and the next best solution. It also compares each of the five interval based techniques (SWS, IBMS, SBS, S&TBS and T&SBS) with the best solution.

Table 6.13: Comparison of Results over 11 Examples

Example	Number of Streams	Best Technique no of techniques)	TAC ($/yr)	Next Best Solution (%)	SWS (%)	IBMS (%)	SBS (%)	S&TBS (%)	T&SBS (%)
1 4SP1	2 H, 2 C, 1 HU, 1 CU	State Space (11)	10,580	+0.11	-	-	+2.02	+1.95	+5.90
2 4S1	2 H, 2 C, 1 HU, 1CU	SWS (7)	235,400	+0.16	0.00	+1.67	+0.20	+0.16	+2.06
3 Linnhoff problem	2 H, 2 C, 1 HU, 1 CU	SWS (7)	80,274	+9.13	0.00	-	+12.7	+12.95	+9.13
4 MAGNETS Problem	5 H, 1 C, 1 HU, 1 CU	GA (8)	573,205	+0.60	+0.60	+1.52	+1.19	+0.77	+1.53
5 Aromatic Plant	4 H, 5 C, 1 HU, 1 CU	Sequential Match Reduction (11)	2,905,000	+0.59	-	-	+2.44	+1.21	+0.59
6 Multiple Utility 1	2 H, 1 C, 3HU, 1CU	SWS (6)	97,079	+0.14	0.00	+0.14	+4.95	+4.95	+4.96
7 Multiple Utility 2	2 H, 3 C, 3HU, 2CU	SWS (6)	1,121,175	+0.38	0.00	+2.61	+0.38	+2.60	+9.42
8 Ammonia removal	4 R, 3 L (2 Process MSAs, 1 External MSA)	SBS (7)	129,901	+1.25	+3.16	+2.63	0.00	+1.87	+1.25
9 Dephenolisation	2 R, 3 L (2 Process MSAs, 1 External MSA)	Insight based (6)	332,000	+0.39	-	+1.86	+2.28	+26.85	-
10 Coke oven gas problem	2 R, 2 L (1 Process MSA,	SWS (6)	429,700	+0.44	0.00	+3.99	+9.37	+22.00	+23.45

	1External MSA)								
11 Dephenolization of coal conversion waste	4 R, 2 L, 1 H (2 Process MSAs, 1 Regenerant)	Insight based (7)	688,000	+0.19	+0.87	+0.19	+0.86	-	-

Table 6.14 below compares the performance of the various interval based techniques in terms of the number of intervals created and the percentage of the intervals used out of those created and the effect on TAC in HENS and MENS. The column for the TAC is arranged from the highest to the lowest as reflected in the percentage differences in TACs, compared to the lowest one in Table 6.13.

Table 6.14: Comparison of interval based results for all examples

Example	Method	No of units	Stream Splits	No of intervals created	No of intervals used.	Percent intervals used (%)	TAC	Percent Difference (%)
1.4SP1	T&SBS	5	2	6	3	50	11,204	5.90
	S&TBS (TYPE 2)	5	1	5	3	60	10,795	2.03
	SBS	5	1	5	3	60	10,794	2.02
	S&TBS (TYPE 1)	5	1	5	4	80	10,786	1.95
2. 4S1	T&SBS	6	3	6	3	50	240,253	2.06
	IBMS (Cold based)	6	3	5	3	60	239,332	1.67
	IBMS (Hot based)	6	2	5	4	80	237,800	1.02
	SBS	6	2	5	4	80	235,931	0.2
	S&TBS (Types 1 and 2)	6	2	6	4	66.67	235,781	0.16
	SWS	6	2	2	2	100	235,400	0.00
3. Linnhoff, *et al.*, 1982	S&TBS (type 1)	5	1	6	3	50	93,391	16.34
	S&TBS (type 2)	5	1	6	3	50	90,672	12.95
	SBS	7	3	4	3	75	90,521	12.77
	T&SBS	5	0	5	4	80	87,611	9.13
	SWS	5	2	2	2	100	80,274	0.00
4. Magnets Problem	Cold based (IBMS)	7	1	3	3	100	595,064	3.81
	T&SBS	7	1	6	4	66.67	581,954	1.53
	Hot based (IBMS)	7	1	7	3	42.86	581,942	1.52
	S&TBS (type 1)	7	1	7	3	42.86	581,942	1.52
	SBS	8	1	6	4	66.67	580,023	1.19
	S&TBS (type 2)	10	1	7	5	71.43	577,602	0.77
	SWS	7	1	5	-	-	576,640	0.6

5. Aromatic Plant	S&TBS (type 1)	13	3	9	5	55.55	2.979	2.55
	SBS	14	6	9	5	55.55	2.976	2.44
	S&TBS (type B)	11	1	9	5	55.55	2.940	1.21
	T&SBS	17	7	10	6	60.00	2.922	0.59
6. Shenoy Multiple Utility 1	T&SBS	7	1	6	5	83.3	101,893	4.96
	S&TBS	6	2	5	4	80	101,889	4.95
	SBS	6	2	5	4	80	101,889	4.95
	IBMS	9	-	-	-	-	97,211	0.14
	SWS	7	-	-	-	-	97,079	0.00
7. Shenoy Multiple Utility 2	T&SBS	8	3	8	4	50	1,226,806	9.40
	IBMS	7	2	7	5	71.43	1,150,460	2.61
	S&TBS	7	1	8	4	50	1,150,436	2.60
	SBS	8	2	8	5	62.5	1,125,417	0.38
	SWS	8	-	-	-	-	1,121,175	0.00
8. Ammonia removal	SWS	8	1	-	-	-	134,000	3.16
	IBMS	7	2	5	3	60	133,323	2.65
	S&TBS (type 1)	9	3	6	3	50	132,372	1.90
	S&TBS (type 2)	9	3	6	3	50	132,331	1.87
	T&SBS	9	3	5	3	60	131,524	1.25
	SBS	9	3	6	5	83.33	129,901	0.00
9. Dephenolization of aqueous waste	S&TBS (type 2)	5	1	4	3	75.00	421,147	26.85
	Lean based 1 (IBMS)	5	0	-	-	-	358,292	7.92
	SBS	6	0	4	4	100	339,579	2.28
	Lean based 2 (IBMS)	6	0	5	5	100	338,168	1.86
10.Coke oven gas	Rich based (IBMS)	4	0	3	3	100	530,471	23.45
	T&SBS	4	2	4	2	50	526,471	22.52
	S&TBS (type 1)	4	2	4	2	50	524,244	22.00
	S&TBS (type 2)	4	2	4	2	50	524,244	22.00
	SBS	5	0	3	3	100	469,968	9.37
	Lean based (IBMS)	4	2	3	2	66.67	446,840	3.99
	SWS	4	2	-	-	-	429,700	0.00
11. Dephenolization of coal	SWS	NA	1	-	-	-	720,000	4.66
	SWS	7	1	-	-	-	694,000	0.87
	SBS	8	1	5	4	80	693,976	0.86
	IBMS	8	1	6	4	66.67	689,300	0.19

6.1 GENERAL DISCUSSION OF RESULTS AND OBSERVATIONS

Tables 6.1 to 6.12 present the summary of comparison of results over each of the examples solved with the superstructures presented in this thesis and other results as presented by different researchers while Table 6.13 summarises the various TACs as obtained by different researchers for each of the examples. The summary of all the TACs over all examples presented in Table 6.13 shows that no particular technique including those presented in this thesis is able to consistently obtain the lowest TAC for the HEN or the MEN task. With particular reference to the superstructures presented in this thesis, for example, out of eleven examples solved, SBS produced the lowest TAC in six of the examples, while the S&TBS produced the lowest TAC once and T&SBS produced the lowest TAC twice. These excluded two of the examples where the solutions could not be obtained with the S&TBS or the T&SBS. In all the interval based superstructures, however, the SWS consistently obtained lowest TAC for HENS as seen in Examples 2, 3,4, 6 and 7 but the adapted SWS could not obtain same for MENS as seen in Example 8 and 11.

Table 6.14 compares the performance of the various interval based approaches in terms of the number of intervals created and the proportion of the intervals used of those created to see the effects on TAC returned for HENS and MENS task. The TACs are arranged relative to the lowest TAC that appeared in Tables 6.1 to 6.312. The motivation stated as part of the goal in this thesis is if, perhaps, one of the partitioning techniques that have been developed for HENS and MENS tasks would consistently produce lower TACs when compared with other techniques. It is, however, evident in Tables 6.13 and 6.14 that none of the partitioning techniques can consistently produce the lowest TAC for the HENS or MENS task.

Generally, it can be inferred from Table 6.14 that a technique that is able to utilise most (or all) of the intervals created would return a lower TAC (based on those techniques whose number of intervals have been reported). This is obviously reflected in some of the cases considered. In Examples 1, 3, 5 and 9, and to large extent in Example 8, the proportion of intervals used increases as the TAC decreases, this trend was also observed in Example 2 while no particular trend was followed in Examples 4, 6 and 7 and 11. Table 6.14 suggests that it is almost always better that a partitioning technique should be able to use most of the intervals created to be able to return a lower TAC.

The SBS, S&TBS and T&SBS partitioning technique mostly produce a higher number of intervals than the other partitioning techniques studied in this thesis. However, Table 6.14 reflects that a higher number of intervals will not always translate to a lower TAC especially if a number of those intervals are not used.

Generally, in some of the examples presented, a particular method can achieve the lowest or close to the lowest TAC for a particular example, and that same method achieve the highest or close to the highest in another example. An example of this is the T&SBS of this study that obtained the second lowest TAC in Examples 3, 5 and 8 and obtained the second highest TACs in Examples 2, 6 and 7. However, there are some of the techniques that feature once or twice over all the examples solved, and such technique perhaps feature the lowest TAC where it is considered, it would be observed that the percentage difference in TAC between such example and the next will be much less than 1%. This therefore demonstrates that, so far, the outcome of various techniques in the literature have been problem specific; no particular technique can claim to be globally or conclusively suitable to obtain the lowest TAC for all HENS/MENS tasks.

Similarly, the number of heat/mass exchanger units as obtained by different researchers is also problem specific. In Examples 1 and 2, all the methods used for each of the examples obtain the same number of units. In all other examples, a method that achieves a lowest number of units or close to the lowest number of units for a one example can feature the highest or close to the highest number of units in another example. Moreover, this research shows that the general notion that the lowest number of units in HEN corresponds to the lowest TAC is not true. This is corroborated by Examples 4 and 5 where the GA of Lewin and the Sequential Match reduction technique of Petersen (2005) that produced the lowest TAC respectively for each example have the highest number of units for each of those examples.

Although the SBS, S&TBS and T&SBS presented in this thesis assume isothermal and iso-composition mixing of split streams at the interval outlets, as in the SWS and IBMS, this is not a limitation in obtaining good solutions as shown in the examples presented. These can be inferred from the solutions of Krishna and Murty (2007) and those of Chen and Hung (2005) that did away with the isothermal and isocomposition assumptions in HENS and MENS respectively. For instance, the solution of Krishna and Murty is just 0.04% lower than the SBS solution in Example 1 but it is 0.68% higher than the solution obtained by the T&SBS in Example 5. In MENS, the solution of Chen and Huang is 0.44% lower than the solution of the pinch technique of Hallale and Fraser (2000a) in Example 10 but it is 0.86%

and 0.67% higher than the solutions of Insight based of Commeaux and the rich based IBMS of Isafiade and Fraser respectively in Example 11. This again shows that the inclusion or the exclusion of the isothermal mixing assumption does not necessarily translate to structures of lowest TAC in HENS and MENS.

Moreover, it seems that inclusion of non linearities such as the equations for the determination of number of stages for stagewise exchanger and the manner of superstructure partitioning can make it more difficult for GAMS with DICOPT++ to return solutions for MENS problems. This could be the reason for the difficulty for the S&TBS and the T&SBS to obtain solutions in at least one of the MEN problems involving the Kremser equation which make the non linearity to be more pronounced in the model.

CHAPTER SEVEN

CONCLUSIONS AND RECOMMENDATIONS

CHAPTER SEVEN: CONCLUSIONS AND RECOMMENDATIONS

7.1 KEY FINDINGS

This thesis presents new methodology for the minimisation of TAC in HENS and MENS. The methodology presented uses the insight from pinch technology and mathematical programming to generate superstructures for HENS and MENS for the minimization of TAC. Some of the findings from the research in this thesis are the following:

1. In order to define the interval boundaries for HENS/MENS for the minimisation of TAC, one or a combination of the key parameters can be used as follows: supply temperatures/compositions of hot/rich streams and cold/lean streams; target temperatures/compositions of hot/rich streams and cold/lean streams; supply temperatures/compositions of hot/rich streams and the target temperatures/compositions of cold/lean streams; target temperatures/compositions of hot/rich streams and the supply temperatures/compositions of cold/lean streams.
2. The use of supply temperature/composition of hot/rich streams and target temperature/compositions for cold/lean streams or the vice versa have the tendency to generate a higher number of intervals in the superstructure formulations for HENS and MENS.
3. The use of target temperature/composition for the definition of superstructure is not feasible because of the constraints imposed by target temperature/composition of streams.
4. The superstructures presented in this thesis have been successfully applied to different HENS and MENS problems including HENS of restricted or forbidden matches, significantly different heat transfer coefficients and those involving multiple utilities,

and MENS problems including one involving regeneration and those involving multiple MSAs.

5. The use of a larger number of intervals in the HEN/MEN superstructure does not translate to a lower TAC in HENS/MENS.
6. The partitioning technique and the number of intervals used in a superstructure impose a limitation on the solution space of HENS and MENS and consequently affects the TAC obtained.
7. The optimum number of intervals to obtain the lowest TAC for HENS/MENS task is problem specific.
8. The outcome of various techniques for the minimisation of TAC or the number of heat/mass exchanger units as presented in the literature by various researchers is problem specific, as no particular technique can consistently obtain the lowest TAC for all the HENS/MENS tasks in the literature.
9. A technique that produces the lowest number of units in HENS/MENS will not necessarily produce the lowest TAC.
10. Both the manner of superstructure partitioning and the inclusion of non-linearities such as the equations for the determination of number of stages for stagewise mass transfer columns have the tendency to increase the difficulties encountered by gradient solver such as GAMS with DICOPT++.
11. Isothermal/Isocomposition assumptions in HENS/MENS do not necessarily translate to high TACs.
12. Supply temperatures of streams appear to be better for use in the definition of superstructures since the SBS is able to solve all the HEN/MEN problems presented in this thesis. The SBS is therefore recommended for use mostly since it is capable of

giving networks that can be among the lowest cost as shown in the examples presented.

13. The method presented in this thesis is not the best when it comes to implementation of multiple utility problems.

It is evident from the results presented in this thesis that the partitioning techniques presented in this thesis do not return global optimal results, this is due to the presence of non linear and non-convex terms in the objective functions and the manner of superstructure partitioning that have been shown to make the solver more or less efficient depending on the problem and the partitioning. However, these factors do not present barriers in getting results that are well comparable with those in the literature.

7.2 RECOMMENDATIONS

The future work that arises from the present studies is the following:

1. The isothermal mixing junctions in this study can be relaxed, and the non linear heat and mass balances equations included in the SBS, S&TBS and T&SBS HEN and MEN model equations. This will allow some solutions that are not possible with isothermal mixing assumptions to be included, such features can possibly produce solutions with lower costs
2. Stream bypass equations can also be included in all the superstructures presented in this thesis so that networks that are possible with this inclusion can be obtained and evaluated for TAC.

3. Branch flow rates can be used to determine the existence or otherwise of matches rather than the use of binary variables.
4. The superstructures presented in this thesis should be extended for evaluation of TACs in multiperiod HENS and MENS.
5. The superstructures presented in this thesis should be investigated for multi-component MENs where the superstructure will be based on the supply and target compositions of the limiting component in all the rich and lean streams present. However, the optimum network found will need to be checked to ensure that it satisfies the requirements for other components.
6. MEN with non convex equilibrium functions should be set up using piece-wise linearization.
7. The current formulation of these superstructures in GAMS should include more conditionals and constraints to accommodate exclusion of very small matches.

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NOMENCLATURE

Abbreviations

ACC	annualised capital costs
AOC	annual operating cost
CE	cold end
AC	area cost coefficient
AE	area exponent cost
CF	exchanger fixed charge
CS	cold start
CUP	cheapest utility principle
CW	cooling water
DFP	driving force plot
EMCD	exchanger minimum composition difference
EMAT	exchanger minimum approach temperature
FCp	heat capacity flowrate
GCC	grand composite curve
HE	hot end
HENS	heat exchanger network synthesis
HMPS	high medium pressure steam
HPS	high pressure steam
HRAT	heat recovery approach temperature
HS	hot start
HTU	height of theoretical units
IBMS	interval based MINLP superstructure
LMTD	logarithmic mean temperature difference
LP	linear programming

LPS	low pressure steam
MENS	mass exchange network synthesis
MER	maximum energy recovery
MILP	mixed integer linear programming
MINLP	mixed integer non linear programming
MOC	minimum operating cost
MPS	medium pressure steam
MSA	mass separating agent
NOK	total number of temperature/composition interval boundaries
NLP	non linear programming
NTU	number of theoretical units
OLD	optimum load distribution
RPA	remaining problem analysis
TAC	total annual cost
SBS	supply based superstructure
S&TBS	supply and target based superstructure
SWS	stagewise superstructure
T&SBS	target and supply based superstructure
TBS	target based superstructure
U	overall heat transfer coefficient

Symbols

	minimum temperature difference
	logarithmic mean temperature difference
	rich stream composition difference
	minimum composition difference in the rich phase
	logarithmic mean composition difference

conditional operator

General notations

DS mass exchanger column cross sectional area

minimum cold utility

minimum hot utility

stream film heat transfer coefficient

overall mass transfer coefficient based on rich stream

equilibrium constant

number of cold stream

number of hot stream

number of rich stream

number of lean stream

temperature of cold stream

temperature of hot stream

mass load of stream

composition of lean stream

composition of rich stream

HENS and MENS notations in Chapter 4

Sets

H hot process and utility streams

C cold process and utility streams

temperature/composition intervals in the superstructure

rich streams

lean streams (process and external mass separating agents)

Indices

hot process or utility streams

cold process or utility streams

index for temperature/composition boundary (k=1, ... NOK+1)

lean stream (process or external mass separating agent)

rich process stream

Parameters

AC_l	annual cost per unit of lean stream l
ACH_{rl}	annual cost per height for continuous contact columns involving rich stream r and lean stream l
ACT_{rl}	annual cost per stage for staged columns involving rich stream r and lean stream l
AFC	area cost coefficient for heat exchangers
b	equilibrium line intercept
	is the existence of cold stream in interval K (between temperature interval boundaries and
CB_{ij}	fixed charge for heat exchangers
CB_{rl}	fixed charge for mass exchanger columns involving rich stream r and lean stream l
CU	cost per unit of cold utility
D	area cost index for heat/mass exchangers

is the existence of hot stream in interval K (between temperature interval boundaries and),

HU cost per unit of hot utility

K_w lumped mass transfer coefficient

m equilibrium constant for the transfer of component from rich stream r to lean stream l

existence of rich stream r in interval K (between composition interval boundary k and $k+1$)

rich stream r start at composition interval boundary k

existence of lean stream l in interval K (between composition interval boundary k and k+1)

lean stream l start at composition interval boundary k

supply temperature of hot stream i

target temperature of hot stream i

supply temperature of cold stream j

target temperature of cold stream j

T_k temperature of interval boundary k

supply composition of lean stream l

target composition of lean stream l

supply composition of rich stream *r*

target composition of rich stream *r*

equilibrium supply composition of lean stream *l*

equilibrium target composition of lean stream *l*

composition of interval boundary *k*

Γ_H upper bound for driving force in match *i*, *j*

upper bound for driving force in match *r*, *l*

ε_{min} minimum composition difference in the lean phase

Ω_H upper bound for heat exchanged in match *i*, *j*

Ω_Z upper bound for mass exchanged in match *r*, *l*

<u>*Binary variables*</u>

variable showing the existence of match *ij* in interval *K* in the network

variable showing the existence of match *rl* in interval *K* in the network

<u>*Positive variables*</u>

heat exchanger driving force for match *ij* in temperature interval *K*

mass exchanger driving force for match *rl* in composition interval *K*

F_i flow rate of hot stream *i*

F_j flow rate of cold stream *j*

G_r rich stream flowrate

L_l lean stream flowrate

heat exchanged between stream *i* and stream *j* in temperature interval *K*

number of stages in staged column *rlk*

heat exchanged between stream *i* and stream *j* in temperature interval *K*

temperature of hot stream *i* at temperature boundary *k*

temperature of cold stream *j* at temperature boundary *k*

composition of rich stream *r* at composition boundary *k*

equilibrium composition of lean stream at composition boundary *k*

APPENDIX A. HEAT EXCHANGER NETWORKS PROBLEM DATA

This appendix presents the examples solved for the heat exchange networks problems in Chapters three to five.

Table A1: Problem specifications for Example 1 (Lee *et al*., 1970)

Stream	T^s(°F)	T^t (°F)	Cp (Btu/(°F))
H1	320	200	16,666.8
H2	480	280	20,000
C1	140	320	14,450.1
C2	240	500	11,530
S1	540	540	-
W1	100	180	-

Hot utility (S1) cost = \$12.76kBTU^{-1} yr^{-1}, Cold utility (W1) cost = \$5.24 kBTU^{-1} yr^{-1}. Heat exchangers annual cost = \$35×Area$^{0.6}$(Area in ft^2). *U*=150 Btu/ft^{2o}F for all matches except those involving steam where *U*=200bBtu/ft^2.

Table A2: Problem specifications for Example 2 (Shenoy, 1995)

Stream	T^s (°C)	T^t (°C)	F (kW°C^{-1})	h (kWm^{-2}°C^{-1})	Costs
H1	175	45	10	0.2	-
H2	125	65	40	0.2	-
C1	20	155	20	0.2	-
C2	40	112	15	0.2	-
HU1	180	179	-	0.2	120
CU1	15	25	-	0.2	10

Annualisation factor=0.322, utility costs in \$ kW^{-1}yr^{-1}.
Capital cost (\$) = 30,000+750[Area (m^2)]$^{0.81}$ for all exchangers

Table A3: Problem specifications for Example 3 (Linnhoff *et al*., 1982).

Stream	T^s (K)	T^t (K)	F (kWK^{-1})	Costs
H1	443	333	30	-
H2	423	303	15	-
C1	293	408	20	-
C2	353	413	40	-
S1	450	450	-	80
W1	293	313	-	20

U=0.8(kWm^{-2}K^{-1}) for all matches except one involving steam
U=1.2(kWm^{-2}K^{-1}) for matches involving steam
Annual cost = 1000 x [area (m^2)]$^{0.6}$

Table A4: Problem specifications for Example 4.

Stream	$T^s(^0K)$	$T^t(^0K)$	Cp(kW/K)	Cost($\$kW^{-1}yr^{-1}$)
H1	500	320	6	-
H2	480	380	4	-
H3	460	360	6	-
H4	380	360	20	-
H5	380	320	12	-
C1	290	660	18	-
S1	700	700	-	140
W1	300	320	-	10

$U(kWm^{-2} K^{-1})=1$ for all matches, annualized area cost= $1200(A)^{0.6}$ for all exchangers where A is the Area(m^2).

Table A5: Problem specifications for Example 5.

Streams	$T^s(^oC)$	$T^t(^oC)$	Cp(kWK-1)	H(kWm-2K-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

Plant Lifetime is five years, rate of interest =0%. Exchanger cost (US\$)=10,000 +350 x S (S is Area in m^2). Hot oil Cost=60 US$\$kW^{-1}yr^{-1}$; Water Cost= 6US$\$kW^{-1}yr^{-1}$.

Table A6: Stream, Utility and cost data for Multiple Utility 1 in Example 6.

Stream	T^s (^oC)	T^t (^oC)	Heat capacity flowrate ($kW/^oC$)	Heat transfer coefficient ($kW/m^2/^oC$)	Cost (£/kW/yr)
H1	105	25	10	0.5	
H2	185	35	5	0.5	
C3	25	185	7.5	0.5	
HP Steam	210	209		5.0	160
MP Steam	160	159		5.0	110
LP Steam	130	129		5.0	50
CW	5	6		2.6	10

Exchanger Capital cost (£) = 800 x area $(m)^2$, Annualization factor = 0.298 (/yr).

Table A7: Stream, Utility and cost data for Multiple Utility 2 in Example 7.

Stream	T^s (°C)	T^t (°C)	Heat capacity flowrate (Kw/°C)	Heat transfer coefficient (kW/m^2/°C)	Cost (£/kW/yr)
H1	155	85	150	0.5	
H2	230	40	85	0.5	
C3	115	210	140	0.5	
C4	50	180	55	0.5	
C5	60	175	60	0.5	
HP Steam	255	254		0.5	70
MP Steam	205	204		0.5	50
LP Steam	150	149		0.5	20
CW	30	40		0.5	10
AC	40	65		0.5	5

Exchanger Capital cost (£) = 13000 + 1000 (area) $^{0.83}$ (m^2), Annualization factor = 0.322(/yr).

APPENDIX B: MASS EXCHANGER NETWORKS PROBLEM DATA

Table B1: Problem specifications for Example 8 (Hallale, 1998)

Rich Stream		G(kg/s)		Y^s		Y^t
R1		2		0.005		0.0010
R2		4		0.005		0.0025
R3		3.5		0.011		0.0025
R4		1.5		0.010		0.0050
R5		0.5		0.008		0.0025
Lean Stream	**L^c(Kg/s)**	**X^s**	**X^t**	**m**	**b**	**Cost($/kg)**
S1	1.8	0.0017	0.0071	1.2	0	0
S2	1.0	0.0025	0.0085	1	0	0
S3	∞	0.0	0.017	0.5	0	0.001

Packed column exchangers, K_W = 0.02 kg NH_3/(s kg), Shell cost = \$618$M^{0.66}$, where M is exchanger mass. Annualisation factor = 0.225; Annual operating time = 8150 hr.

Table B2: Problem specifications for Example 9 (El-Halwagi, 1997)

Rich Stream		R(kg/s)		Y^s		Y^t
R1		2		0.050		0.010
R2		1		0.030		0.006
Lean Stream	**L^c(kg/s)**	**X^s**	**X^t**	**m**	**b**	**Cost($/kg)**
S1	5	0.005	0.015	2.00	0	0
S2	3	0.01	0.030	1.53	0	0
S3	∞	0.0013	0.015	0.71	0.001	0.01

Sieve tray columns, cost per equilibrium stage per year = \$4552/yr (Papalexandri, *et al.*, 1994)

Table B3: Problem specifications for Example 10 (El-Halwagi and Manousiouthakis, 1989)

Rich Stream		R(kg/s)		Y^s		Y^t
R1		0.9		0.070		0.0003
R2		0.1		0.051		0.0001
Lean Stream	**L^C(kg/s)**	**X(s)**	**X(t)**	**m**	**b**	**Cost($/yr)(kg/s)**
S1	2.3	0.0006	0.031	1.45	0	117,360
S2	∞	0.0002	0.0035	0.26	0	176,040

Sieve tray columns, cost per equilibrium stage per year = \$4552/yr (Papalexandri, *et al.*, 1994)

Table B4: Problem specifications for Example 11 (Papalexandri *et. al*., 1994)

Rich streams	G(kg/s)	Y^s (mass fraction)	Y^t (mass fraction)
R1	3.3	0.05	0.0015
R2	0.6	0.07	0.003
R3	1.4	0.02	0.003
R4	0.2	0.03	0.002

MSAs	L^c (Kg/s)	X^s (mass fraction)	X^t (mass fraction)	m	b	Cost ($/yr)/(kg/s)
S1	10	0.0013	0.025	0.71	0.001	58680
S2	10			0.13	0.001	417060
Regen	M^c (Kg/s)	Z^s (mass fraction)	Z^t (mass fraction)	m	b	Cost ($/yr)/(kg/s)
V1	10	0	0.005	1.38	-	88020

Appendix C: Use of Different Approximations for evaluation SBS, S&TBS and the T&SBS

Table C1: Results of Examples 1, 2 and 4 using different LMTD approximations

LMTD Approximations	SBS (TAC)	S&TBS (Type A) (TAC)	S&TBS (Type B) (TAC)	T&SBS (TAC)
Example 1				
First Chen's (1987)	10,794	10,786	10,795	11,204
Second Chen's (1987)	10,629	10,618	10,640	11,195
Underwood (1970)	10,619	10,606	10,630	11,109
Paterson (1984)	10,590	10,604	10,564	11,090
Example 2				
First Chen's (1987)	235,931	235,781	235,781	240,253
Second Chen's (1987)	235,419	2354192	235419	241,290
Underwood (1970)	235,464	235,464	235464	241,339
Paterson (1984)	237,401	235,382	235,382	241,255
Example 4				
First Chen's (1987)	580,023	581,942	577,602	581,954
Second Chen's (1987)	579,011	579,818	575,612	577,460
Underwood (1970)	579,026	579,829	575,637	577,483
Paterson (1984)	586,986	586,989	582,738	582,738

APPENDIX D GAMS CODE

Appendix D1 GAMS code for SBS in Example 7.

```
$Title:  HENS by Supply Based Superstructure
*Optimal SBS for multiple utility Example 7 written by Sarafa Azeez
SETS

 JH        Hot streams and utilities /1*4/
 JC        Cold streams and utilities /1*4/
 DATA       /TIN, TOUT, MCP,H/;


TABLE HOTS (JH,DATA) Hot streams data

      TIN          TOUT     H

 1   155.00        85.00    0.5
 2   230.00        40.00    0.5
 3   255.00        254.00   0.5
 4   205.00        204.00   0.5


TABLE COLDS (JC,DATA) Cold streams data

      TIN          TOUT     H

 1    30.00        40.00    0.5
 2    115.00       210.00   0.5
 3     50.00       180.00   0.5
 4     60.00       175.00   0.5;



TABLE       MHC (JH, JC) forbidden matches for hot and cold streams including utilities

    1   2   3   4
1   1   1   1   1
2   1   1   1   1
3   0   1   1   1
4   0   1   1   1;


SCALAR

NOI Number of intervals in SBS /7/;


SET

I temperature intervals NOI +1   /1*8/;
```

PARAMETERS

HU(JH)	Cost per unit of hot utility
CU(JC)	Cost per unit of cold utility
CB	Fixed charge for units
AFC	Area cost coefficient
D	Area cost index
AF	Annualisation factor
EMAT	Exchange minimum approach temperature
TKH(I)	Temperature location i in SBS
INTERVAL(I)	Intervals in the superstructure
H(JH,I)	Hot stream existence coefficient in interval I
C(JC,I)	Cold stream existence coefficient in interval I
H1(JH,I)	Hot stream supply temperature coefficients
H2(JH,I)	Hot stream supply temperature coefficients
H3(JH,I)	Hot stream supply temperature coefficients
H4(JH,I)	Hot stream supply temperature coefficients
C1(JC,I)	Cold stream supply temperature coefficients
C2(JC,I)	Cold stream supply temperature coefficients
C3(JC,I)	Cold stream supply temperature coefficients
C4(JC,I)	Cold stream supply temperature coefficients
FTB1(I)	First temperature boundary in superstructure
FTB2(I)	Second temperature boundary in superstructure
FTB3(I)	Third temperature boundary in superstructure
FTB4(I)	Fourth temperature boundary in superstructure
FTB5(I)	Fifth temperature boundary in superstructure
FTB6(I)	Sixthtemperature boundary in superstructure
FTB7(I)	Seventh temperature boundary in superstructure
LTB(I)	Last temperature boundary in superstructure
MAXDT(JH,JC)	
AREA(JH,JC,I)	Area of exchanger between hot stream and cold stream in interval I;

CB=13000;   AFC = 1000;   D = 0.83;   AF= 0.322;
HUC('1')=0;   HUC('2')=0;   HUC('3')=70;   HUC('4')=50;
CUC('1')=10; CUC('2')=0; CUC('3')=0;   CUC('4')=0;

Supply temperature locations

TKH('1') = 255.00; TKH('2') = 230.00; TKH('3') = 205.00; TKH('4') = 155.00;
TKH('5') = 115.00; TKH('6') = 60.00; TKH('7') = 50.00;   TKH('8') =30.00;

MAXDT(JH,JC)=

MAX(0,COLDS(JC,'TIN')-HOTS(JH,'TIN'),COLDS(JC,'TIN')-HOTS(JH,'TOUT'),
          COLDS(JC,'TOUT')-HOTS(JH,'TIN'),COLDS(JC,'TOUT')-HOTS(JH,'TOUT'));

```
INTERVAL(I)$(ORD(I) LT CARD(I)) =1;
FTB1(I)$(ORD(I) EQ 1) =1;
FTB2(I)$(ORD(I) EQ 2) =1;
FTB3(I)$(ORD(I) EQ 3) =1;
FTB4(I)$(ORD(I) EQ 4) =1;
FTB5(I)$(ORD(I) EQ 5) =1;
FTB6(I)$(ORD(I) EQ 6) =1;
FTB7(I)$(ORD(I) EQ 7) =1;
LTB(I)$(ORD(I) EQ CARD(I))=1;


H(JH,I)$(INTERVAL(I) AND HOTS(JH,'TIN') GE TKH(I)) = 1;
C(JC,I)$(INTERVAL(I) AND COLDS(JC,'TIN') LE TKH(I)) =1;


H1(JH,I)$(HOTS(JH,'TIN') EQ TKH(I))=1;
H2(JH,I)$(HOTS(JH,'TIN') EQ TKH(I))=1;
H3(JH,I)$(HOTS(JH,'TIN') EQ TKH(I))=1;
H4(JH,I)$(HOTS(JH,'TIN') EQ TKH(I))=1;
C1(JC,I)$(COLDS(JC,'TIN') EQ TKH(I))=1;
C2(JC,I)$(COLDS(JC,'TIN') EQ TKH(I))=1;
C3(JC,I)$(COLDS(JC,'TIN') EQ TKH(I))=1;
C4(JC,I)$(COLDS(JC,'TIN') EQ TKH(I))=1;


POSITIVE VARIABLES

TH(JH,I)            Temperature of hot stream JH as it enters interval I
TC(JC,I)            Temperature of cold stream as it leaves interval I
AVHOT(JH)           Heat content of JH
AVCOLD(JC)          Heat content of JC
Q(JH,JC,I)          Energy exchanged between JH and JC in interval I
DTHC(JH,JC,I)       Approach temperature between JH and JC in interval I
MCP1(JH)            Heat capacity flowrate of JH
MCP2(JC);           Heat capacity flowrate of JC


VARIABLE

TAC                 Total annual cost;


BINARY VARIABLES

NHC(JH,JC,I)        is one if the match between JH and JC exists in interval I;
```

```
EQUATIONS
AVHOT1(JH)
AVCOLD1(JC)
ENBHSBS(JH)
ENBCSBS(JC)
EBHSBS(JH,I)
EBCSBS(JC,I)

UTHSBS(JH,I)
UTCSBS(JC,I)

SBSH1(JH,I)
SBSH2(JH,I)
SBSH3(JH,I)
SBSH4(JH,I)
SBSC1(JC,I)
SBSC2(JC,I)
SBSC3(JC,I)
SBSC4(JC,I)

CONSTHS(JH,I)
CONSTHLB(JH,I)
CONSTCS(JC,I)
CONSTCFB(JC,I)
BOUNDQS(JH,JC,I)

DTHEQNS(JH,JC,I)
DTCEQNBJH,JC,I)
FORBHCS(JH,JC,I)


OBJ             Total annual Cost;

*=================================================================

*Available energy in hot stream JH

AVHOT1(JH)..  AVHOT(JH)=E=MCP1(JH)*(HOTS(JH,'TIN') - HOTS(JH,'TOUT'));


*Available energy in cold stream JC

AVCOLD1(JC)..  AVCOLD(JC)=E=MCP2(JC)*(COLDS(JC,'TOUT') - COLDS(JC,'TIN'));

*=================================================================

*Overall energy balance for hot stream JH

ENBHSBS(JH)..
  AVHOT(JH) =E=SUM((JC,I)$(INTERVAL(I) AND(H(JH,I) EQ 1 AND C(JC,I) EQ
1)),Q(JH,JC,I));
```

Overall energy balance for cold stream JC

```
ENBCSBS(JC)..
  AVCOLD(JC)=E=SUM((JH,I)$(INTERVAL(I)AND (H(JH,I) EQ 1 AND C(JC,I) EQ
1)),Q(JH,JC,I));
*=====================================================================

*Interval energy balance for hot stream JH

EBHSBS(JH,I)$(INTERVAL(I) AND H(JH,I))..
  MCP1(JH)*(TH(JH,I)-TH(JH,I+1))=E=SUM(JC$(C(JC,I)),Q(JH,JC,I));


*Interval energy balance for cold stream JC

EBCSBS(JC,I)$(INTERVAL(I) AND C(JC,I))..
  MCP2(JC)*(TC(JC,I)-TC(JC,I+1))=E=SUM(JH$(H(JH,I)),Q(JH,JC,I));
*=====================================================================

*Hot stream temperatures at the first temperature location

UTHSBS(JH,I)$FTB1(I)..
  HOTS(JH,'TIN')=E=TH(JH,I);

*Cold stream temperatures at the last temperature locations

UTCSBS(JC,I)$(LTB(I) AND C4(JC,I))..
  COLDS(JC,'TIN')=E=TC(JC,I);
*=====================================================================

*Assignment of superstructure interval temperatures using hot and cold stream supply
temperatures

SBSH1(JH,I)$(FTB1(I) AND H1(JH,I) AND H(JH,I))..
 HOTS(JH,'TIN')=E=TH(JH,I);

SBSH2(JH,I)$(FTB2(I) AND H2(JH,I) AND H(JH,I))..
 HOTS(JH,'TIN')=E=TH(JH,I);

SBSH3(JH,I)$(FTB3(I) AND H3(JH,I) AND H(JH,I))..
 HOTS(JH,'TIN')=E=TH(JH,I);

SBSH4(JH,I)$(FTB4(I) AND H4(JH,I) AND H(JH,I))..
 HOTS(JH,'TIN')=E=TH(JH,I);

SBSC1(JC,I)$(FTB5(I) AND C1(JC,I) AND C(JC,I))..
  COLDS(JC,'TIN')=E=TC(JC,I);

SBSC2(JC,I)$(FTB6(I) AND C2(JC,I) AND C(JC,I))..
  COLDS(JC,'TIN')=E=TC(JC,I);
```

```
SBSC3(JC,I)$(FTB7(I) AND C3(JC,I) AND C(JC,I))..
  COLDS(JC,'TIN')=E=TC(JC,I);

SBSC4(JC,I)$LTB(I)..
  COLDS(JC,'TIN')=E=TC(JC,I);
*==========================================================================

*The following constraints guarantee that temperatures decrease from the first to the last temperature interval boundary

CONSTHS(JH,I)$(INTERVAL(I)AND H(JH,I))..
  TH(JH,I)=G=TH(JH,I+1);

CONSTHLB(JH,I)$(LTB(I))..
  TH(JH,I)=E=HOTS(JH,'TOUT');

CONSTCS(JC,I)$(INTERVAL(I)AND C(JC,I))..
  TC(JC,I)=G=TC(JC,I+1);

CONSTCFB(JC,I)$FTB1(I)..
  COLDS(JC,'TOUT')=E=TC(JC,I);
*==========================================================================

*Logical constraints

BOUNDQS(JH,JC,I)$(INTERVAL(I)) ..
 Q(JH,JC,I)-MIN(AVHOT(JH),AVCOLD(JC))*NHC(JH,JC,I)=L=0;


*==========================================================================

*Approach temperatures

DTHEQNS(JH,JC,I)$INTERVAL(I)..
 DTHC(JH,JC,I)=L=TH(JH,I) - TC(JC,I)+MAXDT(JH,JC)*(1 - NHC(JH,JC,I)) ;

DTCEQNB(JH,JC,I)$INTERVAL(I)..
 DTHC(JH,JC,I+1)=L=TH(JH,I+1)-TC(JC,I+1)+MAXDT(JH,JC)*(1 - NHC(JH,JC,I)) ;
```

```
*Forbidden Mathes

FORBHCS(JH,JC,I)$(MHC(JH,JC) EQ 0)..
    Q(JH,JC,I) =E=0;
*==========================================================================

Objective function

 OBJ..
       TAC=E=   AF*((CB*(SUM((JH,JC,I)$(INTERVAL(I)),NHC(JH,JC,I))))+

AFC*SUM((JH,JC,I)$(INTERVAL(I)),(Q(JH,JC,I)*(1/HOTS(JH,'H')+1/COLDS(JC,'H'))/
```

```
((((1e6)**3+(DTHC(JH,JC,I)*DTHC(JH,JC,I+1))*((DTHC(JH,JC,I)+DTHC(JH,JC,I+1))*0.
5))**0.3333)+1E-6)+(1E-6))**COEFFC))

 +  SUM((JH,JC,I),Q(JH,JC,I)*HU(JH))+SUM((JH,JC,I),Q(JH,JC,I)*CU(JC));
*=====================================================================

MODEL MULTIPLE UTILITY EXAMPLE 7 /ALL/;

*Upper/lower bounds and initialisation

MCP1.L('1')=150;       MCP1.LO('1')=150;      MCP1.UP('1')=150;
MCP1.L('2')=85;        MCP1.LO('2')=85;       MCP1.UP('2')=85;
MCP1.L('3')=1;         MCP1.LO('3')=1;        MCP1.UP('3')=20000;
MCP1.L('4')=1;         MCP1.LO('4')=1;        MCP1.UP('4')=30000;
MCP2.L('1')=1.00;      MCP2.LO('1')=1.00;     MCP2.UP('1')=30000.00;
MCP2.L('2')=140;       MCP2.LO('2')=140;      MCP2.UP('2')=140;
MCP2.L('3')=55;        MCP2.LO('3')=55;       MCP2.UP('3')=55;
MCP2.L('4')=60;        MCP2.LO('4')=60;       MCP2.UP('4')=60;

EMAT =.18;    DTHC.LO(JH,JC,I)=TMAPP;     DTHC.UP(JH,JC,I)=1000000;

*Resetting some GAMS options

OPTION LIMROW =500;      OPTION ITERLIM=1000

SOLVE AUTIL USING MINLP MINIMIZING TAC;

*Calculating areas for units in superstructure

AREA(JH,JC,I)$(INTERVAL(I) AND H(JH,I) AND Q.L(JH,JC,I) )=

  Q.L(JH,JC,I)*(1/HOTS(JH,'H')+1/COLDS(JC,'H'))/((((1e-
6)**3+(DTHC.L(JH,JC,I)*DTHC.L(JH,JC,I+1))*((DTHC.L(JH,JC,I)+DTHC.L(JH,JC,I+1))
*0.5))**0.3333)+1E-6)+1E-6;

DISPLAY AREA
```

Appendix D2 GAMS code for S&TBS in Example 7.

```
$Title:  HENS by Supply and Target Based Superstructure
*Optimal S&TBS for multiple utility Example 7 written by Sarafa Azeez

SETS

 JH        Hot streams and utilities /1*4/
 JC        Cold streams and utilities /1*4/
 DATA       /TIN, TOUT, MCP,H/;

TABLE HOTS(JH,DATA) Hot streams data

     TIN          TOUT     H

 1   155.00       85.00    0.5
 2   230.00       40.00    0.5
 3   255.00       254.00   0.5
 4   205.00       204.00   0.5

TABLE COLDS(JC,DATA) Cold streams data

     TIN          TOUT     H

 1    30.00      40.00     0.5
 2    115.00     210.00    0.5
 3     50.00     180.00    0.5
 4     60.00     175.00    0.5;



TABLE       MHC(JH,JC)  forbidden matches for hot and cold streams including utilities

    1  2  3  4
1   1  1  1  1
2   1  1  1  1
3   0  1  1  1
4   0  1  1  1;

SCALAR

NOI Number of intervals in SBS /8/;
```

SET

I temperature intervals NOI +1 /1*9/;

PARAMETERS

HU(JH)	Cost per unit of hot utility
CU(JC)	Cost per unit of cold utility
CB	Fixed charge for units
AFC	Area cost coefficient
D	Area cost index
AF	Annualisation factor
EMAT	Exchange minimum approach temperature
TKH(I)	Temperature location i in SBS
INTERVAL(I)	Intervals in the superstructure
H(JH,I)	Hot stream existence coefficient in interval I
C(JC,I)	Cold stream existence coefficient in interval I
H1(JH,I)	Hot stream supply temperature coefficients
H2(JH,I)	Hot stream supply temperature coefficients
H3(JH,I)	Hot stream supply temperature coefficients
H4(JH,I)	Hot stream supply temperature coefficients
C1(JC,I)	Cold stream supply temperature coefficients
C2(JC,I)	Cold stream supply temperature coefficients
C3(JC,I)	Cold stream supply temperature coefficients
C4(JC,I)	Cold stream supply temperature coefficients
C5(JC,I)	Cold stream supply temperature coefficients
FTB1(I)	First temperature boundary in superstructure
FTB2(I)	Second temperature boundary in superstructure
FTB3(I)	Third temperature boundary in superstructure
FTB4(I)	Fourth temperature boundary in superstructure
FTB5(I)	Fifth temperature boundary in superstructure
FTB6(I)	Sixth temperature boundary in superstructure
FTB7(I)	Seventh temperature boundary in superstructure
FTB8(I)	Eight temperature boundary in superstructure
LTB(I)	Last temperature boundary in superstructure
MAXDT(JH,JC)	
AREA(JH,JC,I)	Area of exchanger between hot stream and cold stream in interval I;

CB=13000; AFC = 1000; D = 0.83; AF= 0.322;
HUC('1')=0; HUC('2')=0; HUC('3')=70; HUC('4')=50;
CUC('1')=10; CUC('2')=0; CUC('3')=0; CUC('4')=0;

Supply temperature locations

TKH('1') = 255.00; TKH('2') = 230.00; TKH('3') = 210.00; TKH('4') = 205.00;
TKH('5') = 180.00; TKH('6') = 175.00; TKH('7') = 155.00; TKH('8') = 40.00;
TKH('9') =30.00;

MAXDT(JH,JC)=

```
MAX(0,COLDS(JC,'TIN')-HOTS(JH,'TIN'),COLDS(JC,'TIN')-HOTS(JH,'TOUT'),
          COLDS(JC,'TOUT')-HOTS(JH,'TIN'),COLDS(JC,'TOUT')-HOTS(JH,'TOUT'));


INTERVAL(I)$(ORD(I) LT CARD(I)) =1;
FTB1(I)$(ORD(I) EQ 1) =1;
FTB2(I)$(ORD(I) EQ 2) =1;
FTB3(I)$(ORD(I) EQ 3) =1;
FTB4(I)$(ORD(I) EQ 4) =1;
FTB5(I)$(ORD(I) EQ 5) =1;
FTB6(I)$(ORD(I) EQ 6) =1;
FTB7(I)$(ORD(I) EQ 7) =1;
FTB8(I)$(ORD(I) EQ 8) =1;
LTB(I)$(ORD(I) EQ CARD(I))=1;


H(JH,I)$(INTERVAL(I) AND HOTS(JH,'TIN') GE TKH(I)) = 1;
C(JC,I)$(INTERVAL(I) AND COLDS(JC,'TIN') LE TKH(I)) =1;


H1(JH,I)$(HOTS(JH,'TIN') EQ TKH(I))=1;
H2(JH,I)$(HOTS(JH,'TIN') EQ TKH(I))=1;
C1(JC,I)$(COLDS(JC,'TIN') EQ TKH(I))=1;

H3(JH,I)$(HOTS(JH,'TIN') EQ TKH(I))=1;
C2(JC,I)$(COLDS(JC,'TIN') EQ TKH(I))=1;
C3(JC,I)$(COLDS(JC,'TIN') EQ TKH(I))=1;
H4(JH,I)$(HOTS(JH,'TIN') EQ TKH(I))=1;
C4(JC,I)$(COLDS(JC,'TIN') EQ TKH(I))=1;
C5(JC,I)$(COLDS(JC,'TIN') EQ TKH(I))=1;


POSITIVE VARIABLES

TH(JH,I)            Temperature of hot stream JH as it enters interval I
TC(JC,I)            Temperature of cold stream as it leaves interval I
AVHOT(JH)           Heat content of JH
AVCOLD(JC)          Heat content of JC
Q(JH,JC,I)          Energy exchanged between JH and JC in interval I
DTHC(JH,JC,I)       Approach temperature between JH and JC in interval I
MCP1(JH)            Heat capacity flowrate of JH
MCP2(JC);           Heat capacity flowrate of JC


VARIABLE

TAC                 Total annual cost;
```

BINARY VARIABLES

NHC(JH,JC,I) is one if the match between JH and JC exists in interval I;

EQUATIONS
AVHOT1(JH)
AVCOLD1(JC)
ENBHSBS(JH)
ENBCSBS(JC)
EBHSBS(JH,I)
EBCSBS(JC,I)

UTHSBS(JH,I)
UTCSBS(JC,I)

SBSH1(JH,I)
SBSH2(JH,I)
SBSH3(JH,I)
SBSH4(JH,I)
SBSC1(JC,I)
SBSC2(JC,I)
SBSC3(JC,I)
SBSC4(JC,I)
SBSC5(JC,I)
CONSTHS(JH,I)
CONSTHLB(JH,I)
CONSTCS(JC,I)
CONSTCFB(JC,I)
BOUNDQS(JH,JC,I)

DTHEQNS(JH,JC,I)
DTCEQNBJH,JC,I)
FORBHCS(JH,JC,I)

OBJ Total annual Cost;

*==

*Available energy in hot stream JH

AVHOT1(JH).. AVHOT(JH)=E=MCP1(JH)*(HOTS(JH,'TIN') - HOTS(JH,'TOUT'));

*Available energy in cold stream JC

AVCOLD1(JC).. AVCOLD(JC)=E=MCP2(JC)*(COLDS(JC,'TOUT') - COLDS(JC,'TIN'));

*==

*Overall energy balance for hot stream JH

```
ENBHSBS(JH)..
  AVHOT(JH) =E=SUM((JC,I)$(INTERVAL(I) AND(H(JH,I) EQ 1 AND C(JC,I) EQ
1)),Q(JH,JC,I));


Overall energy balance for cold stream JC

ENBCSBS(JC)..
  AVCOLD(JC)=E=SUM((JH,I)$(INTERVAL(I)AND (H(JH,I) EQ 1 AND C(JC,I) EQ
1)),Q(JH,JC,I));
*===================================================================

*Interval energy balance for hot stream JH

EBHSBS(JH,I)$(INTERVAL(I) AND H(JH,I))..
  MCP1(JH)*(TH(JH,I)-TH(JH,I+1))=E=SUM(JC$(C(JC,I)),Q(JH,JC,I));


*Interval energy balance for cold stream JC

EBCSBS(JC,I)$(INTERVAL(I) AND C(JC,I))..
  MCP2(JC)*(TC(JC,I)-TC(JC,I+1))=E=SUM(JH$(H(JH,I)),Q(JH,JC,I));
*===================================================================

*Hot stream temperatures at the first temperature location

UTHSBS(JH,I)$FTB1(I)..
  HOTS(JH,'TIN')=E=TH(JH,I);
*Cold stream temperatures at the last temperature locations

UTCSBS(JC,I)$(LTB(I) AND C4(JC,I))..
  COLDS(JC,'TIN')=E=TC(JC,I);
*===================================================================

*Assignment of superstructure interval temperatures using hot and cold stream supply
temperatures

SBSH1(JH,I)$(FTB1(I) AND H1(JH,I) AND H(JH,I))..
 HOTS(JH,'TIN')=E=TH(JH,I);

SBSH2(JH,I)$(FTB2(I) AND H2(JH,I) AND H(JH,I))..
 HOTS(JH,'TIN')=E=TH(JH,I);

SBSC1(JC,I)$(FTB3(I) AND C1(JC,I) AND C(JC,I))..
  COLDS(JC,'TIN')=E=TC(JC,I);

SBSH3(JH,I)$(FTB4(I) AND H3(JH,I) AND H(JH,I))..
 HOTS(JH,'TIN')=E=TH(JH,I);

SBSC2(JC,I)$(FTB5(I) AND C2(JC,I) AND C(JC,I))..
  COLDS(JC,'TIN')=E=TC(JC,I);

SBSC3(JC,I)$(FTB6(I) AND C3(JC,I) AND C(JC,I))..
```

```
  COLDS(JC,'TIN')=E=TC(JC,I);

SBSH4(JH,I)$(FTB7(I) AND H4(JH,I) AND H(JH,I))..
 HOTS(JH,'TIN')=E=TH(JH,I);

SBSC4(JC,I)$(FTB8(I) AND C4(JC,I) AND C(JC,I))..
  COLDS(JC,'TIN')=E=TC(JC,I);

SBSC5(JC,I)$LTB(I)..
  COLDS(JC,'TIN')=E=TC(JC,I);
*===================================================================

*The following constraints guarantee that temperatures decrease from the first to the last
temperature interval boundary

CONSTHS(JH,I)$(INTERVAL(I)AND H(JH,I))..
  TH(JH,I)=G=TH(JH,I+1);

CONSTHLB(JH,I)$(LTB(I))..
  TH(JH,I)=E=HOTS(JH,'TOUT');

CONSTCS(JC,I)$(INTERVAL(I)AND C(JC,I))..
  TC(JC,I)=G=TC(JC,I+1);

CONSTCFB(JC,I)$FTB1(I)..
  COLDS(JC,'TOUT')=E=TC(JC,I);
*===================================================================

*Logical constraints

BOUNDQS(JH,JC,I)$(INTERVAL(I)) ..
 Q(JH,JC,I)-MIN(AVHOT(JH),AVCOLD(JC))*NHC(JH,JC,I)=L=0;


*===================================================================

*Approach temperatures

DTHEQNS(JH,JC,I)$INTERVAL(I)..

DTHC(JH,JC,I)=L=TH(JH,I) - TC(JC,I)+MAXDT(JH,JC)*(1 - NHC(JH,JC,I)) ;

DTCEQNB(JH,JC,I)$INTERVAL(I)..
 DTHC(JH,JC,I+1)=L=TH(JH,I+1)-TC(JC,I+1)+MAXDT(JH,JC)*(1 - NHC(JH,JC,I)) ;
```

```
*Forbidden Matches

FORBHCS(JH,JC,I)$(MHC(JH,JC) EQ 0)..
    Q(JH,JC,I) =E=0;
*===================================================================
```

Objective function

```
 OBJ..
        TAC=E=    AF*((CB*(SUM((JH,JC,I)$(INTERVAL(I)),NHC(JH,JC,I))))+

AFC*SUM((JH,JC,I)$(INTERVAL(I)),(Q(JH,JC,I)*(1/HOTS(JH,'H')+1/COLDS(JC,'H'))/

((((1e6)**3+(DTHC(JH,JC,I)*DTHC(JH,JC,I+1))*((DTHC(JH,JC,I)+DTHC(JH,JC,I+1))*0.
5))**0.3333)+1E-6)+(1E-6))**COEFFC))

 +  SUM((JH,JC,I),Q(JH,JC,I)*HU(JH))+SUM((JH,JC,I),Q(JH,JC,I)*CU(JC));
*=====================================================================

MODEL MULTIPLE UTILITY EXAMPLE 7 /ALL/;


*Upper/lower bounds and initialisation

MCP1.L('1')=150;      MCP1.LO('1')=150;      MCP1.UP('1')=150;
MCP1.L('2')=85;       MCP1.LO('2')=85;       MCP1.UP('2')=85;
MCP1.L('3')=1;        MCP1.LO('3')=1;        MCP1.UP('3')=20000;
MCP1.L('4')=1;        MCP1.LO('4')=1;        MCP1.UP('4')=30000;
MCP2.L('1')=1.00;     MCP2.LO('1')=1.00;     MCP2.UP('1')=30000.00;
MCP2.L('2')=140;      MCP2.LO('2')=140;      MCP2.UP('2')=140;
MCP2.L('3')=55;       MCP2.LO('3')=55;       MCP2.UP('3')=55;
MCP2.L('4')=60;       MCP2.LO('4')=60;       MCP2.UP('4')=60;


EMAT =.76;    DTHC.LO(JH,JC,I)=TMAPP;     DTHC.UP(JH,JC,I)=1000000;

*Resetting some GAMS options


OPTION LIMROW =50;      OPTION ITERLIM=100

SOLVE AUTIL USING MINLP MINIMIZING TAC;


*Calculating areas for units in superstructure

AREA(JH,JC,I)$(INTERVAL(I) AND H(JH,I) AND Q.L(JH,JC,I) )=

  Q.L(JH,JC,I)*(1/HOTS(JH,'H')+1/COLDS(JC,'H'))/((((1e-
6)**3+(DTHC.L(JH,JC,I)*DTHC.L(JH,JC,I+1))*((DTHC.L(JH,JC,I)+DTHC.L(JH,JC,I+1))
*0.5))**0.3333)+1E-6)+1E-6;


DISPLAY AREA
```

Appendix D3 GAMS code for T&SBS in Example 7.

```
$Title:  HENS by Target and Supply Based Superstructure
*Optimal T&SBS for multiple utility Example 7 written by Sarafa Azeez

SETS

 JH       Hot streams and utilities /1*4/
 JC       Cold streams and utilities /1*5/
 DATA      /TIN, TOUT, MCP,H/;

TABLE HOTS(JH,DATA) Hot streams data

      TIN         TOUT    H

 1   155.00       85.00    0.5
 2   230.00       40.00    0.5
 3   255.00       254.00   0.5
 4   205.00       204.00   0.5

TABLE COLDS(JC,DATA) Cold streams data

      TIN         TOUT     H

 1    30.00       40.00    0.5
 2    40.00       65.00    0.5
 3    115.00      210.00   0.5
 4     50.00      180.00   0.5
 5     60.00      175.00   0.5;


TABLE       MHC(JH,JC)  forbidden matches for hot and cold streams including utilities

    1  2  3   4    5
1   1  1  1   1    1
2   1  1  1   1    1
3   0  0  1   1    1
4   0  0  1   1    1;

SCALAR

NOI Number of intervals in SBS /8/;


SET

I temperature intervals NOI +1   /1*9/;
```

PARAMETERS

HU(JH)	Cost per unit of hot utility
CU(JC)	Cost per unit of cold utility
CB	Fixed charge for units
AFC	Area cost coefficient
D	Area cost index
AF	Annualisation factor
EMAT	Exchange minimum approach temperature
TKH(I)	Temperature location i in SBS
INTERVAL(I)	Intervals in the superstructure
H(JH,I)	Hot stream existence coefficient in interval I
C(JC,I)	Cold stream existence coefficient in interval I
H1(JH,I)	Hot stream supply temperature coefficients
H2(JH,I)	Hot stream supply temperature coefficients
H3(JH,I)	Hot stream supply temperature coefficients
H4(JH,I)	Hot stream supply temperature coefficients
H5(JH,I)	Hot stream supply temperature coefficients
C1(JC,I)	Cold stream supply temperature coefficients
C2(JC,I)	Cold stream supply temperature coefficients
C3(JC,I)	Cold stream supply temperature coefficients
C4(JC,I)	Cold stream supply temperature coefficients
FTB1(I)	First temperature boundary in superstructure
FTB2(I)	Second temperature boundary in superstructure
FTB3(I)	Third temperature boundary in superstructure
FTB4(I)	Fourth temperature boundary in superstructure
FTB5(I)	Fifth temperature boundary in superstructure
FTB6(I)	Sixth temperature boundary in superstructure
FTB7(I)	Seventh temperature boundary in superstructure
FTB8(I)	Eight temperature boundary in superstructure
LTB(I)	Last temperature boundary in superstructure
MAXDT(JH,JC)	
AREA(JH,JC,I)	Area of exchanger between hot stream and cold stream in interval I;

CB=13000;   AFC = 1000;   D = 0.83;   AF= 0.322;
HUC('1')=0;   HUC('2')=0;   HUC('3')=70;   HUC('4')=50;
CUC('1')=10; CUC('2')=5; CUC('3')=0;   CUC('4')=0; CUC('5')=0;

Supply temperature locations

TKH('1') = 255.00; TKH('2') = 254.00; TKH('3') = 204.00; TKH('4') = 115.00;
TKH('5') = 85.00; TKH('6') = 60.00; TKH('7') = 50.00; TKH('8') = 40.00;
TKH('9') =30.00;

MAXDT(JH,JC)=

MAX(0,COLDS(JC,'TIN')-HOTS(JH,'TIN'),COLDS(JC,'TIN')-HOTS(JH,'TOUT'),
COLDS(JC,'TOUT')-HOTS(JH,'TIN'),COLDS(JC,'TOUT')-HOTS(JH,'TOUT'));

```
INTERVAL(I)$(ORD(I) LT CARD(I)) =1;
FTB1(I)$(ORD(I) EQ 1) =1;
FTB2(I)$(ORD(I) EQ 2) =1;
FTB3(I)$(ORD(I) EQ 3) =1;
FTB4(I)$(ORD(I) EQ 4) =1;
FTB5(I)$(ORD(I) EQ 5) =1;
FTB6(I)$(ORD(I) EQ 6) =1;
FTB7(I)$(ORD(I) EQ 7) =1;
FTB8(I)$(ORD(I) EQ 8) =1;
LTB(I)$(ORD(I) EQ CARD(I))=1;


H(JH,I)$(INTERVAL(I) AND HOTS(JH,'TOUT') LE TKH(I)) = 1;
C(JC,I)$(INTERVAL(I) AND COLDS(JC,'TIN') LE TKH(I)) =1;


H1(JH,I)$(HOTS(JH,'TIN') EQ TKH(I))=1;
H2(JH,I)$(HOTS(JH,'TIN') EQ TKH(I))=1;
H3(JH,I)$(HOTS(JH,'TIN') EQ TKH(I))=1;
H4(JH,I)$(HOTS(JH,'TIN') EQ TKH(I))=1;
C1(JC,I)$(COLDS(JC,'TIN') EQ TKH(I))=1;
H5(JH,I)$(HOTS(JH,'TIN') EQ TKH(I))=1;
C2(JC,I)$(COLDS(JC,'TIN') EQ TKH(I))=1;
C3(JC,I)$(COLDS(JC,'TIN') EQ TKH(I))=1;
C4(JC,I)$(COLDS(JC,'TIN') EQ TKH(I))=1;


POSITIVE VARIABLES

TH(JH,I)          Temperature of hot stream JH as it enters interval I
TC(JC,I)          Temperature of cold stream as it leaves interval I
AVHOT(JH)         Heat content of JH
AVCOLD(JC)        Heat content of JC
Q(JH,JC,I)        Energy exchanged between JH and JC in interval I
DTHC(JH,JC,I)     Approach temperature between JH and JC in interval I
MCP1(JH)          Heat capacity flowrate of JH
MCP2(JC);         Heat capacity flowrate of JC


VARIABLE

TAC               Total annual cost;

BINARY VARIABLES

NHC(JH,JC,I)      is one if the match between JH and JC exists in interval I;
```

```
EQUATIONS
AVHOT1(JH)
AVCOLD1(JC)
ENBHSBS(JH)
ENBCSBS(JC)
EBHSBS(JH,I)
EBCSBS(JC,I)

UTHSBS(JH,I)
UTCSBS(JC,I)

SBSH1(JH,I)
SBSH2(JH,I)
SBSH3(JH,I)
SBSH4(JH,I)
SBSH5(JH,I)
SBSC1(JC,I)
SBSC2(JC,I)
SBSC3(JC,I)
SBSC4(JC,I)
SBSC5(JC,I)
CONSTHS(JH,I)
CONSTHLB(JH,I)
CONSTCS(JC,I)
CONSTCFB(JC,I)
BOUNDQS(JH,JC,I)

DTHEQNS(JH,JC,I)
DTCEQNBJH,JC,I)
FORBHCS(JH,JC,I)


OBJ           Total annual Cost;



*=====================================================================

*Available energy in hot stream JH

AVHOT1(JH)..  AVHOT(JH)=E=MCP1(JH)*(HOTS(JH,'TIN') - HOTS(JH,'TOUT'));

*Available energy in cold stream JC

AVCOLD1(JC)..  AVCOLD(JC)=E=MCP2(JC)*(COLDS(JC,'TOUT') - COLDS(JC,'TIN'));

*=====================================================================

*Overall energy balance for hot stream JH

ENBHSBS(JH)..
```

```
  AVHOT(JH) =E=SUM((JC,I)$(INTERVAL(I) AND(H(JH,I) EQ 1 AND C(JC,I) EQ
1)),Q(JH,JC,I));
```

Overall energy balance for cold stream JC

```
ENBCSBS(JC)..
  AVCOLD(JC)=E=SUM((JH,I)$(INTERVAL(I)AND (H(JH,I) EQ 1 AND C(JC,I) EQ
1)),Q(JH,JC,I));
*=====================================================================

*Interval energy balance for hot stream JH

EBHSBS(JH,I)$(INTERVAL(I) AND H(JH,I))..
  MCP1(JH)*(TH(JH,I)-TH(JH,I+1))=E=SUM(JC$(C(JC,I)),Q(JH,JC,I));


*Interval energy balance for cold stream JC

EBCSBS(JC,I)$(INTERVAL(I) AND C(JC,I))..
  MCP2(JC)*(TC(JC,I)-TC(JC,I+1))=E=SUM(JH$(H(JH,I)),Q(JH,JC,I));
*=====================================================================

*Hot stream temperatures at the first temperature location

UTHSBS(JH,I)$FTB1(I)..
  HOTS(JH,'TIN')=E=TH(JH,I);
*Cold stream temperatures at the last temperature locations

UTCSBS(JC,I)$(LTB(I) AND C4(JC,I))..
  COLDS(JC,'TIN')=E=TC(JC,I);
*=====================================================================

*Assignment of superstructure interval temperatures using hot and cold stream supply
temperatures

SBSH1(JH,I)$(FTB1(I) AND H1(JH,I) AND H(JH,I))..
 HOTS(JH,'TIN')=E=TH(JH,I);

SBSH2(JH,I)$(FTB2(I) AND H2(JH,I) AND H(JH,I))..
 HOTS(JH,'TIN')=E=TH(JH,I);

SBSH3(JH,I)$(FTB3(I) AND H3(JH,I) AND H(JH,I))..
 HOTS(JH,'TIN')=E=TH(JH,I);

SBSC1(JC,I)$(FTB5(I) AND C1(JC,I) AND C(JC,I))..
  COLDS(JC,'TIN')=E=TC(JC,I);

SBSH4(JH,I)$(FTB4(I) AND H4(JH,I) AND H(JH,I))..
 HOTS(JH,'TIN')=E=TH(JH,I);
SBSC2(JC,I)$(FTB7(I) AND C2(JC,I) AND C(JC,I))..
  COLDS(JC,'TIN')=E=TC(JC,I);
```

```
SBSC3(JC,I)$(FTB8(I) AND C3(JC,I) AND C(JC,I))..
   COLDS(JC,'TIN')=E=TC(JC,I);

SBSH5(JH,I)$(FTB6(I) AND H5(JH,I) AND H(JH,I))..
  HOTS(JH,'TIN')=E=TH(JH,I);

SBSC4(JC,I)$LTB(I)..
   COLDS(JC,'TIN')=E=TC(JC,I);
*=================================================================
```

*The following constraints guarantee that temperatures decrease from the first to the last temperature interval boundary

```
CONSTHS(JH,I)$(INTERVAL(I)AND H(JH,I))..
   TH(JH,I)=G=TH(JH,I+1);

CONSTHLB(JH,I)$(LTB(I))..
   TH(JH,I)=E=HOTS(JH,'TOUT');

CONSTCS(JC,I)$(INTERVAL(I)AND C(JC,I))..
   TC(JC,I)=G=TC(JC,I+1);

CONSTCFB(JC,I)$FTB1(I)..
   COLDS(JC,'TOUT')=E=TC(JC,I);
*=================================================================
```

*Logical constraints

```
BOUNDQS(JH,JC,I)$(INTERVAL(I)) ..
  Q(JH,JC,I)-MIN(AVHOT(JH),AVCOLD(JC))*NHC(JH,JC,I)=L=0;


*=================================================================
```

*Approach temperatures

```
DTHEQNS(JH,JC,I)$INTERVAL(I)..

DTHC(JH,JC,I)=L=TH(JH,I) - TC(JC,I)+MAXDT(JH,JC)*(1 - NHC(JH,JC,I)) ;

DTCEQNB(JH,JC,I)$INTERVAL(I)..
  DTHC(JH,JC,I+1)=L=TH(JH,I+1)-TC(JC,I+1)+MAXDT(JH,JC)*(1 - NHC(JH,JC,I)) ;
```

---

*Forbidden Matches

```
FORBHCS(JH,JC,I)$(MHC(JH,JC) EQ 0)..
     Q(JH,JC,I) =E=0;
*=================================================================
```

Objective function

```
OBJ..
    TAC=E=   AF*((CB*(SUM((JH,JC,I)$(INTERVAL(I)),NHC(JH,JC,I))))+

AFC*SUM((JH,JC,I)$(INTERVAL(I)),(Q(JH,JC,I)*(1/HOTS(JH,'H')+1/COLDS(JC,'H'))/

((((1e6)**3+(DTHC(JH,JC,I)*DTHC(JH,JC,I+1))*((DTHC(JH,JC,I)+DTHC(JH,JC,I+1))*0.
5))**0.3333)+1E-6)+(1E-6))**COEFFC))

 +  SUM((JH,JC,I),Q(JH,JC,I)*HU(JH))+SUM((JH,JC,I),Q(JH,JC,I)*CU(JC));
*==========================================================================


MODEL MULTIPLE UTILITY EXAMPLE 7 /ALL/;


*Upper/lower bounds and initialisation

MCP1.L('1')=150;     MCP1.LO('1')=150;     MCP1.UP('1')=150;
MCP1.L('2')=85;      MCP1.LO('2')=85;      MCP1.UP('2')=85;
MCP1.L('3')=1;       MCP1.LO('3')=1;       MCP1.UP('3')=20000;
MCP1.L('4')=1;       MCP1.LO('4')=1;       MCP1.UP('4')=30000;
MCP2.L('1')=1;       MCP2.LO('1')=1;       MCP2.UP('1')=30000;
MCP2.L('2')=1;       MCP2.LO('2')=1;       MCP2.UP('2')=30000.00;
MCP2.L('3')=140;     MCP2.LO('3')=140;     MCP2.UP('3')=140;
MCP2.L('4')=55;      MCP2.LO('4')=55;      MCP2.UP('4')=55;
MCP2.L('5')=60;      MCP2.LO('5')=60;      MCP2.UP('5')=60;


EMAT =.15;   DTHC.LO(JH,JC,I)=TMAPP;    DTHC.UP(JH,JC,I)=1000000;

*Resetting some GAMS options


OPTION LIMROW =50000;    OPTION ITERLIM=10000

SOLVE AUTIL USING MINLP MINIMIZING TAC;


*Calculating areas for units in superstructure

AREA(JH,JC,I)$(INTERVAL(I) AND H(JH,I) AND Q.L(JH,JC,I) )=

  Q.L(JH,JC,I)*(1/HOTS(JH,'H')+1/COLDS(JC,'H'))/((((1e-
6)**3+(DTHC.L(JH,JC,I)*DTHC.L(JH,JC,I+1))*((DTHC.L(JH,JC,I)+DTHC.L(JH,JC,I+1))
*0.5))**0.3333)+1E-6)+1E-6;

DISPLAY AREA
```

Appendix D4. GAMS code for Example 8.

```
$Title:  MENS by Supply based Superstructure
*Program Name:  MENS Example 8.
*Program written by Azeez Sarafa



SETS
I       Hot streams and utilities /1*5/
J       Cold streams and utilities/1*3/
DATA        /YIN,YOUT,G/;



TABLE   RICH (I,DATA) Rich streams data
        YIN         YOUT        G
1       0.00500       0.00100     2.00
2       0.00500       0.00250     4.00
3       0.01100       0.00250     3.50
4       0.01000       0.00500     1.50
5       0.00800       0.00250     0.50;



TABLE   LEAN(J,DATA)   Lean stream data
         YIN         YOUT
1       0.00204       0.00852
2       0.00250       0.00850
3       0.00000       0.00850;



SCALAR


NOK     Number of intervals in the superstructure /6/;


SET

K  concentration intervals NOI+1  /1*7/

PARAMETERS

AF                      Annualisation factor
ACH                     Annual cost per height for continuous contact columns
D                       Area cost exponent for mass exchangers
KW                      Lumped mass transfer coefficient
AC(J)                   Annualised (operating) cost per unit of lean stream
EMCD                    Exchanger minimum composition difference
W
TKH(K)                  Composition at interval location K
```

```
AVRICH(I)            Mass content of rich stream I
INTERVAL(K)          Intervals in superstructure
C(J,K)               Lean stream existence in interval K
R(I,K)               Rich stream existence of rich stream
C1(J,K)              Lean stream supply composition coefficients
C2(J,K)              Lean stream supply composition coefficients
C3(J,K)              Lean stream supply composition coefficients
R1(I,K)              Rich stream supply composition coefficients
R2(I,K)              Rich stream supply composition coefficients
R3(I,K)              Rich stream supply composition coefficients
R4(I,K)              Rich stream supply composition coefficients
FCB1(K)              First composition boundary in the superstructure
FCB2(K)              Second composition boundary in the superstructure
FCB3(K)              Third composition boundary in the superstructure
FCB4(K)              Fourth composition boundary in the superstructure
FCB5(K)              Fifth composition boundary in the superstructure
FCB6(K)              Sixth composition boundary in the superstructure
LCB(K)               Last composition boundary in the superstructure
MAXDC(I,J)           The upper bound for composition difference
TCC Number of stages of exchangers between streams I and J in interval I K;

ACH=618;  D=0.66;   AC('1')=0;  AC ('2')=0;  AC ('3')=14670;  KW=0.02;
AF=0.225;  W=.01;



TKH('1') = 0.01100;  TKH('2')= 0.01000;  TKH('3')= 0.00800; TKH('4')= 0.00500;
TKH('5')= 0.00250;  TKH('6')= 0.00204;  TKH('7')= 0.00000;


AVRICH(I) = RICH(I,'G')*(RICH(I,'YIN')-RICH(I,'YOUT'));


MAXDC(I,J)=MAX(0,LEAN(J,'YIN')-RICH(I,'YIN'),LEAN(J,'YIN')-RICH(I,'YOUT'),
         LEAN(J,'YOUT')-RICH(I,'YIN'),LEAN(J,'YOUT')-RICH(I,'YOUT'));



INTERVAL(K)$(ORD(K) LT CARD(K)) =1;
FCB1(K)$(ORD(K) EQ 1) =1;
FCB2(K)$(ORD(K) EQ 2) =1;
FCB3(K)$(ORD(K) EQ 3) =1;
FCB4(K)$(ORD(K) EQ 4) =1;
FCB5(K)$(ORD(K) EQ 5) =1;
FCB6(K)$(ORD(K) EQ 6) =1;
LCB(K)$(ORD(K) EQ CARD(K))=1;



R(I,K)$(STAGE(K) AND RICH(I,'YIN') GE TKH(K))=1;
C(J,K)$(STAGE(K) AND LEAN(J,'YIN') LE TKH(K))=1;
```

```
R1(I,K)$(RICH(I,'YIN') EQ TKH(K))=1;
R2(I,K)$(RICH(I,'YIN') EQ TKH(K))=1;
R3(I,K)$(RICH(I,'YIN') EQ TKH(K))=1;
R4(I,K)$(RICH(I,'YIN') EQ TKH(K))=1;
C1(J,K)$(LEAN(J,'YIN') EQ TKH(K))=1;
C2(J,K)$(LEAN(J,'YIN') EQ TKH(K))=1;
C3(J,K)$(LEAN(J,'YIN') EQ TKH(K))=1;


POSITIVE VARIABLES
CR(I,K)            Composition of rich stream I as it enters composition interval K
CL(J,K)            Composition of lean stream J as it leaves composition interval K
AVLEAN(J)          Mass content of lean stream J
M(I,J,K)           Mass exchanged between rich stream I and lean stream J in interval K
L(J)               Flowrate of lean stream J
DCRC(I,J,K)        Approach composition between I and J in interval K
NHC(I,J,K)         Relaxed binary variable
PNHC(I,J,K)        Positive tolerance
SNHC(I,J,K)        Negative tolerance;


VARIABLE
TAC                Total annual cost;


BINARY VARIABLES
NNHC(I,J,K)        is one if a match exist between I and J in interval K;


EQUATIONS
MABALRS(I)
MABALLS(J)
MBRSTS(I,K)
MBLSTS(J,K)
AVLEANS1(J)

UTILR(I,K)
UTILL(J,K)

CINL1(J,K)
CINL2(J,K)
CINL3(J,K)


CINR1(I,K)
CINR2(I,K)
CINR3(I,K)
CINR4(I,K)
```

CONSCL(J,K)
CONSCRL(J,K)
CONSCLR(I,K)
CONSCLF(I,K)
BOUNDM(I,J,K)

DTREMN1(I,J,K)
DTREMN2(I,J,K)
DTLEMN1(I,J,K)
DTLEMN2(I,J,K)

N1(I,J,K)
P(I,J,K)
S(I,J,K)

OBJ;
*===

Mass content of lean stream J

AVLEAN1(J).. AVLEAN(J)=E=L(J)*(LEAN(J, 'YOUT')- LEAN(J,'YIN'));

*===
Total mass balance for rich stream I
MABALRS(I)..
((RICH(I,'YIN')-RICH(I,'YOUT'))*RICH(I,'G'))=E=SUM((J,K)$(INTERVAL(K) AND (R(I,K) EQ 1 AND C(J,K) EQ 1)),M(I,J,K));

Total mass balance for lean stream J
MABALLS(J)..
AVLEAN(J)=E=SUM((I,K)$(INTERVAL(K) AND (R(I,K) EQ 1 AND C(J,K) EQ 1)),M(I,J,K));
*===
Interval mass balance for rich stream I
MBRSTS(I,K)$(INTERVAL(K) AND R(I,K))..
RICH(I,'G')*(CR(I,K)-CR(I,K+1))=E=SUM(J$(C(J,K)),M(I,J,K));

Interval mass balance for lean stream J
MBLSTS(J,K)$(INTERVAL(K) AND C(J,K))..
L(J)*(CL(J,K)-CL(J,K+1))=E=SUM(I$(R(I,K)),M(I,J,K));

*===
Composition of rich stream at first composition boundary

UTRSBS(I,K)$FCB1(K)..
RICH(I,'YIN')=E=CR(I,K);
Composition of lean stream at last composition boundary

```
UTLSBS(J,K)$(LCB(K) AND C3(J,K))..
 LEAN(J,'YIN')=E=CL(J,K);

*=====================================================================
Assignment of SBS interval composition using supply composition of rich and lean streams
SBSR1(I,K)$(FCB1(K) AND R1(I,K) AND R(I,K))..
 RICH(I,'YIN')=E=CR(I,K);
SBSR2(I,K)$(FCB2(K) AND R2(I,K) AND R(I,K))..




RICH(I,'YIN')=E=CR(I,K);
SBSR3(I,K)$(FCB3(K) AND R3(I,K) AND R(I,K))..
 RICH(I,'YIN')=E=CR(I,K);
SBSR4(I,K)$(FCB4(K) AND R4(I,K) AND R(I,K))..
 RICH(I,'YIN')=E=CR(I,K);
SBSL1(J,K)$(FCB5(K) AND C1(J,K) AND C(J,K))..
 LEAN(J,'YIN')=E=CL(J,K);
SBSL2(J,K)$(FCB6(K) AND C2(J,K) AND C(J,K))..
 LEAN(J,'YIN')=E=CL(J,K);
SBSL3(J,K)$LCB(K)..
 LEAN(J,'YIN')=E=CL(J,K);
*=====================================================================
*The following guarantee decrease in composition from the first to the last composition boundary
CONSCLRB(I,K)$(STAGE(K) AND R(I,K))..
  CR(I,K)=G=CR(I,K+1);
CONSCLFB(I,K)$(LCB(K))..
  CR(I,K)=E=RICH(I,'YOUT');
CONSCLB(J,K)$(STAGE(K))..
  CL(J,K)=G=CL(J,K+1);
CONSCRLB(J,K)$FCB1(K)..
  LEAN(J,'YOUT')=E=CL(J,K);
*=====================================================================
Logical constraint
BOUNDMS(I,J,K)$(STAGE(K))..
  M(I,J,K)-MIN(AVRICH(I),AVLEAN(J))*NHC(I,J,K)=L=0;
*=====================================================================
*Approach compositions
DTREMNS1(I,J,K)$(STAGE(K))..
  DCRC(I,J,K)=L=CR(I,K)-CL(J,K)+MAXDC(I,J)*(1-NHC(I,J,K));
DTREMNS2(I,J,K)$(INTERVAL(K))..
  DCRC(I,J,K)=G=CR(I,K)-CL(J,K)-MAXDC(I,J)*(1-NHC(I,J,K));
DTLEMNS1(I,J,K)$(INTERVAL(K))..
  DCRC(I,J,K+1)=L=CR(I,K+1)-CL(J,K+1)+MAXDC(I,J)*(1-NHC(I,J,K));
DTLEMNS2(I,J,K)$INTERVAL(K)..
  DCRC(I,J,K+1)=G=CR(I,K+1)-CL(J,K+1)-MAXDC(I,J)*(1-NHC(I,J,K));

*=====================================================================
```

```
P(I,J,K)$(INTERVAL(K) AND C(J,K))..
PNHC(I,J,K)=E=.0000000001;

S(I,J,K)$(INTERVAL(K) AND C(J,K))..
SNHC(I,J,K)=E=.0000000001;

N1(I,J,K)$(INTERVAL(K) AND C(J,K))..


NHC(I,J,K)=E=NNHC(I,J,K)+(PNHC(I,J,K)-SNHC(I,J,K));

*==================================================================

*Objective function
OBJ..


 TAC=E=AF*(ACH*SUM((I,J,K)$(INTERVAL(K)),(M(I,J,K)*(1/KW)/((((1E-
6)**3+(DCRC(I,J,K)*DCRC(I,J,K+1))*((DCRC(I,J,K)+DCRC(I,J,K+1))*0.5))**0.3333)+
1E-6)+1E-6)**D))
         + SUM((J),L(J)*AC(J)) + W*(SUM((I,J,K),PNHC(I,J,K)+SNHC(I,J,K)));

*==================================================================


MODEL SBS MENS EXAMPLE 8 /ALL/;


*Upper/lower bounds and initialisation

*INTERVAL 1

L.L('1')=1;           L.LO('1')=1;              L.UP('1')=1.5;
L.L('2')=.1;            L.LO('2')=.1;            L.UP('2')=1;
L.L('3')=1;            L.LO('3')=1;               L.UP('3')=10;



EMAC = .000096;

DCRC.LO(I,J,K)=EMAC;
DCRC.UP(I,J,K)=1;
*Resetting some GAMS options

OPTION LIMROW =50;

SOLVE AUTIL USING MINLP MINIMISING TAC;
```

```
* Calculating areas for units in superstructure


HEIGHT(I,J,K)$(INTERVAL(K)AND   R(I,K)   AND   C(J,K))=(M.L(I,J,K)*(1/KW)/((((1E-
6)**3+
(DCRC.L(I,J,K)*DCRC.L(I,J,K+1))*((DCRC.L(I,J,K)+DCRC.L(I,J,K+1))*0.5))**0.3333)+
1E-6)+1E-6) ;


OPTION  AVRICH:5;   DISPLAY AVRICH;
OPTION CR:5:1:1;        DISPLAY CR.L;
OPTION CL:5:1:1;        DISPLAY CL.L;
OPTION M:5;             DISPLAY M.L;
OPTION L:5;             DISPLAY L.L;
```