Water Conservation Through Energy Conservation

Report to the
Water Research Commission

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EXECUTIVE SUMMARY

Background

South Africa has amongst the cheapest energy supplies in the world and it is rich in mineral resources. Economic considerations have resulted in a relatively inefficient use of resources including thermal energy when bench-marked against world best practice. While this may provide a temporary economic competitive advantage, it results in poor environmental performance and has led to South Africa being classified as environmentally dirty. Furthermore, South Africa has limited water resources and measures are being taken to conserve the water that is available. Most of the water is used for agriculture and irrigation (59%), forestry (4%), rural (4%), urban (25%), power generation (2%) and mining and bulk industry (6%). (Mukheibir and Sparks, 2003)

Industries with thermal processes (as opposed to electrical processes and excluding electrical power generation), are a significant sub-class of the industrial water-using sector. Energy which is consumed in excess has to be dissipated. This is frequently through the use of wet cooling towers, where the excess energy is used to evaporate water. This results in a two-fold problem for the aqueous environment. Firstly the evaporated water is lost from the national water cycle. Secondly, the salts contained in the cooling water remain behind for discharge or disposal as cooling tower blow-down. The blow-down consists of highly soluble sodium or chloride ions and of less soluble calcium and magnesium cations, and sulphate and carbonate anions. The soluble salts contribute to the salination of the aquatic system, while the sparingly soluble salts contribute to scaling problems either where the blow-down is being treated, or in the receiving water.

Two separate but similar process integration techniques (thermal pinch analysis and water pinch analysis) have been developed to optimise the thermal efficiency or the water efficiency in industrial complexes. These techniques have evolved to meet the needs for increased thermal efficiency (firstly because of the first "energy crisis" in the 1970s and then the subsequent global warming / carbon dioxide issue of the 1990s) and for reduced water consumption (primarily intake water volume in well endowed, water rich regions). Thermal pinch is a mature technique, while water pinch is evolving rapidly. Combining these two techniques could result in significant energy and water savings in South African industries.

Objectives of the study

The overall aim of this project was to promote both water and energy savings in the South African process industry through more efficient use of both process water and cooling and heating utilities. This was to be achieved by creating awareness of potential water and energy savings in the process industry and through the development and promotion of tools incorporating water and thermal pinch and mathematical modelling for the optimisation of water and heat exchanger networks. Specific objectives were:

1. Conserve the use of water by the process industry through thermal energy conservation.
2. Reduction of salination through the reduced cooling need by the process industry.
3. Develop a rigorous and rational technique to optimize cooling circuits for simultaneous water and energy conservation.

Approach

Water and energy conservation in the process industry is an inherently multidimensional problem. Optimising the use of these resources requires a very careful definition of the problem to be considered. In general, process water and heating/cooling requirements as well as effluent production are functions of process design and operation and may be interdependent. This is particularly true in the case of mass transfer operations which involve aqueous process streams since mass transfer efficiency is generally a function of temperature. In addition, cooling tower performance depends on the temperature and chemical quality of the cooling water (dissolved and suspended solids levels), the former being determined by process thermal requirements and the latter being constrained by fouling considerations. Changes in process operation or design can therefore affect cooling tower performance. Consequently, achieving the maximum overall savings in water and energy requires a better understanding of the interactions between the various subsystems and an integrated approach to the design of entire industrial process systems (including reactors, mass transfer and heat transfer networks, cooling towers etc.).

The approach taken in this study was to develop models of the interactions between various subsystems in the process industry and tools in the form of computer packages and graphical methods for their design and optimisation. The work was carried out by two independent research groups: Professor Duncan Fraser's Environmental and Process Systems Engineering Group at the University of Cape Town (UCT) and Professor Thokozani Majozi's group at the University of Pretoria (UP). The approach taken by each group was determined by their existing expertise.

The UCT group's expertise is in the field of analysis and design of heat and mass transfer networks. This group therefore focused on working towards the development of a methodology and tools for the analysis and design of systems in which the heat and mass exchanger networks are not independent, but interact with each other, with a view to being able to apply these techniques to systems in water conservation could be achieved through energy conservation.

Professor Thokozani Majozi has a background in process optimisation in general, and water pinch analysis in particular. The UP contribution was to undertake a case study of a site with the potential for water savings through the optimisation of the operation of the cooling circuit. During the course of the study, a cooling water network design was developed for systems with multiple cooling water systems. The technique is an extension of that developed by Kim and Smith (2001) for cooling water networks with a single cooling water source.

The following sections describe in the work done and results obtained by each team.

Development of Procedures for the Design of Combined Heat and Mass Exchange Systems (University of Cape Town)

The contribution of the University of Cape Town is presented in Part 1 of this report. Considerable progress has been made towards the objective of having a generalised methodology and tools to handle situations in which both heat transfer and mass transfer occur, but there remain areas that still need to be resolved.

In this study UCT have identified two basically different types of systems. In the first type of system either the heat or mass exchange system may be used to enhance the performance of the other system. In this case the system which is optimised by the other one is termed the foundation problem.

The most common example of this type is a water-using (or mass exchange) operation that can be improved by use of heat exchange, with the heat exchange being supplied by hot and cold utilities. Here the water-using (or mass transfer) system is the foundation problem, and its performance would be enhanced by changing the temperatures of the water-using streams (or the mass separating agents). Something which would be less common would be a heat exchange system which is improved by means of utility water or utility mass separating agents.

In the second type of system there is both a water-using (or mass transfer) system as well as hot and cold process streams (the heat exchange system), and there is interaction between them, so neither can be used as the foundation problem.

Design approaches developed

Problems in which energy utilities are used to enhance water use or mass exchange

Several different types of problems where water is used as a MSA have been considered. Based on the three different *Combined Heat and Mass Exchange Network Synthesis* (CHAMENS) problems considered in Section 3 of Part 1, a synthesis algorithm for achieving optimal designs in problems in which energy utilities are used to enhance water use or mass exchange can be described as follows:

Mass Exchange Network Synthesis (MENS) problems with one MSA

- Identify the most dominant variable and discretise (each being a topology), in this case, the mass exchange temperature is the most dominant of the variables and is not influenced by other variables. The search for the optimum is carried out within each of these temperature options (topologies) with the supply temperature for the only available MSA being the first topology while the lowest working temperature for the MSA is the last.
- Within each topology, the optimum *minimum concentration driving force* ε is identified and for each optimum ε the $\Delta T_{\min}$ is optimized. The best $\Delta T_{\min}$ is noted so that it can then be compared with the best $\Delta T_{\min}$ from other ε. The least combination in terms of cost of ε - $\Delta T_{\min}$ is taken as the best for the concerned topology.
- The second step is repeated for all the temperature topologies and the least ε - $\Delta T_{\min}$ combination is taken as the optimum solution.

Note, however, that this is beneficial in situations in which the *Heat Exchange Network* (HEN)-cost is not dominant. However, this approach is still good in that it helps to identify the dominant network in terms of costs between the HEN and MEN since a thorough search is carried out at all the variables that affect the costs of each of these networks so that the least combined cost of HEN and MEN can be easily compared with the MENS base problem (i.e. at the supply conditions with no option of introducing HENS).

MENS problems with non-overlapping MSAs

Each of the MSAs in this type of MENS problem is restricted to each side of the pinch, the process MSA being above while the external is below. The procedure highlighted above for MENS problems with one MSA is followed for each side of the pinch division here as well. But for cases in which the process MSA at a low mass exchange temperature is not able to take away alone the entire mass load, the following steps should be followed:

- Identify temperature topologies for both process and external MSAs, i.e. above and below the pinch.
- Carry out a one-one mapping of the two temperature topologies at each mass exchange temperature and then follow the procedure stated for the MENS problem with just one MSA.

MENS problems with overlapping MSAs

The procedure for the MENS problems with non-overlapping MSAs is also followed here, the difference lies in the fact that the mapping of the temperature topologies would result in a matrix which will be somewhat difficult to handle manually since within each topology there still exists variables which need to be optimized.

Problems in which process energy streams are used to enhance water use or mass exchange

Two approaches of combining the synthesis of heat and mass exchanger networks have been considered and applied to a test problem. It can be deduced from the second technique that combined heat and mass exchange network problems are highly interactive and that there exists opportunities for saving costs. This test problem, through the sequential synthesis approach, has revealed the many topologies which exist in the combined network and also gives the designer a feel of how each of these topologies contribute to the CHAMENS total annual cost.

It has been demonstrated that the heat exchange *grand composite curve* could be used as a framework for optimising the combined system since the best positioning of the MSA streams as utility in the heat exchange operation could easily be identified on the grand composite curve.

Also, it is shown that combining the synthesis of heat and mass exchangers is beneficial not only to the mass exchanger network, but also to the heat exchanger network. This is because the use of the MSA as a utility in the heat exchanger network helps in reducing the utility need of the heat exchange operation, also the capital cost of the HEN is reduced because the MSA streams are operating at a reduced heat capacity flowrate.

Water pinch analysis

The technique known as water pinch analysis has a somewhat wider scope than the use of water as a MSA, since water is used in processes for many diverse purposes other than mass separation, including its use as a heat transfer medium. The approach used in water pinch analysis to handle this diversity of application has been to require that all process requirements be expressed purely in terms of quantity and quality constraints for the water streams, so that the analysis does not have to consider the nature of the processes which give rise to the constraints. The preceding development of CHAMENS therefore does not fully address the water pinch problem, and further work is required to include all aspects of water use into the methodology. In section 5.3 of Part 1, a start has been made by including water pinch capability into the targeting software.

Software Development

UCT have written a software package that will analyse both heat and mass exchange networks independently. They have also added the capability to analyse water pinch networks. The main software package was developed as a master's degree project by Khaya Ndwandwe, and the water pinch targeting component was added by Prashant Bansal as a research internship.

As it stands, this computer package can be used for analysis of heat and mass exchange systems on their own, in order to establish which system dominates. It is also useful for iterative calculations to establish the interaction between the heat and mass exchange systems. This is based on the presumption that comparing targets provides a valid determination of what could be achieved in the design of such systems. This approach is justified on the basis of experience that has shown that it is always possible to achieve the utility targets (whether energy utilities or *Mass Separating Agent* (MSA) utilities), and that capital costs targets for both energy and mass exchange systems can be approached to within less than 10%.

Work in Progress

A fundamentally different approach is being developed for the situations in which there is interaction between the water-using (or mass transfer) and energy-using (or energy transfer) systems. This requires a more complex methodology in which conceptual Pinch Technology techniques are combined with mathematical programming optimisation techniques, such as Mixed-Integer Non-Linear Programming (MINLP).

Training

It should be noted that three students have had a major hand in the work of this part of the overall project, all of whom have been black (but only one of them is South African):

- Khaya Ndwandwe – M.Sc.(Eng), Black South African Male
- Prashant Bansal – Research Internship for IIT Bombay, Indian Male
- Adeniyi Isafiade – Ph.D., Nigerian Male

Technology Transfer

UCT produced the following outputs, mainly in the form of publications related to the work of this project:

Computer software (1)

Targeting package for the analysis of heat and mass exchange systems, including special section on water pinch. This package runs on Excel.

Journal Publications (4)

"Determination of Mass Separating Agent Flows Using the Mass Exchange Grand Composite Curve," Duncan Fraser, Michael Howe, Andre Hugo and Uday Shenoy, 83(A12), 1381-1390, *Chem Eng Research and Design*, 2005.

"The influence of particle size on energy consumption and water recovery in comminution and dewatering systems", Mwale, A.H., Musonge, P., and Fraser, D.M., *Minerals Engineering*, 18, 915-926, 2005.

"A New Method For Sizing Mass Exchange Units Without The Singularity Of The Kremser Equation", Fraser, D.M., and Shenoy, U.V., *Computers and Chem Eng*, **28**(11), 2331-2335, 2004.

"A New Formulation of the Kremser Equation for Sizing Mass Exchangers", Shenoy, U.V., and Fraser, D.M., *Chemical Engineering Science*, **58**(22), 5121-5124, 2003.

Theses (1)

"A Spreadsheet-Based Tool For The Synthesis Of Heat And Mass Exchange Networks", Ndwandwe, K.P., M.Sc.(Eng), 2003.

Conference publications (9)

Six papers were presented at international conferences and three papers at local conferences. Full details of these are given Part 3 of the main report.

Water Conservation Through Energy Conservation Case Study: African Explosives, Modderfontein (University of Pretoria)

The contribution of the University of Pretoria is presented in Part 2 of the main report. The site chosen for use as the case study was Unit 11 at the African Explosives Limited (AEL) factory in Modderfontein. The facility produces nitric acid, which is one of the intermediate products used in the production of ammonium nitrates, fertilizer and explosives for the mining industry.

Objectives

After assessing the case study which was chosen for the project, the objectives of the project were adapted. The specific aim of the project was to develop a graphical methodology to target and design cooling water networks, using basic principles of Pinch Analysis, for systems with multiple cooling water sources. The refocusing of the research project objectives was motivated by the observation that the case study system had two cooling water sources and could not be fully analysed using the techniques currently available, which only address systems with single cooling water sources.

Approach

This research project was undertaken by Ms Nongezile Nyathi, a full-time M.Eng. student at the University of Pretoria, under the supervision of Professor Thokozani Majozi. At the start of the project in July 2004, literature review was conducted to find out what techniques could be used to achieve the objectives of the project. Then the data required for the analysis was collected from the production team, headed by Mr Alan Pikor at AEL. This was followed by preliminary calculations which were done using heat exchanger network (HENs) design, to investigate the possibility of reducing the utilities used. This investigation showed that the process was a threshold process where only cooling water is required as an external utility. Consequently, the investigation was focused on the low temperature end of the process, which involves a cooling tower and the associated cooling water network. The cooling water network design techniques were used during the investigation. The possibility to reduce the amount effluent produced in the cooling tower in the form of blowdown was also investigated.

During the course of the project, four feedback sessions where held at the AEL production facility in Modderfontein to update the production staff on the progress of the project and gather more data.

Results and Discussion

A cooling water network design was developed for systems with multiple cooling water systems. The technique is an extension of that developed by Kim and Smith (2001) for cooling water networks with a single cooling water source. Furthermore, a cooling tower model was used to investigate the impacts of the new cooling water conditions on the performance of the cooling tower.

Cooling Water Network Design

The cooling water network design technique developed is divided into two parts, namely targeting and design. Figure 1 shows the targeting technique used to obtain the optimal amount of cooling water required to cool the process.

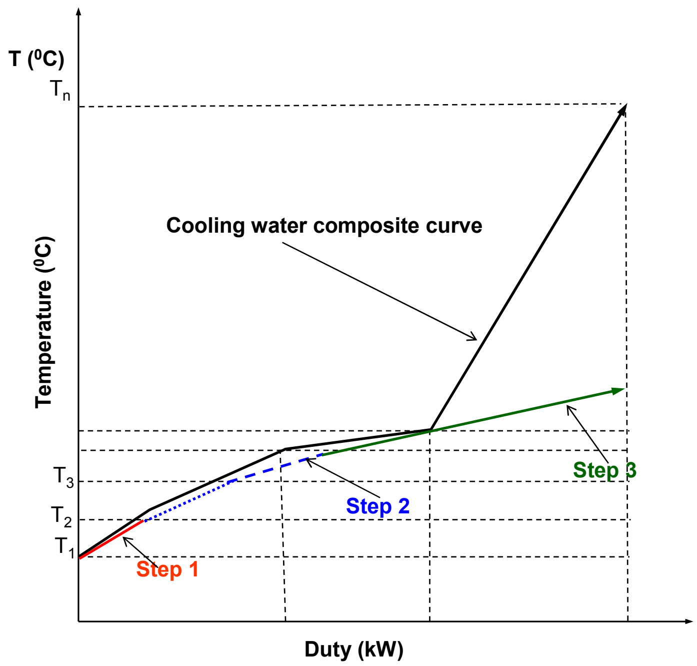

Figure 1: Targeting steps for systems with multiple cooling water sources

The targeting technique is performed in three steps. The first step is for the cooling water source with the lowest supply temperature, i.e. the primary source and the second step is for the intermediate cooling water sources. The main aim is to maximize the amount of cooling water used from the cooling water sources with the minimum and intermediate supply temperatures. The change in the gradient of the cooling water supply line indicates that there is an additional cooling water source and an increase in the cooling water flowrate. The third step is for the cooling water source with the maximum supply temperature. In order to minimize the overall amount of cooling water used, the amount of water used from the last cooling water source, i.e. the source with the highest supply temperature, should be minimized.

The cooling water network design which meets the target was designed using the technique given by Kim and Smith (2001). The advantage of this technique is that several designs which meet the target can be obtained. Table 1 shows the current cooling water flowrates used in the heat exchangers and the new flowrates based on the new design.

Table 1: Cooling water requirements for the improved cooling water network

Heat Exchanger	T_{supply} (°C)	T_{target} (°C)	Flowrate (t/h)	New Flowrate (t/h)
1	24	28	2 290	2 290
2	28	44	2 390	895
3	24	42	1 450	643
4	24	29	60	51
5	32	44	450	59
6	32	46	900	269
7	35	34	1 700	214

A cooling tower model based on the model by Kim and Smith (2001) was used to assess the impacts of the new cooling water flowrate on the performance of the cooling tower. The results indicated that increasing the inlet cooling water temperature to the cooling tower from 34°C to 37°C increases the evaporation by 4%. However, the objective of the investigation of reducing the effluent produced by the cooling tower, in the form of blowdown is achieved as the amount of cooling water blowdown is reduced by 47%. The makeup stream is also reduced by 10%.

The main results of the analysis were:

1. The results obtained from the analysis showed that there is a possibility to reduce the blowdown rate by 47% and the freshwater makeup by 10 %.
2. The reduction in the blowdown rate has a potential to reduce the blowdown treatment costs by almost R480 000 per year.
3. The results also showed that there exists a potential to reduce the overall cooling water requirement from 3900 t/h to 2984 t/h, i.e. 23% reduction. This reduction is concomitant with a slight increase in the return temperature from 34°C to 37°C.
4. The cooling tower model developed by Kim and Smith (2001) was used to demonstrate that the high return temperature of 37°C obtained with the new cooling water network would not adversely affect the supply temperature to the cooling water network. The results from the model indicated that when the return temperature was 37°C, the inlet cooling water temperature to the cooling water network was 23.4°C. This is lower than the current value of 24°C, which shows that more heat is removed by the cooling tower, thus the performance of the cooling tower is improved.
5. To obtain the optimum solution when using multiple cooling towers with different supply temperatures, all the cooling water from the primary source should be used first before using water from any other cooling water source. The target for the cooling tower with the highest supply temperature is set by the pinch.
6. The amount of salination was reduced although the heat duty remains the same because the amount of salts discharged to the water system is reduced as the amount of blowdown leaving the cooling tower is reduced.

Recommendations

1. Heat exchanger network design (HEN) should be done prior to designing the cooling water network, to investigate the possibility of reducing the overall amount of external utilities that are required by the process thus saving energy and reducing operating costs.
2. The cycles of concentration of the cooling tower have a significant impact on the amount of effluent produced, thus the optimal value should be investigated as another way of reducing the amount of effluent produced.
3. The graphical technique presented in this report is such that the return temperature is not fixed, i.e. there is no limit to the value of the return temperature. In reality, one

finds that the maximum return temperature is set by either fouling considerations, corrosion or design considerations of the cooling tower packing. In these instances, the final water supply line is set by the maximum acceptable return temperature. It is possible that this line would not form a pinch with the limiting cooling water composite curve, thus it will not be possible to obtain the minimum cooling water requirement directly. The water mains method presented is based on the concept of the pinch point and can not be readily applied to cases where there is no pinch. In this case, the pinch migration method suggested by Kim and Smith (2001) can be adopted. In this method, the limiting cooling water composite curve is allowed to move along the temperature axis until a new pinch is formed. The details of how to find the new pinch point and how to modify the composite curve are given in Kim and Smith (2001). The pinch migration and temperature shift method enables design with any target temperature (Kim and Smith, 2001). The cooling water flowrate obtained this way may be minimum but not necessarily optimal.

4. The graphical technique as presented in chapter 3 of this report assumes that premixing and post mixing are acceptable. Premixing refers to a situation where, cooling water from different cooling water sources is mixed before it is used in any water-using operation. Post mixing refers to a situation where cooling water which has been used in the cooling water using operations is mixed before it is returned to the cooling water sources. There may exist situations where premixing is not acceptable due to geographical constraints or maximum supply temperature acceptable. Moreover, there may be situations where post mixing is not allowed due to the maximum return temperatures acceptable for the various cooling water sources or due to the process layout. For these reasons, there is a need to investigate a way of incorporating these constraints to the graphical technique. However, it is possible to set these constraints when mathematical formulation is used.

Technology Transfer

Routine feedback sessions with AEL were held during the course of the project. The following summarizes the presentations and publications related to this research project:

Majozi T. and N. Nyathi, Process Design and Process Integration, *PRES'05 8th Conference on Process Integration, Modeling and Optimization for Energy Saving and Pollution Reduction, Giardini di Naxos, Sicily, 15-18 May 2005*: (Poster Presentation)

Majozi, T and N. Nyathi, "On cooling water and effluent reduction in systems with multiple cooling water sources – a pinch design philosophy", *Chemical Technology Innovations Awards,* November 2005 – *3rd Prize*

Two journal articles have since been submitted to international journals.

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The members of the steering committee are thanked for their time and input. The members of the committee were:

Mr GN Steenveld	Water Research Commission (Chairman)
Prof CA Buckley	University of KwaZulu-Natal
Prof R Bharuthram	University of KwaZulu-Natal
Mr CJ Brouckaert	University of KwaZulu-Natal
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PART 1

Development of Procedures for the Design of Combined Heat and Mass Exchange Systems

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PART 1

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2 LIST OF SYMBOLS

Symbol	Meaning
A	Heat transfer area
c	Heat exchange cost coefficient
C	Cost of utility
CP	Set of cold process streams
CP_{C}	Heat capacity of the cold stream OR
CP_{H}	Heat capacity of the hot stream
CU	Set of cold utility streams
$EMAT$	Minimum approach temperature = ΔT_{min}
FCp	Heat capacity flowrate
G	Rich stream flowrate
H	Stream film heat transfer coefficient
H_{min}	Minimum packing height target for a network
HP	Set of hot process streams
$HRAT$	Heat recovery approach temperature
HTU	Height of a transfer unit
HU	Set of hot utility streams
K	Enthalpy interval
$K_y a$	Mass transfer coefficient
K_{W}	Lumped coefficient for calculating required exchanger mass
L	Lean stream flowrate
L_j^c	Upper bound on the available flowrate of the j^{th} MSA

m_j	Linear equilibrium coefficient
M	Mass of an exchanger
N	Number of equilibrium stages in a mass exchanger
N_{real}	Number of real stages in a mass exchanger
N_{C}	Number of cold streams
N_{H}	Number of hot streams
N_R	Number of rich streams
N_S	Number of lean streams
N_{SP}	Number of external MSA streams
N_{SP}	Number of process MSA streams
N_{Shells}	Number of shells
NTU	Number of transfer units
N_{units}	Number of heat/mass exchanger units
O_{ij}	Mass exchanger connecting streams *i* and *j*
q	Enthalpy change of a given stream
Q	Enthalpy change
Q^C	Heat transferred to cold process streams
$\mathrm{Q}_{\mathrm{Cmin}}$	Minimum cold utility target
Q^H	Heat transferred from hot process streams
$\mathrm{Q}_{\mathrm{Hmin}}$	Minimum hot utility target
QS	Heat transferred from hot utility streams
QW	Heat transferred to cold utility streams
R_k	Residual heat from the k^{th} interval
S	Number of streams for heat/mass transfer or mass transfer column cross section
TI	Set of all temperature intervals

TIAT	Temperature interval approach temperature
U	Overall heat transfer coefficient
$U_{i,j,m}$	Upper bound on exchangeable mass between *i* and *j* in subnetwork *m*
w_i	Mass load of stream *i*
W_k	Mass transferred in interval *k*
x_i	Composition of lean stream in contact with rich stream *i*
x_i^s	Inlet composition of lean stream *i*
x_i^t	Target composition of lean stream *i*
x_i*	Composition of lean stream in equilibrium with rich stream *i*
y_i	Composition of rich stream *i*
y_i^s	Inlet composition of rich stream *i*
y_i^t	Target composition of rich stream *i*
δ_k	Residual mass from the k^{th} interval
ε	Minimum allowable composition difference = minimum allowable difference $x_i* - x_i$ for feasible mass transfer
ΔT_{lm}	Log mean temperature difference
ΔT_{min}	Minimum approach temperature
Δy_{lm}	Log mean concentration difference in the rich stream
Δy_{min}	Minimum concentration difference expressed in terms of the rich stream
$\left(\sum G\right)_k$	Total rich stream flowrate in interval *k*
$\left(\sum L\right)_k$	Total lean stream flowrate in interval *k*

3 LIST OF ABBREVIATIONS

AOC	Annual operating cost
ACC	Annual capital cost
CHAMENS	Combined heat and mass transfer networks synthesis
DFP	Driving force plot
GCC	Grand composite curve
GUI	Graphical user interface
LP	Linear programming
MILP	Mixed integer linear programming
MINLP	Mixed integer non-linear programming
MSA	Mass separating agent
NLP	Non linear programming
RPA	Remaining problem analysis
TAC	Total annual cost
UCT	University of Cape Town

GLOSSARY

Enthalpy intervals

Composite curves

Grand composite curve (GCC)

Grassroots network synthesis

Lean stream

Pinch

Retrofit networks systems

Rich streams

Shells

Superstructure/hyperstructure

Supertargeting

Targeting

Vertical heat transfer

INTRODUCTION

This report highlights what has been achieved by the UCT team in the course of this project. Water conservation through energy conservation is a specific application of the general subject of combined heat and mass exchange. The expertise of the UCT team is in the area of analysis and design of heat and mass exchanger networks.

The contribution of the UCT team to this project was therefore to develop a methodology and tools for the analysis and design of systems in which the heat and mass exchanger networks are not independent, but interact with each other, with a view to being able to apply these techniques to systems in water conservation could be achieved through energy conservation.

Considerable progress has been made towards the objective of having a methodology and tools to handle all conceivable situations in which both heat transfer and mass transfer occur, but there remain areas that still need to be resolved.

We had a good start with the development of the basic computer package for separate heat and mass exchange networks by Khaya Ndwandwe (this was his master's degree project). This was further developed by Prashant Bansal who added Water Pinch functionality to the package (done as a research internship for the Indian Institute of Technology, Bombay).

We struggled to find a suitable student to continue the work, until we were able to recruit Adeniyi Isiafaide from Nigeria to do a doctorate on the topic of combined heat and mass exchange. While this will ultimately achieve the objectives we set for this study, the nature of doctoral research meant starting from a fundamental and general point of view, rather than an applied and specific point of view.

So we have made some good progress in terms of development of the general methodology and tools, but have yet to reap the full benefits of this in terms of the specific application to water conservation through energy conservation.

It should be noted that most of the example problems that have been tackled in this project have been problems in which water was the mass separating agent used for removal of contaminants (Examples 3.1, 3.3 and 4.1).

In this study we have identified two basically different types of systems. In the first type of system either the heat or mass exchange system may be used to enhance the performance of the other system. In this case the system which is optimised by the other one is termed the foundation problem.

The most common example of this type is a water-using (or mass exchange) operation that can be improved by use of heat exchange, with the heat exchange being supplied by hot and cold utilities. Here the water-using (or mass transfer) system is the foundation problem, and its performance would be enhanced by changing the temperatures of the water-using streams (or the mass separating agents). Something which would be less common would be a heat exchange system which is improved by means of utility water or utility mass separating agents.

In the second type of system we have both a water-using (or mass transfer) system as well as hot and cold process streams (the heat exchange system), and there is interaction between them, so neither can be used as the foundation problem.

In this report we will highlight what has been achieved by the UCT team in the course of this project. Considerable progress has been made towards the objective of having a methodology and tools to handle all conceivable situations in which both heat transfer and mass transfer occur, but there remain areas that still need to be resolved.

The report will start with a review of the literature on the general topic of combined heat and mass exchange network synthesis, with particular emphasis on the different methodologies for analysis and design of such systems.

The report will then cover application of these methods to the two different types of combined heat and mass exchange problems. Implicit in all the methods is optimisation of the systems under consideration.

The final section of the report will detail the software developed in support of these methods.

In the conclusion we will summarise what has been achieved in this part of the project. References and Appendices follow after the conclusions.

1.1 Process Synthesis

The conversion of raw materials to chemical products goes through many steps such as, reaction, separation, mixing, heating, cooling, etc. These steps are individual transformation steps which have to be interconnected so as to form a complete process that meets the desired overall transformation. The process of selecting these steps and choosing the interconnection pattern is known as process synthesis (Smith, 2005); the resulting interconnection grid is called a flowsheet.

The individual steps involved in chemical processes (based on traditional synthesis techniques) could be arranged in an order of hierarchy with the reaction stage (if one is needed) being the core or starting point of a synthesis methodology. Raw materials are converted into products, alongside, by-products and unreacted feed are produced, and these mixture needs to be separated. In essence, the reactor design defines the separation system requirements, these two stages in turn define the heating and cooling systems configuration and how much of process heat recovery is achieved determines the external heating and cooling utilities requirements. This hierarchy according to Smith (2005) could be represented symbolically by the layers of the "onion diagram" illustrated in Figure 1.1 below. Note that the separation step in Figure 1.1 involves both primary and secondary separations.

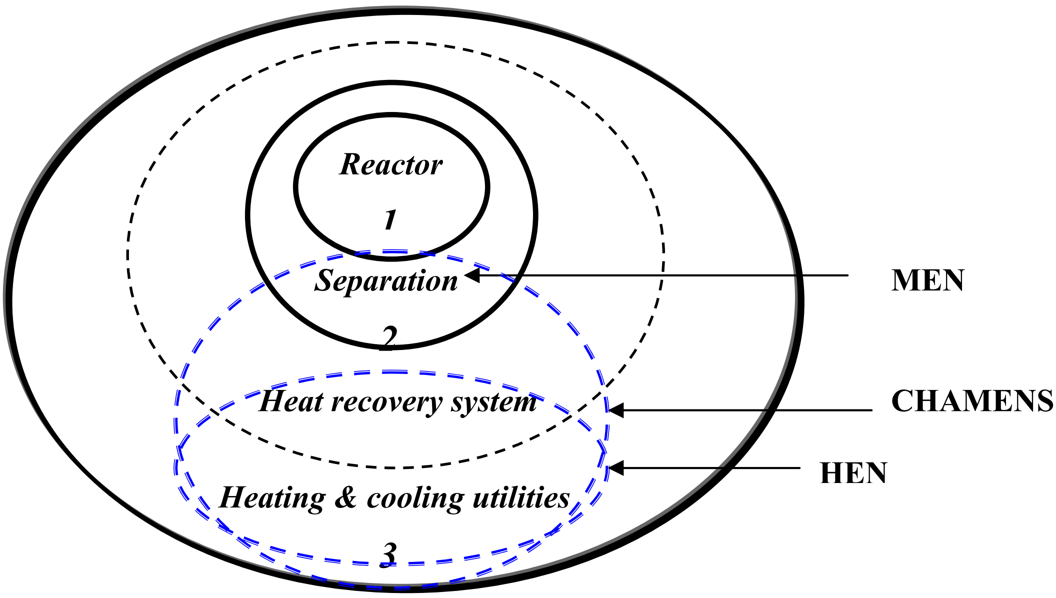

Figure 1.1: The onion model of process design (Smith, 2005).

1.2 Synthesis of Subsystems and Combination of Sub-Systems

The traditional approach in the design of chemical processes has had to do with focussing attention on the design of individual items of equipment that makes up the whole chemical process, items such as: heat exchangers, reactors, mass exchangers, etc The starting point of such designs has been from the centre of the "onion diagram" while the interconnection of these equipments and processes with one another has been accomplished by trial and error and heuristics. With time, subsystems were identified and connections of equipments and processes within the same subsystems were synthesized by various techniques, with heuristics, physical and thermodynamic insights and mathematical programming being the most common of them. Of these subsystems, heat exchanger network synthesis has received the most attention (Gundersen & Naess, 1988; Linnhoff, 1993) while mass exchanger network synthesis is following suit (El-Halwagi, 1997; Hallale & Fraser, 1998, 2000a, & 2000b; Fraser & Shenoy, 2005; Fraser and Hallale, 2000). Reactor networks synthesis is gaining ground too (Smith, 2005) while heat induced separation systems (such as distillation columns) and heat and power systems are being integrated into site's heat exchange operations (Shenoy, 1995). In all, design of chemical processes aims at total site integration.

The identification and subsequent synthesis of subsystems has gone a long way in helping to attain optimal networks design, but this is restricted to such subsystems as there are still interactions among different subsystems such as energy and mass (because some streams may require heating/cooling). So in order to meet desired criteria such as economics, yield improvement, pollution abatement, flexibility etc. in the design and operation of chemical processes, efforts should be focused not only on design of individual items of equipments (Hallale, 1998) or the synthesis of subsystems but also on the techniques with which to select and connect these equipments from more than one layer of the chemical process.

There are so many process alternatives in the light of the different process variables (such as temperatures, pressures, flowrates, compositions etc) as well as performance criterions at the disposal of the design engineer, these calls for a conceptual understanding of the interaction among these process variables (in essence the layers) so as to be able to establish design and synthesis techniques that would tackle the problem systematically in achieving the desired goals.

This study aims to reinforce the third level of chemical process design (as illustrated in Figure 1.2 below) which is a combined synthesis of two of the layers of the onion diagram which are the separation (secondary) and the heat requirement sub-systems, the interaction between these two is critical in meeting the philosophy of total site integration. The study will establish trade-off techniques for parameters (that determine the performance criteria) within the two different layers of the onion diagram.

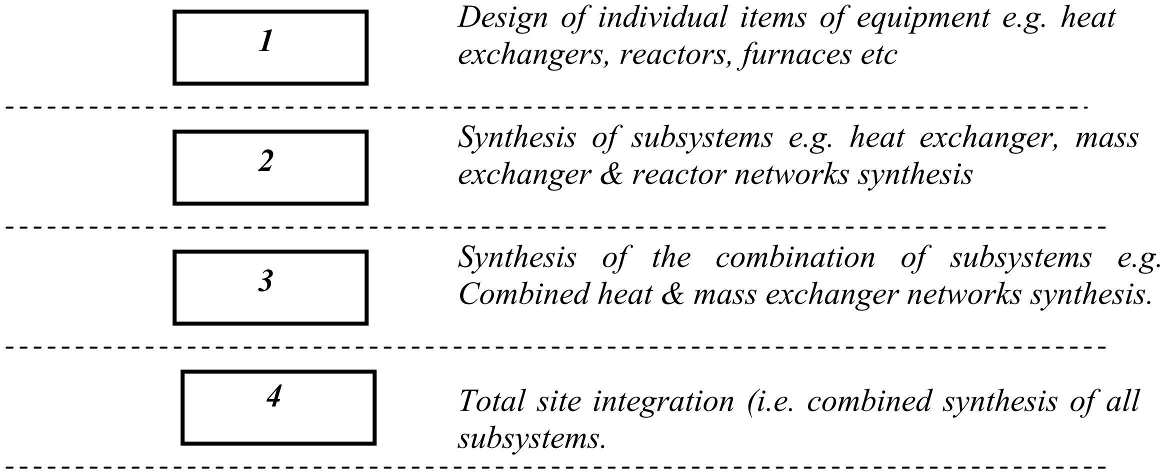

Figure 1.2: Design and synthesis procedures of chemical processes.

An example for the potential improvement which the synthesis of combined subsystems can have on a process could be found in combining the synthesis of heat and mass exchanger networks. This is because absorption processes are mostly better accomplished at lower temperatures while stripping at higher temperature conditions (Seader and Henley, 1998). Exploiting these alternatives would produce an effect on the final network in terms of the operating conditions (e.g. MSA/Utility requirements) as well as the structural configuration. But in meeting these temperature conditions, heating or cooling would be required and heat exchangers would be needed to accomplish such heat exchange. There has to be a conceptual understanding of the interaction between mass and energy in chemical processes so as to be able to develop a systematic way in which trade-offs would be established among these competing alternatives.

Heat and mass exchanger network synthesis have been accomplished using techniques which are insight-based and mathematically-based (Hallale, 1998). Also, there have been studies that established a hybrid of the two techniques for the synthesis (Msiza and Fraser, 2003). The insight-based technique entails the use physical and thermodynamic insights while the mathematically-based methods involve formulating as a mathematical model, the heat or mass exchange operation as a single task and subjecting the model to some material, energy and logical constraints for subsequent optimisation for the best. The few studies that have been carried out on combined heat and mass exchanger networks synthesis (CHAMENS) have used both the insight and mathematically-based techniques. These techniques (as would be explained in section two) are fraught with some drawbacks. The drawbacks prompts this study which would be carried out using first, pinch analysis only and then a sequential optimisation of the pinch analysis.

1.3 Pinch Technology

Pinch technology is a synthesis technique whose concept is based on physical and thermodynamic insights for the design of overall heat/material requirements of a process. The synthesis technique started in the late 1970s with heat exchanger networks (Linnhoff and Flower, 1978). The procedure entails identification of the most thermodynamically constrained part of a network otherwise known as the *pinch*. The pinch position automatically sets the maximum energy/mass that could be recovered as well as the utilities/external mass separating agents that would be needed in addition. The corresponding structural configuration (in terms of equipment size and their interconnections) needed to accomplish this energy/mass transfer can be predicted simultaneously (Townsend and Linnhoff, 1984; Hallale, 1998). The two predictions could be done before actual design in a process known as *targeting*. The resulting network can be optimised by simply trading off the two targets against one another, the technique is known as supertargeting. The minimum temperature approach, $\Delta T_{\min}$/composition difference, ε that corresponds to the least total annual cost (sum of annual operating and annualized capital costs) gives the optimal target before design. The design is subsequently initialized with the targeted $\Delta T_{\min}/\varepsilon$ and there would be very little or no evolution required in arriving at designs that would meet the targeted costs.

The ability to target ahead of actual design is one of the key advantages of pinch analysis, this is because there is assurance that such targets are the best possible as far as the process is concerned. This helps to do away with the traditional optimization technique which involves repeated design and subsequent costing of such designs with the aim of regarding the design with the least cost as the best. Such approaches lack the yardstick with which to measure the goodness of designs irrespective of the amount of network evolution carried out as it might have been initialized from a wrong network topology.

1.4 Mathematical Programming

Mathematical programming usage in process synthesis has been of two natures, the sequential and the simultaneous approaches. The sequential approach basically, is a formulation of the pinch concept as a mathematical model which is subsequently optimised. While the simultaneous approach formulates as a mathematical model the heat/mass exchange network as a single task using objective functions which aims to minimize in a single step all the competing costs. The sequential techniques entails three steps, the being the use of linear programming (LP) to target for the minimum utility/MSA requirements and the pinch location. The minimum number of units that meets the targeted utility/MSA in the first stage is targeted using mixed integer linear programming (MILP) as the second step (Papoulias & Grossmann, 1983). The vertical MILP model of Gundersen and Grossmann (1990) has the ability to discriminate among the different networks that meet the same utility target in terms of their heat load distribution as well as the degree to which they are able to transfer heat vertically on the composite curves. These automation procedures make the targeting for the total annual cost TAC to be done ahead of design just like in pinch analysis. The final step is the network generation and subsequent optimization using non linear programming (NLP) and this was developed by Floudas *et al*., (1986) for heat exchanger network synthesis (HENS). No study has addressed the automation of the capital cost targeting techniques for mass exchange networks of Hallale (1998) so as to be able to discriminate among all the networks that would meet the same MSA targets in terms of their mass load distributions and ability to transfer mass vertically on the composite curves. Also the subsequent network generation and optimization using NLP is yet to be addressed.

The simultaneous approaches use mixed integer non-linear programming (MINLP) for the synthesis of heat and mass exchanger networks by setting up superstructures (or hyperstructures) which is believed to embed all the potential configurations and operating conditions that the synthesis problem at hand could have, this superstructure is then optimized for the best structure in the light of the aforementioned performance criterion (Floudas and Ciric, 1989; Papalexandri *et al.,* (1994). It carries out the trade-offs of all the necessary parameters simultaneously unlike the sequential technique. But there is not usually a guarantee of global optimum due to the presence of non-convexities of relations. Also, the engineer has to be clever enough to include within the parent superstructure all the potential optimal configurations of the proposed network. The merits and demerits of each of these techniques are discussed in section two of this study.

1.5 Combined Heat and Mass Exchanger Network Synthesis (CHAMENS)

El-Halwagi, (1992/1993) introduced the concept of Combined Heat and Mass Exchanger Network Synthesis (CHAMENS). This is a system having rich streams from which species has to be removed by lean streams and at the same time may be required to carry out a heat transfer duty. MINLP was used by Srinivas and El-Halwagi (1994) to target for the minimum operating cost solution as well as the minimum number of heat and mass exchangers that corresponds to this operating cost. This same approach characterized the early days of HENS and MENS in which there were no capital cost targets for the heat and mass exchangers that correspond to the targeted minimum utility/MSAs respectively. Extending this technique to CHAMENS will result in networks that can not be guaranteed to be the best possible in terms of total cost.

CHAMENS is an aspect of process synthesis that is yet to receive much attention. Papalexandri & Pistikopoulos (1994) on one hand and Bagajewicz et al. (1998) on the other hand also used MINLP in synthesizing CHAMENs. Papalexandri & Pistikopoulos (1994) set up a hyperstructure which is believed to embed all the potential structural and operational network configurations of both heat and mass exchangers. The hyperstructure was subsequently optimised for the minimum total annual cost (TAC) using a composite objective function which is a sum of the operating cost (for the hot and cold utilities as well as mass separating agents) and annual capital cost (sum of the heat and mass exchangers).

Bagajewicz et al. (1998) used the state space approach which involves the use of operators such as assignment and pinch. The state space is a special case of network superstructure. These authors applied the pinch operator to solve the problem of combined heat and mass exchanger networks. But the aim of this approach is to design for the minimum utility (i.e. heating/cooling and mass separating agents) cost requirements.

1.6 Objectives and Methodology

This study will develop synthesis techniques for both grassroots and retrofit CHAMENS using three approaches which are: graphical, sequential optimisation and simultaneous approaches. The frameworks of the graphical approach are the established pinch analysis techniques for heat exchanger network synthesis (Linnhoff et al., 1982; Linnhoff & Ahmad, 1990; Ahmad & Smith, 1989) and mass exchanger network synthesis (El-Halwagi & Manousouthakis, 1989; Hallale, 1998).

The sequential optimization would be an automation of the graphical approach. The first step will be the use of linear programming to target for the minimum utility and MSA requirements simultaneously. The second step will include the development of MILP models that embed the verticality of mass transfer and ability to discriminate among the different potential networks that would meet the same MSA targets as well as the same or close number of units in terms of their mass load distributions and ability to transfer mass vertically on the composite curves (as done by Gundersen & Grossmann, 1990, for HENS). This model will establish a common basis for the automated targeting of both heat and mass exchanger's capital cost requirements. Setting the two targets out on the same basis is necessary so as to be able to form a composite objective function that will aim to minimize simultaneously the size requirements of the heat and mass exchangers without numerical difficulties.

The final step in the sequential optimization would be the combined network generation using non linear programming (NLP). The first two steps are targets setting steps. Targets setting for the synthesis of combined sub-systems have advantages. First, MENS targets can be used to suggest process improvements for HENS (and vice versa) and second with targets for CHAMENS, it becomes easier to screen quickly many process alternatives and hence design options for the overall process.

The simultaneous approach will entail the use of mixed integer non linear programming for the proposed synthesis. This approach will contribute to the field of process synthesis due to the fact that it proposes to use the mass exchanger sizing equations of Hallale (1998) which is based on mass and volume.

1.7 Scope and Structure of this Report

This report will develop a systematic technique for the synthesis of combined heat and mass exchange networks for both new and retrofit designs. The new designs will involve no overlapping and multiple overlapping MSAs as well as linear equilibria and variable exchanger specifications. The results of the developed techniques will be compared with those of previous works wherever possible.

Section 2

The relevant theory for this study is reviewed in this section. The review covers the applications of pinch analysis and mathematical programming (sequential and simultaneous) techniques to the synthesis of heat and mass exchanger networks separately. The vertical MILP model of Gundersen and Grossmann (1990) and the capital cost targeting techniques for mass exchanger networks of Hallale (1998) will be dwelt upon extensively in this section because these techniques would be the basis for the proposed synthesis methods.

Section 3

This section opens with the reasons for which this study has to be carried out and the presentation of the CHAMENS problem statement. After this, the first synthesis method for CHAMENS which is a simple graphical technique using pinch analysis only is demonstrated, Targeting techniques are first presented after which design methods follow and this is applied to CHAMENS problems in which MENS is the foundation problem with HENS being used to enhance the mass exchange. This section is wrapped up with the merits and demerits of the pinch analysis.

Section 4

CHAMENS problems in which both the HENS and MENS are foundation problems would be addressed in this section using pinch technology just as was done in Section 3. The heat exchange network synthesis grand composite curve will be used to evaluate the different approaches of integrating MENS with HENS.

Section 5

This section discusses the software tools developed with emphasis on water pinch targeting.

2 LITERATURE REVIEW

2.1 Introduction

Combined heat and mass exchange network synthesis (CHAMENS) is composed of heat exchanger networks (HENs) and mass exchanger networks (MENs). Pinch analysis has been employed in the synthesis of both HENs and MENs, so also is mathematical programming. So this section will review the literatures on the synthesis of HENs and MENs using the aforementioned synthesis techniques. The mathematical programming techniques will be reviewed in the light of how they have been applied to HENS and MENS synthesis. The aim of this study is to synthesize CHAMENs, and so much effort will be devoted to discussing the established CHAMENs synthesis techniques.

2.2 Heat Exchanger Network Synthesis, HENS

Heat exchanger network synthesis (HENS) is an aspect of process synthesis that has been studied extensively (Shenoy, 1995; Linnhoff, 1993; Gundersen & Naess, 1988). Pinch analysis and mathematical programming have been applied widely to its synthesis.

The HENS problem statement can be stated as follows (El-Halwagi, 1997 and Floudas, 1995)

> *Given a number N_H of hot process streams (to be cooled) and a number N_C of cold process streams (to be heated), it is desired to synthesize a cost effective network of heat exchangers which can transfer heat from the hot streams to the cold streams. Also given are the heat capacity flowrate (flowrate × specific heat) of each process hot stream, FCp, supply temperature, T^s, and target temperature T^t, of each stream. Available for service are heating and cooling utilities whose costs, supply temperatures, and target temperatures are also given.*

Key questions to be answered by the synthesis are:

- Which heating/cooling utilities should be employed?
- What is the optimal heat load to be removed/added by each utility?
- How should the hot and cold streams be matched (i.e. stream pairings)?
- What is the optimal network configuration (e.g. how should the heat exchangers be arranged? Should there any stream splitting and mixing?, etc)
- What should be the heat load of each heat exchanger?

- What are the area requirements of each heat exchanger?

The subsections that follow are reviews on pinch technology and mathematical programming as applied to heat exchanger network synthesis.

2.2.1 Pinch Technology as applied to HENS

The energy crisis of the 1970s prompted the extensive study in the area of heat exchanger network synthesis using pinch technology (Linnhoff, 1993). At that time, the aim was to design for energy optimal networks and this was accomplished with the identification of the pinch. Emphasis then shifted from merely designing for energy optimal networks to cost optimal networks in which trade-off between the operating and investment costs are established through targeting techniques before actual design is carried out (Gundersen & Naess, 1988).

2.2.1.1 Energy targets

Pinch technology energy targeting has been accomplished using the graphical and algebraic approaches. The graphical technique entails the use of a tool known as the composite curves plot (Linnhoff et al., 1982) which is a representation of the composites of the hot and cold streams plots on temperature versus cumulative enthalpy graphs. As illustrated by Figure 2.1 below, the hot composite is plotted on the same axes as the cold composite and they are shifted horizontally against one another until the closest temperature approach becomes exactly equal to the desired ΔT_{min}.

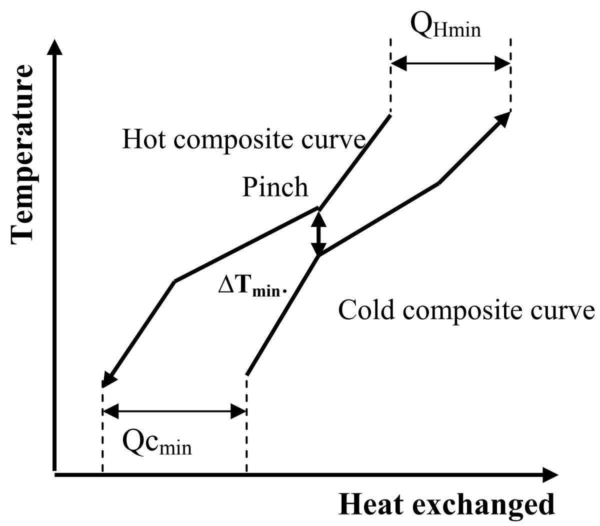

Figure 2.1: Construction of hot and old composite curves on the same axes showing pinch location and minimum energy targets

The hot and cold composite curves are a representation of the overall energy potential of the individual hot and cold streams. The points of inflection on each of these curves corresponds to the supply and target temperatures of the streams. Also sections of equal slopes on the curves are the sum of the FCp (heat capacity flowrate) of each of the participating streams and are known as temperature or enthalpy intervals. The region of overlap of the two composite curves is known as the area of maximum heat recovery by process to process heat transfer. While the section of overshoot of the cold composite curve over the hot composite curve indicates the minimum hot utility target (Q_{Hmin}) and the overshoot of the hot composite curve over the cold composite curve represents the minimum cold utility target (Qc_{min}). These are the targets because further process heat recovery is not possible in the overlap regions. Thus the pinch represents a bottleneck to process heat recovery and in essence divides the network into two thermodynamically independent regions. These are: above the pinch (containing all streams or part of streams hotter than the pinch temperature) and below the pinch (containing all streams or part of streams colder than the pinch temperature). The above the pinch region is in enthalpy balance with the minimum hot utility requirement while the below the pinch region is in enthalpy balance with the minimum cold utility required. For designs to meet these minimum utility targets, no additional heat other than the targeted one should be used above the pinch and no additional cooling other than the one targeted should be used below the pinch. Also, no heat should be transferred across the pinch (Smith, 2005).

The algebraic approach uses a tool known as the problem table analysis which can also identify the pinch and target for the minimum utilities required. This tool is described by Linnhoff et al. (1982).

Illustrated in Figure 2.2 below is a grid representation of the streams relative to the pinch temperature. It represents the stream populations above and below the pinch thereby allowing for design procedures that meet targeted utilities. The pinch temperature is represented by the broken lines. The grid structure depicts the countercurrent nature of the heat exchange problem which makes for easy check on heat exchanger temperature feasibility. Also, the stream matches (which are represented by two circles joined by vertical lines in the grid) can be placed in either order without having to redraw the stream system; this cannot be accomplished in the flowsheet representation (Linnhoff et al., 1982).

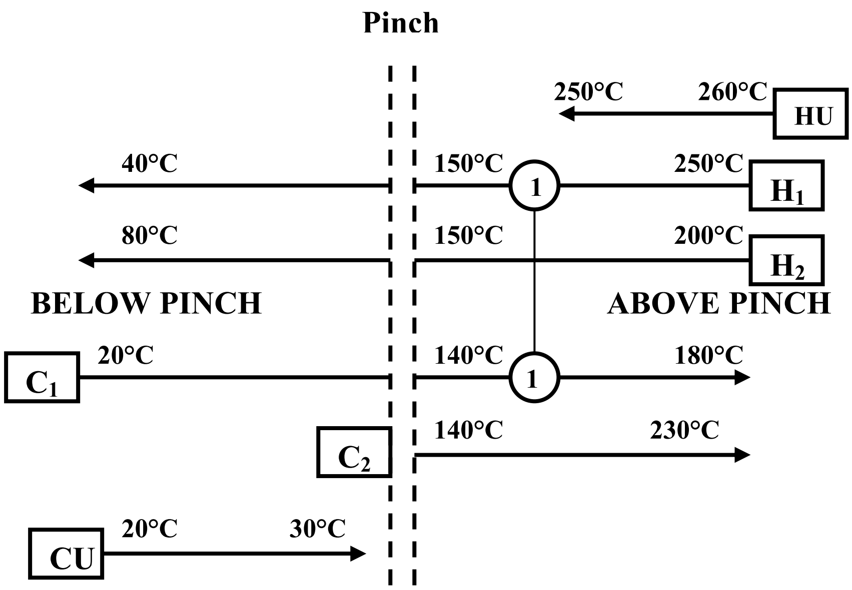

Figure 2.2: Grid representation of streams relative to the pinch temperature. ΔT_{min} is 10°C.

There could be so many network designs meeting the same energy and number of units targets (to be discussed later) at a specific ΔT_{min}, but they would have different capital costs because of the differences in their matches selection. Each of the designs is costed and the one with the least cost is chosen as the optimal network (Linnhoff *et al.*, 1982). This approach has some shortcomings in that it is tedious because repeated designs is done for different ΔT_{min}, and there could be the problem of a topology trap in the perceived optimal ΔT_{min}. These prompted Townsend and Linnhoff, (1984) to develop targeting techniques for the capital requirements not only in terms of the number of units but also based on the area requirements of these units.

The HENS Grand Composite Curve, GCC

The heat transfer grand composite curve, (GCC) is reviewed in this study because it comes in handy as a tool for developing sequential synthesis techniques for CHAMENs based on pinch technology. Plotting interval temperatures versus the cumulative heat cascaded gives the grand composite curve of Linnhoff et al. (1982). This curve depicts the region of process to process heat transfer and the section which needs external heating and cooling. This is illustrated by Figure 2.3 below.

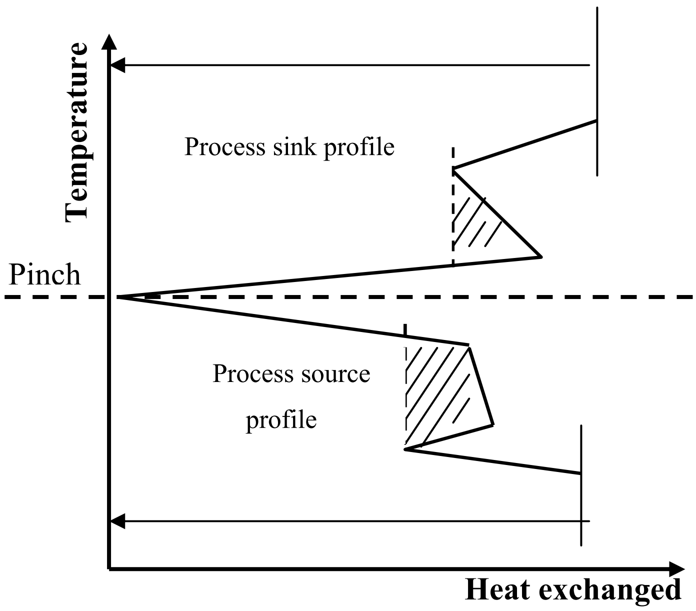

Figure 2.3: The grand composite curve illustrates the heat sources and heat sinks and region of process-process heat transfer and zero heat flow.

The pinch temperature is indicated on the diagram which is the point of zero net heat flow. Above the pinch is the process sink profile with temperature and enthalpy increase and below the pinch is the process source profile with temperature decrease but increasing enthalpy (contrary to convention, Shenoy, 1995). The GCC is useful in the sense that it does not just indicate that a utility is needed but it shows the temperature level at which it is needed. It also comes in handy for profile matching for total energy integration.

2.2.1.2 Capital Cost Targets

In determining the optimal network out of the alternatives, the traditional approach requires picking the design that meets the energy target with the least capital cost out of a range of ΔT_{min} as the optimal network but such networks are not always synonymous to the optimal. This is because there is no proper accounting of the competing cost which is: the utility costs and the heat exchanger costs in terms of the size. So ability to target for the capital cost before design goes a long way in making for an easy optimization procedure. The capital cost of a heat exchanger network depends on the following: the number of heat exchange units, total heat exchange area, number of shells, material of construction and pressure rating. Some of these will be discussed in the following sections.

Number of Units Target

A small number of units is desirable because it allows for simple and practical network designs. Also exchanger costs are correlated as concave functions of heat exchange area, so for an equivalent area, reducing the number of units results in a lower capital cost. One of the key concepts of pinch technology is the ability to target for the minimum number of units recognizing the pinch division. The minimum number of units without the pinch division is given by (Linnhoff et al., 1982):

$$N_{units} = S - 1 \tag{2.1}$$

S is the number of streams including utilities.

The minimum number of units is one less the total number of streams and utilities. This is for the whole network and unpinched problems but since the pinch divides the whole network into two thermodynamic distinct regions (above and below the pinch) Equation 2.1 can be applied to each of these regions separately. This gives the minimum number of units with the pinch division (Linnhoff et al., 1982):

$$N_{units,\ pinch} = (S\text{-}1)_{\text{Above pinch}} + (S\text{-}1)_{\text{Below pinch}} \tag{2.2}$$

Partitioning at the pinch leads to an increase in the number of units because some of the streams cross the pinch and they would be counted twice. Prior to the setting up of the capital cost targeting techniques for heat exchanger network synthesis (discussed in the following section), designs were geared towards the minimum number of units in an attempt to minimize the capital cost (Linnhoff et al., 1982). But this is not always the case because minimum number of units is not synonymous to the minimum size (area) of exchangers.

Heat Exchange Area Target

The position of the hot and cold composite curves relative to one another on the graph has been exploited by Townsend and Linnhoff (1984) to target for the total heat exchange area requirement in a network corresponding to a specified energy target and ΔT_{min}. This is possible because the vertical distance between any two points (along the temperature axis) depicts the driving force (temperature difference) at that particular point and it is smallest at the pinch. Drawing vertical lines at each point in which there is a change in slope (including the regions to be serviced by the utilities) on each of the composite curves creates the boundaries for what is known as enthalpy intervals as illustrated in Figure 2.4 below.

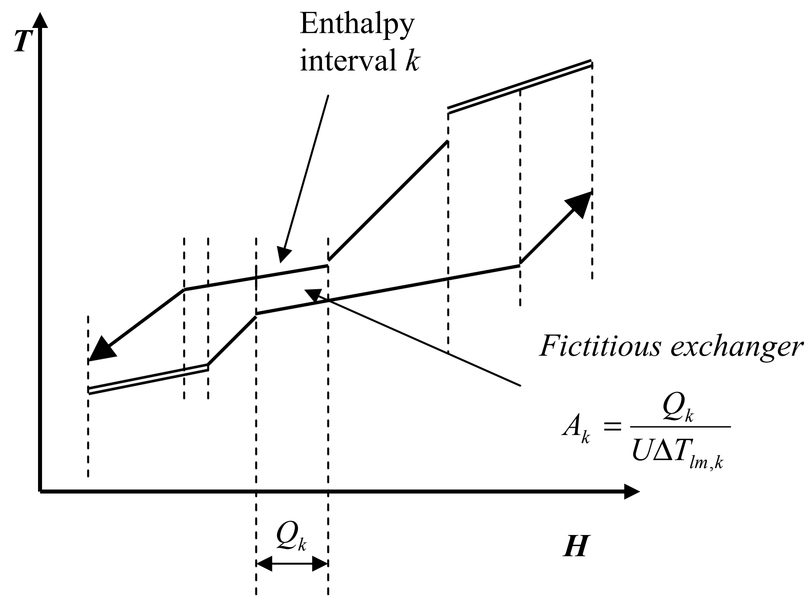

Figure 2.4: Division of the balanced composite curve into enthalpy intervals (*Smith, 2005*)

These intervals could be regarded as fictitious heat exchangers and treated as one by calculating an ideal area for them. The ideal area, *A*, for a countercurrent heat exchanger is given as:

$$A = \frac{Q}{U \Delta T_{lm}} \tag{2.3}$$

where: Q is the enthalpy change

U is the overall heat transfer coefficient

ΔT_{lm} is the log mean temperature difference

k is the enthalpy interval

For a constant heat transfer coefficient throughout the process, the minimum total network area can be obtained by applying Equation 2.3 to each of the enthalpy intervals and summing (Smith, 2005) to obtain:

$$A_{\min,Network} = \frac{1}{U} \sum_{k}^{Intervals,K} \frac{Q_k}{\Delta T_{lm,k}} \tag{2.4}$$

where: K is the total number of enthalpy intervals

Equation 2.4 assumes vertical heat transfer as well as a constant overall heat transfer coefficient which is not always the case in realistic situations because the heat transfer coefficient is usually stream dependent. The respective heat transfer coefficients of each stream can be accounted for by virtue of the fact that the heat transfer coefficient resistances are additive:

$$\frac{1}{U} = \frac{1}{h_i} + \frac{1}{h_j} \tag{2.5}$$

where: h is the stream film heat transfer coefficient

i is the hot stream

j is the cold stream

Applying Equation 2.5 to 2.4, the total minimum area requirement becomes:

$$A_{\min,Network} = \sum_{k}^{Intervals} \frac{1}{\Delta T_{lm,k}} \left[\sum_{i}^{\substack{Hot\\streams}} \frac{q_i}{h_i} + \sum_{j}^{\substack{Cold\\streams}} \frac{q_j}{h_j} \right]_k \tag{2.6}$$

where q is the enthalpy change of each stream. Equation 2.6 is called the *Bath formula* of Townsend & Linnhoff (1984).

The grid diagram as illustrated by Figure 2.5 below also depicts the enthalpy intervals as well as which streams are present in each interval.

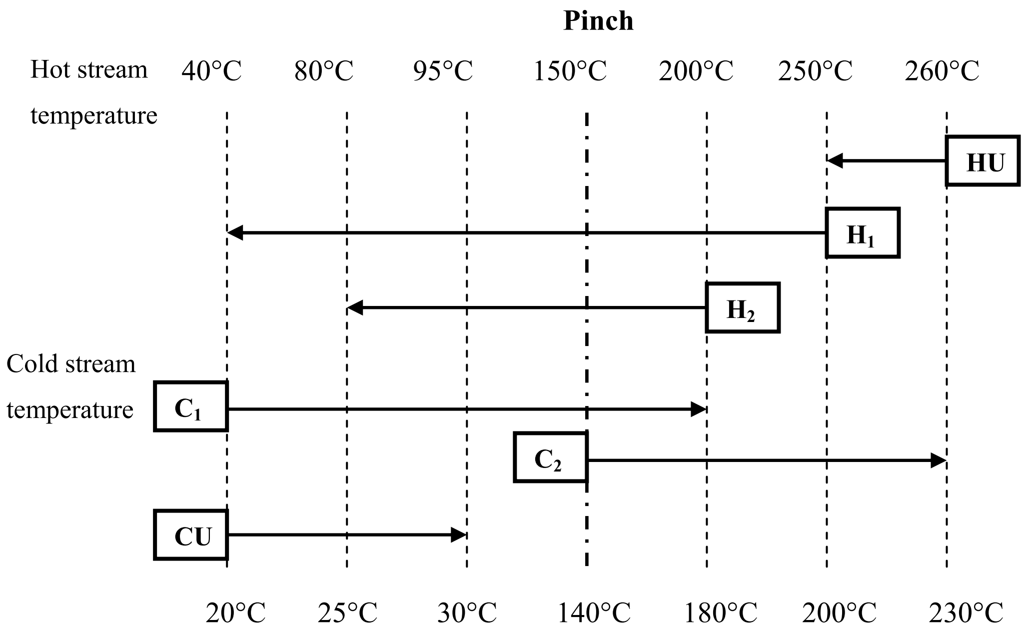

Figure 2.5: Grid representation for enthalpy interval stream populations.

Equation 2.6 would target for the rigorous total minimum area in cases where the stream film heat transfer coefficients are identical. For situations in which film coefficients differ by only an order of magnitude, Equation 2.6 predicts the total minimum area within 10 percent of the actual minimum (Ahmad, 1985; Smith 2005). But if the film coefficients are very different, then the strict vertical matching rule has to be relaxed and deviation from verticality employed so as to achieve the minimum area. This is discussed below and illustrated by Figure 2.6.

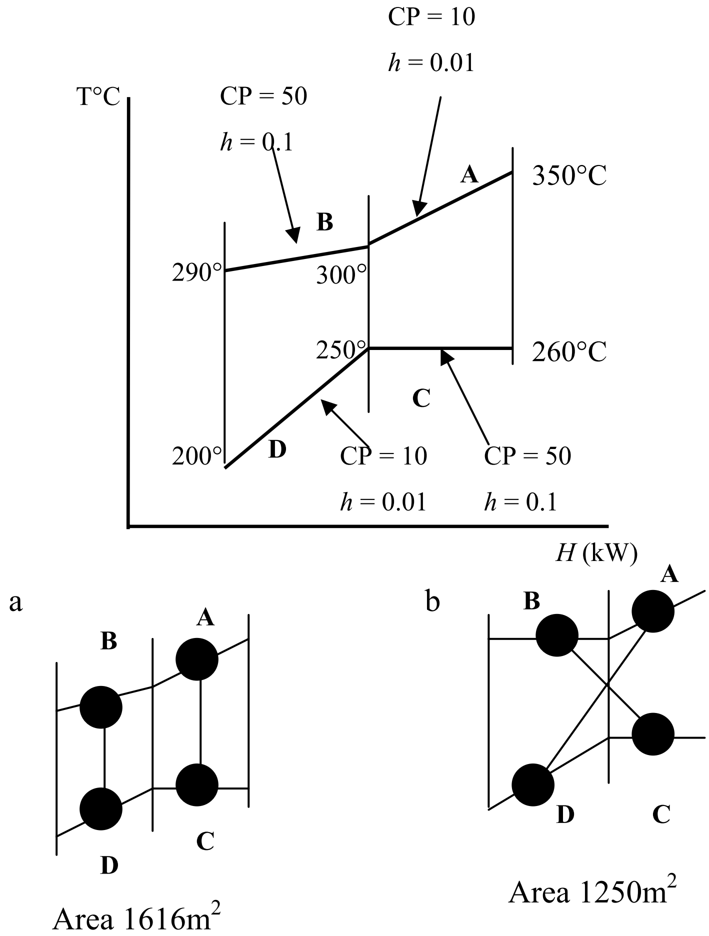

Figure 2.6: Vertical and non-vertical (criss-crossing) heat transfer matching (Linnhoff & Ahmad, 1990)

In Figure 2.6, hot stream A has a low film coefficient and it exists in interval 1, cold stream C has a high film coefficient and it also exists in interval 1. Hot stream B has a high heat transfer coefficient and it exists in interval 2 while cold stream D has a low heat transfer coefficient and it exists in interval 2 as well.

Vertical heat transfer requires that hot stream A which is in interval 1 be matched with cold stream C which is also in interval 1. This is because such a match (heat exchanger) would use temperature driving force exactly the way it is used in the interval (thus appearing vertical on the composite curve). If there are more streams within this same interval, they all have to be matched with one another in the interval, but if there are more hot streams than cold streams or vice versa then stream splitting is required so as to meet the condition of verticality of heat transfer. Following these rules religiously would result in a kind of design known as the spaghetti design (Linnhoff & Ahmad, 1990).

The spaghetti design (as the name implies) produces very complex networks with so many stream splits because of the requirement of individual matching of each stream within each interval so as to meet the verticality of heat transfer as depicted by the composite curves. This is the ideal matching pattern but it is not very practical because of the many stream splits and heat exchangers that would result thereby requiring a high capital cost (for the installation of each exchanger) and a complex layout. But it can serve as a theoretical basis for area targeting in the sense that the ideal matching pattern can first be produced after which it can be reduced to a simpler network by evolution through breaking of loops and exploiting paths, but this might result in incurring a small penalty in area.

Matching stream A with stream C and B with D gives a total area requirement as $1616m^2$ as illustrated in Figure 2.4a. But matching stream A with stream D and B with C (this type of matching is known as criss-crossing, Linnhoff & Ahmad, 1990) gives a minimum area requirement as $1250m^2$ which is less than the first area. The A-D match (both having low heat transfer coefficients) uses temperature driving forces far more than are available on the composite curves while the B-C match uses less.

The stream film heat transfer coefficients can be obtained from tabulated experience values or by assuming fluid velocity, fluid physical properties with heat transfer correlations (Smith, 2005).

Equation 2.1 which states that the total minimum number of units requirement is one less than the sum of the number of all the streams including hot and cold utilities was applied to each enthalpy intervals as well by Ahmad and Smith (1989). This enables one to achieve vertical heat transfer. So summing the number of units within each interval gives the total minimum number of units required for the entire network. It results in a low total area because it maximizes the use of driving forces but on the other hand, it increases cost because the area is shared among so many units as explained above.

Equation 2.6 also assumes that the ΔT_{min} is not stream dependent. But in cases in which it is stream dependent, the *pseudo-Bath formula* has been put forth by Ahmad (1985) to handle such cases because there will no longer be a single log-mean temperature difference within each interval. For such cases, the target for minimum area is given by

$$A_{\min,Network} = \sum_{k}^{Intervals} \left[\sum_{i}^{\substack{Hot \\ streams}} \sum_{j}^{\substack{Cold \\ streams}} \frac{1}{\Delta T_{lm,ij}} \frac{q_{ij}}{h_i} + \sum_{j}^{\substack{Cold \\ streams}} \sum_{i}^{\substack{Hot \\ streams}} \frac{1}{\Delta T_{lm,ji}} \frac{q_{ji}}{h_j} \right]_k \tag{2.7}$$

where: $q_{ij} = qi \dfrac{q_j}{Q_k}$ and $q_{ji} = q_j \dfrac{q_i}{Q_k}$

Equation 2.7 splits the heat from each hot stream in an interval among all the cold streams in proportion to their enthalpy change relative to the total for the interval; this is also carried out for the cold streams in relation to the hot streams. Equations 2.4, 2.6 and 2.7 are very useful for area targeting before actual design, but they need to be converted into costs, the equations for estimating such costs are presented in later sections.

Number of Shells Target

For cases in which heat exchangers are perfect countercurrent type, the number of units equals the number of shells in as much as no shell exceeds some practical upper size limit (Smith, 2005). More common exchanger types in chemical processes are the 1-2 design i.e. 1 shell pass, 2 tube passes. For severe temperature crosses in a pair of streams, the following inequality normally holds (Ahmad and Smith 1989):

$$N_{Shells} \geq N_{Units} \tag{2.8}$$

The flow in this case is a combination of countercurrent and cocurrent. More than one shell is needed in a unit so as to guide against temperature crossing. Ahmad and Smith (1989) proposed targeting techniques for cases of this nature because it has a considerable influence on the capital cost requirements. They still employed the concept of vertical heat transfer by dividing the composite curves into enthalpy intervals just as was done for area targeting.

They gave the number of shells target as:

$$N_{Shells} = \sum_{k}^{Intervals} N_{Shells,k}\left(S_k - 1\right) \tag{2.9}$$

where: N_{Shells} is the total number of shells in all k enthalpy intervals

S_k is the number of streams in enthalpy interval k

Equation 2.9 is applied to both sides of the pinch separately so as to be consistent with the maximum energy recovery and minimum number of units target. See Ahmad and Smith (1989) for total number of shells target based on streams contributions.

Capital Cost Estimation

Procedures for converting the different targets discussed earlier are reviewed in this section. Networks in which all exchangers have the same specifications in terms of their materials of construction and pressure rating are discussed. For exchangers with non-uniform specifications, see Hall et al. (1990) and Jegede and Polley (1992).

For network capital cost prediction, it is assumed that a single heat exchanger can be costed by the following relation:

$$\text{Cost (installed)} = a + bA^c \tag{2.10}$$

where a,b,c are cost law constants which depend on material of construction, pressure rating and type of exchanger. The cost is a non-linear concave function of area because the exponent c is usually less than 1. This implies that the cost of a network of exchangers depends on the number of exchangers as well as the distribution pattern of the area among them. But this distribution pattern is not yet known at the targeting stage and so the assumption is made that the targeted area is distributed evenly among all the exchangers. This is given as:

$$\text{Network Capital Cost} = N\left[a + b\left(\frac{A_{\min}}{N}\right)^{c}\right] \tag{2.11}$$

where N is the number of units or shells (whichever is appropriate).

To ensure consistency between the capital cost target and energy target, Equation 2.11 should be applied separately to the sections above and below the pinch and the cost added so as to provide the total target for the network (Fraser, 1991). Equation 2.11, despite being based on the assumption that the total area is evenly distributed among the exchangers has been found to predict capital cost targets which can be approached to within typically 5 percent in design (Ahmad, 1985).

2.2.1.3 Supertargeting

The techniques with which to target for the minimum energy requirement as well as the corresponding capital cost has been discussed in the previous sections, but these targets are carried out at a particular $\Delta T_{\min}$. If the value of $\Delta T_{\min}$ is increased, there would be a corresponding increase in the utility requirement (see Figure 2.1) and a reduction in the heat exchange surface area needed to accomplish the energy recovery because driving forces are increased. To check the effect (in terms of cost) of varying $\Delta T_{\min}$ on networks, the capital cost target is annualized and then added to the corresponding annual operating (energy) cost target at the specified $\Delta T_{\min}$ so as to give the total annual cost (TAC) target. Doing this at different values of $\Delta T_{\min}$ would locate the $\Delta T_{\min}$ that corresponds to the least total annual cost, such is the optimum $\Delta T_{\min}$. This procedure is known as supertargeting and is illustrated by Figure 2.8 below.

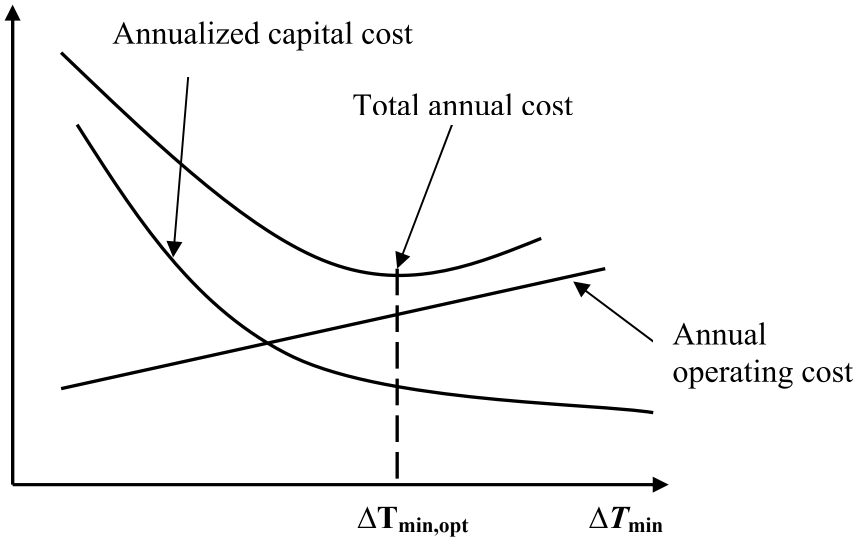

Figure 2.8: The supertargeting curve for HENS optimization.

With capital cost targets, optimization can be carried out before actual design unlike what used to be the case in the early days of pinch technology when design was carried out for each energy target repeatedly and costing done on each design so as to identify that which is minimum in terms of cost. Figures 2.9 and 2.10 below both illustrate the previous and the improved optimization algorithms.

Figure 2.9, as stated earlier depicts much repeated design and costing tasks so as to identify the minimum total annual cost. This is not the case with Figure 2.10 in which it is the targets that need to be carried out repeatedly over a range of $\Delta T_{\min}$ so as to identify the $\Delta T_{\min}$ that corresponds to the minimum TAC. The network design is then initialized with this $\Delta T_{\min,\text{opt}}$, such designs usually require very little evolution before arriving at the final design whose cost is usually very close to the targeted total annual cost. Also the improved optimization procedure is independent of any network structure and this reduces greatly the chances of falling into topology traps (Linnhoff & Ahmad, 1990). Supertargeting for stream dependent $\Delta T_{\min,\text{opt}}$ is a multivariable optimization; Fraser (1989) proposed reducing it to single variable optimization introduction of minimum flux.

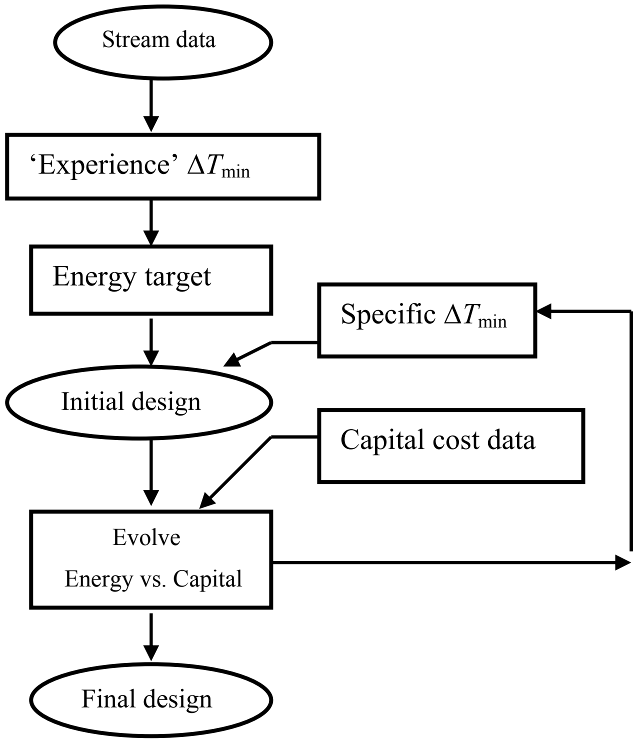

Figure 2.9: Previous pinch technique for optimising heat exchanger networks (Linnhoff et al., 1982)

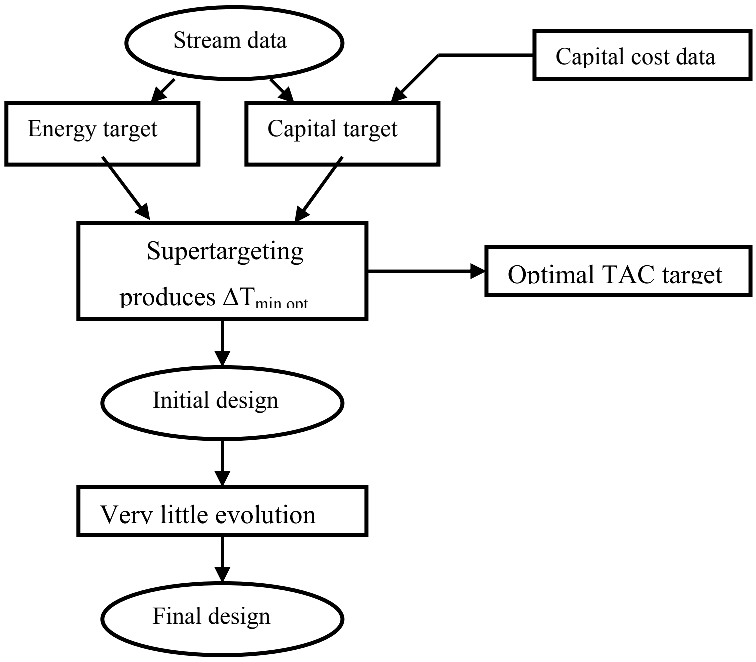

Figure 2.10: Improved pinch technique for heat exchanger network optimization, supertargeting (Linnhoff & Ahmad, 1989)

2.2.1.4 Retrofit Targeting

The discussions have so far been centred on new or grassroots heat exchanger networks but there is often a need to retrofit existing heat exchanger networks. This might be as a result of the desire to reduce the energy consumption of the existing network, increase its throughput, etc. Heat duties may need to be changed within the existing network. Retrofitting is reviewed extensively in this study because the proposed techniques would be applied to CHAMENS retrofit problems.

Tjoe and Linnhoff (1986) proposed a retrofit technique for heat exchanger networks that does not aim to achieve the optimum by synthesizing networks for the minimum TAC, but instead it tries to save the greatest amount of energy possible subject to a specified payback period or investment limit. Their procedure also entails two steps (targeting and design) but these are done in the light of the existing units (since no one would want to throw away already installed plant items). In reducing the energy consumption of a plant, more area needs to be installed, the relationship between the energy that could be saved and additional area that would need to be installed to achieve this energy saving has to be predicted along with the associated cost. This is considered in the light of the payback period for the additional capital investment (area installed). Tjoe and Linnhoff (1986) defined an area efficiency, *α,* which is the ratio of the minimum area (targeted) to that actually used for a certain energy recovery. They assumed that the area efficiency is constant throughout the retrofit but it can also have an incremental efficiency of unity according to Ahmad and Polley (1990).

$$\alpha = \left(\frac{A_{\min}}{A_{existing}} \right)_{\text{existing energy}} \tag{2.12}$$

Tjoe and Linnhoff (1986) approach which is based on the assumption that α is constant throughout the full energy span makes the identification of a region in which a good retrofit should fall possible. The constant α is then used to give a conservative to obtain what savings could be made from different levels of investments at specified payback periods. These give the targets and the subsequent designs are carried out by identifying the corresponding pinch location for the targets and then carrying out the necessary modifications which could involve doing away with cross-pinch heat transfer (this could be as a result of process to process heat exchange or inappropriate use of utilities) and reconnections while still retaining as much as possible the existing items.

While this retrofit technique would help in saving energy it is however fraught with some problems (Smith, 2005) which have to do with which $\Delta T_{\min}$ is to be used, and how to avoid neglecting the constraints associated with the existing network. Also existing equipment is only reused in an ad hoc way and the retrofit procedure will most likely end up with many modifications being done to the existing network.

Smith (2005) recommends a better approach which has to do with identifying the most critical changes which are cost effective that have to be carried out on the network. This is accomplished by identifying and overcoming the *pinching match* in a network, the point at which this occurs in a network is known as the *network pinch*. This is the point at which heat recovery is limited for the existing heat exchanger network. Overcoming the network pinch could be accomplished in four different ways which are by resequencing units, repiping (which is similar to resequencing), inserting a new match and introducing an additional stream. Each of these procedures results in a modified network. A cost optimization still has to be carried out for the network so as to obtain a correct setting for capital-energy trade-off.

2.2.1.5 Network Design

This section reviews the design aspect of the pinch technology which is carried out after the respective targetings. The design technique is known as the *pinch design method*. It is a systematic design technique which is interactive and enables the use of physical insights thereby putting the designer in control. This systematic procedure ensures that the targeted energy, capital and total costs are achieved or closely approached in design.

The design is done using the grid diagram as explained earlier. The pinch design method usually starts off by initializing the design with the assumption that no individual exchanger would have a temperature difference less than $\Delta T_{\min}$ and then abiding by the rule of no transfer of heat across the pinch either by process to process heat transfer or inappropriate use of utilities. Hot utilities should not be used below the pinch neither should cold utilities be used above the pinch. This would ensure meeting in design the energy targets. Also in meeting the area target, there are rules which have to be adhered to; these rules are discussed in subsequent sections (Smith, 2005).

Design to Achieve Minimum Energy Target

In designing for the energy target, the network of streams represented in a grid form (Figure 2.2) should be divided at the pinch and the design done separately for each of the two subnetworks. So it is only above the pinch that hot utility should be used and cold utility below the pinch. The following criteria should be used for the matching of the streams (Smith, 2005).

1. *Start the design at the pinch*. The design should start at the pinch since it is the most constrained part of the network: this is because the $\Delta T_{\min}$ exists between all hot and cold streams and so the number of feasible matches at this region is strictly limited, failure to establish some key matches within the pinch region will result in penalties such as the use of temperature differences less than $\Delta T_{\min}$ or too much use of utilities. Starting the design at the pinch enables early decisions to be made at the most constrained part of the network.

2. *Stream population*. A good way of starting the design at the pinch is to bring all the hot streams to their pinch temperature immediately above the pinch by matching each with a cold stream (or part thereof) which is also at its pinch temperature. This helps to do away with the use of cold utility above the pinch. With this procedure, the $\Delta T_{\min}$ will not be violated. For this to be accomplished, the following condition above the pinch has to hold,

$$N_{\text{H,above pinch}} \leq N_{\text{C, above pinch}} \tag{2.13}$$

   where N_{H} and N_{C} are the number of hot and cold streams respectively.

   The opposite of this condition should hold immediately below the pinch as well for the cold streams. That is

$$N_{\text{H,below pinch}} \geq N_{\text{C, below pinch}} \tag{2.14}$$

This condition is known as the number count criterion. Situations in which the number count does not hold will require splitting of either the hot or cold streams at the pinch.

3. *CP inequality.* Temperature differences at the pinch are exactly equal to ΔT_{min} and so all matches at this region will have this temperature difference at the pinch side. All other regions away from the pinch will only experience temperature differences either equal to or greater than the ΔT_{min}. For this condition to hold, match selection immediately above the pinch must be based on the following criterion:

$$CP_{\text{H, above pinch}} \leq CP_{\text{C, above pinch}} \tag{2.15}$$

For immediately below the pinch too, the opposite has to hold, that is

$$CP_{\text{H, below pinch}} \geq CP_{\text{C, below pinch}} \tag{2.16}$$

where CP_H is the heat capacity of the hot stream and CP_C is that of the cold stream.

If these conditions do not hold, then stream splitting may be necessary.

Further matching away from the pinch could be accomplished with more lack of restrictions but with capital cost still being kept at a minimum. This is carried on till all process-to-process heat has been recovered after which utilities are used to make up for the remaining heat duty. The above and below the pinch designs are then combined so as to arrive at the complete network.

The above set of guidelines if followed will make for designs that meet only the targeted utility. For each utility target, there can be many corresponding designs meeting the same number of units. This would require repeated costing of each design so as to narrow down to the minimum and so studies were carried out so as to establish design techniques that meet not only the targeted utility but the capital cost as well and these are discussed in the next section.

Design to Achieve Minimum Capital Cost Target

In the early days of heat exchanger network synthesis, the utility target that corresponds to the minimum number of units was regarded as being the optimum design (Linnhoff and Hindmarsh, 1983). At such times, the *tick-off heuristics* was used to design for networks having the minimum utility target in the minimum number of units. This is accomplished by ticking off in each match the heat duty requirement of one stream. But this can have an implication in the overall design.

Design for vertical heat transfer achieves the minimum area target but with the attendant problem of too many units and stream splits (i.e. the spaghetti network as discussed earlier) and this would be impractical. Some techniques have been developed (Shenoy, 1995; Linnhoff & Ahmad, 1990) to avoid the spaghetti networks by designs which approach the vertical heat transfer as much as possible in a low number of units and stream splits. This is good in that the network is simplified but might result in a larger area requirement. These techniques are discussed below.

The FCP rule

This rule entails using the ratio of the *FCPs* of the hot and cold streams on the composite curve as a measure for selecting the pinch matches in the design. This is because driving forces are lowest at the region closest to the pinch and so most of the network area is concentrated here.

The Driving Force Plot, DFP

This technique is used to design networks that will approach as closely as possible the minimum area target with the minimum number of units target. It comes in as the guideline to follow for cases in which the *FCP* rule is not sufficient and also takes care of other regions of low driving forces apart from the pinch as this also contributes greatly to the capital cost of a network.

It is a plot which shows the vertical temperature differences, ΔT, between the hot and cold composite curves all through. This difference is represented by plotting the cold temperature, T_c, on the abscissa (or T_h) and the temperature difference, ΔT, on the ordinate. The point with the smallest vertical distance from the abscissa corresponds to the pinch. This is illustrated in Figure 2.11 below.

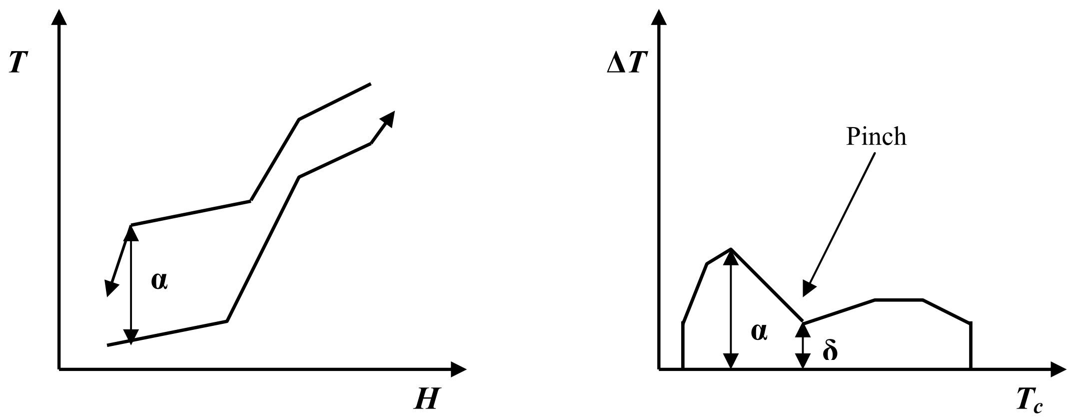

Figure 2.11: Driving force plot construction from the composite curves.

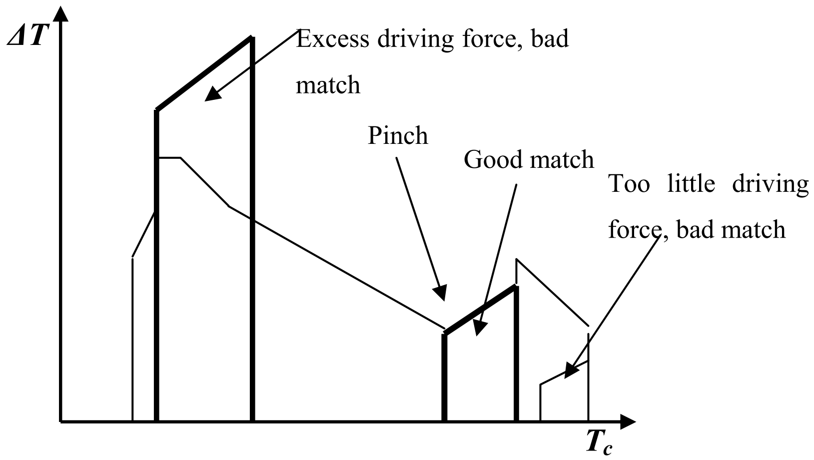

Figure 2.12: Matches assessment with the driving force plot (Shenoy, 1995).

The plot prescribes what driving forces should be used by each match (which is the ideal case) and so each of the potential matches is superimposed on the plot so as to see how it deviates from ideality, or vertical heat transfer. “Good” matches exactly or closely fits the plot while “bad” matches either use too little or too much driving forces (as illustrated in Figure 2.12 above). Too little use of driving forces relative to the ideal forces available will result in increased surface area requirements while those that use excess driving force will require less area but by this less driving force is left for other potential matches and this generally results in an overall increase in network area requirement.

The DFP provides a quick means of screening matches. It employs the model of vertical heat transfer and since this model is the basis of area and shell targeting, designs that approach the DFP should approach as well area and shells targets in design.

The Remaining Problem Analysis, RPA

This technique analyses a match not only based on temperatures (as it is in driving force plot) but on the heat duty as well. Remaining problem analysis as the name implies is a tool which can be used to investigate the penalty incurred for every individual match relative to the final network meeting the targets without having to complete the network (Ahmad and Smith, 1989).

Given that a match M is placed in a network design process, and the area used up is A_M, the remaining area is analysed and denoted as $A_{min,\ remaining}$. Where A_{min} is the ideal total minimum area targeted. A_M is then added to $A_{min,\ remaining}$ and A_{min} subtracted from the total to give the area penalty incurred by the match M. This penalty is the extra area required over and above the target A_{min}, due to the non-ideal match. For perfect matches, the area penalty will be zero. This penalty could be analysed in terms of an efficiency, α_{match}, which is defined as:

$$\alpha_{match} = \frac{A_{min}}{\sum_{M}^{Matches} A_M + A_{min,\ remaining}} \tag{2.17}$$

For matches that are good, the efficiency would be close to unity while those that are not so good would deviate from unity, this is as a result of the extra area incurred.

The remaining problem analysis is a very powerful tool for network designs, its major use is in comparing two alternatives. But it requires much computational effort since the efficiency of each match has to be analysed one after the other and the order in which to go about the matching is not usually known before hand. It has been applied to shells design as well (Ahmad and Smith, 1989), and it will find good use for energy, cost and other criteria which have to be considered in network designs.

The Hidden Pinch Phenomenon and Diverse Pinch Concept

The tick off heuristic is not always a guarantee for meeting the targeted utility in design due to what has been termed "the hidden pinch" (Shenoy, 1995). The remaining problem analysis can be used in determining the hidden pinch as well as the allowable heat load. Also the concept of the diverse pinch has been developed to tackle cases in which there is considerable difference in the heat transfer coefficients of streams (Rev and Fonyo, 1991).

Design for Total Annual Cost

A key rule that has to be followed so as to approach the targets discussed so far is to initialize designs with the optimal $\Delta T_{\min}$ alongside the pinch designed techniques discussed previously. These would result in designs that meet the energy targets precisely, it can also meet exactly the area and number of shells target or at least approach it very closely. Cases in which this is not the case can be handled by evolutionary methods which involve the exploitation of loops, utility paths and stream splitting (Linnhoff and Ahmad, 1990).

Design for Retrofit

The design for achieving the retrofit targets of Tjoe and Linnhoff (1986) can be accomplished using the pinch design methods as well as that recommended by Smith (2005) which was discussed earlier.

This section has reviewed extensively pinch technology as applied to heat exchanger network synthesis. Mathematical programming has equally found wide usage for the synthesis of heat exchanger networks and it is discussed in the next section.

2.2.2 Mathematical Programming as Applied to HENS

Before the entry of the pinch concept into the synthesis of processes, heat exchanger networks were synthesized as a single task problem. But with the identification of the pinch point, this ceased to be the case and the syntheses were done sequentially by decomposing the problem into simpler subtasks which were developed through thermodynamic, heuristic, and optimization approaches. This sequential approach introduced by the pinch technique is what divided mathematical programming techniques as applied to heat exchanger network synthesis into two major synthesis methods (Floudas, 1995), the first being the superstructure based (S based) or simultaneous approach and the second, the superstructure independent, SI, or sequential approach (Msiza, 2001). The SI could still be subdivided based on the degree to which the problem is decomposed.

The HENS problem generally has nonlinear relations and many discrete decisions to be made so it is more or less a mixed integer nonlinear programming (MINLP) problem (Gundersen and Grossmann, 1990). The decomposition approach to HENS synthesis gained recognition due to the combinatorial nature of the HENS problem and the lack of solver environments for the algorithms generated.

The sequential approach is more or less an automation of the pinch technology by virtue of the fact that it tackles the HENs synthesis problem by decomposing the task based on the pinch division into the following subtasks:

i. Minimum utility cost
ii. Minimum number of matches
iii. Minimum investment cost network configurations

The first and second tasks involve targets setting, just as it is with pinch technology. The minimum utility cost target for constrained and unconstrained matches has been accomplished using the linear programming (LP) transportation model of Cerda et al. (1983) and the LP transshipment model of Papoulias and Grossmann (1983). The modified transhipment model of Viswanathan and Evans (1987) has been used as well.

The minimum number of matches that corresponds to the minimum utility cost target has been tackled by the mixed integer linear programming (MILP) transportation model of Cerda and Westerberg (1983) as well as the MILP transhipment model of Papoulias and Grossmann (1983). Gundersen and Grossmann (1990) went further to model the verticality of heat transfer based on the composite curves by the use of the vertical MILP model. This model can be used to discriminate among the various set of matches that meet the same minimum utility and number of units targets. The discrimination is based on their ability to transfer heat vertically between the composite curves thereby giving the corresponding minimum area target in the network.

The generation and subsequent optimization of the corresponding network that meets the targets (i) and (ii) above in terms of the minimum investment cost, has been achieved by the non-linear program, (NLP) of Floudas et al. (1986).

The above sequential approach has advantages in that the decomposition into simpler subtasks enables the designer to be in control of the synthesis. But the competing design variables are not traded-off simultaneously and so this can produce suboptimal networks. These limitations prompted the S-based approach which is a simultaneous optimization approach and it came to be in the late 1980s and early 1990s. This method treats the HEN synthesis as a single task problem. This ensures that the various design variables are traded-off simultaneously (Floudas, 1995). But is also has some limitations which would be discussed in a later section.

Targets (ii) and (iii) have been treated simultaneously by Floudas and Ciric (1989) using a mixed integer nonlinear programming model. They went ahead in 1990 to apply the simultaneous approach still to targets (ii) and (iii) using the pseudo-pinch concept. Subsequent to this, the whole of the HENs synthesis problem has been tackled simultaneously (including target, i), much research has been carried out on this (Floudas, 1995).

Temperature Approaches

The pinch technology approach for HENs uses a single global minimum approach temperature (ΔT_{min}) for all the heat exchangers but this is not the case in practice. This is due to the manual nature of the pinch technology technique. The mathematical programming approach due to the automation nature has the potential to implement some other approach temperatures. These are discussed below (Floudas, 1995).

The approach temperatures are:

Heat recovery approach temperature, HRAT

This is used to identify the pinch temperature so as to determine the minimum utility requirement.

Temperature interval approach temperature, TIAT

This is used to partition the temperature range into intervals and controls the temperature flows into and out of the intervals.

Minimum approach temperature, $\Delta T_{\min}$ *or EMAT*

This is specific to each heat exchanger and it specifies the minimum temperature difference between the two stream exchanging heat inside an exchanger.

These three temperature approaches are related by the inequality,

$$HRAT \geq TIAT \geq EMAT$$

For a strict pinch case, *TIAT* is set equal to *HRAT* while for the pseudo-pinch case, it can be set to a constant value less than *HRAT*. *EMAT* on the other hand can be set to a small positive value, ε, which can also be as low as zero.

A sentence which should be included in the problem statement under pinch technology techniques is "*Each of the process streams, hot and cold has a specific heat capacity flowrate, their respective supply and target temperatures can be specified too or stated as inequalities*" (Floudas, 1995).

The above statement was not included in the problem statement under pinch technology because pinch technology being a very manual approach cannot easily accommodate the supply and target temperatures of the hot and cold process streams as inequalities unlike the mathematical programming approach. If the effect of change in inlet or exit temperatures of process streams on the overall network need to be examined the whole process of problem table analysis or composite curves has to be repeated over again.

2.2.2.1 Sequential Approach

The different tasks that make up the overall synthesis procedure for the sequential approach have been stated above.

Minimum Energy Targets

The minimum utility requirement has been targeted using the LP transportation model (Cerda et al., 1983) as well as the LP transhipment model (Papoulias and Grossmann 1983). The LP transhipment model will be reviewed because it has fewer variables and constraints than the transportation model (Floudas, 1995).

Heat exchange modelling using the LP Transhipment Model

Papoulias and Grossmann (1983) formulated the HENS problem as an LP transhipment model. They established analogies between the transhipment model and the HEN. In their model, heat was regarded as the commodity which is being shipped from the hot process streams (and hot utilities, which are the sources) to the cold process stream (and cold utilities, which are the destinations), the temperature intervals are regarded as the shipping route i.e. the warehouse. So the aim is to determine the optimum network for this distribution operation. See Figures 2.13 and Table 2.1 below for illustrations. Floudas (1995) discusses the temperature partitioning procedure which ensures only a feasible transfer of heat in each temperature interval.

Table 2.1: Analogies between the transhipment model and the heat exchanger network synthesis problem (*Floudas, 1995*).

Transhipment model		**HEN**
Commodity	=	Heat
Intermediate nodes (i.e. warehouses)	=	Temperature intervals
Sources	=	Hot process streams and hot utilities
Destinations	=	Cold process streams and cold utilities

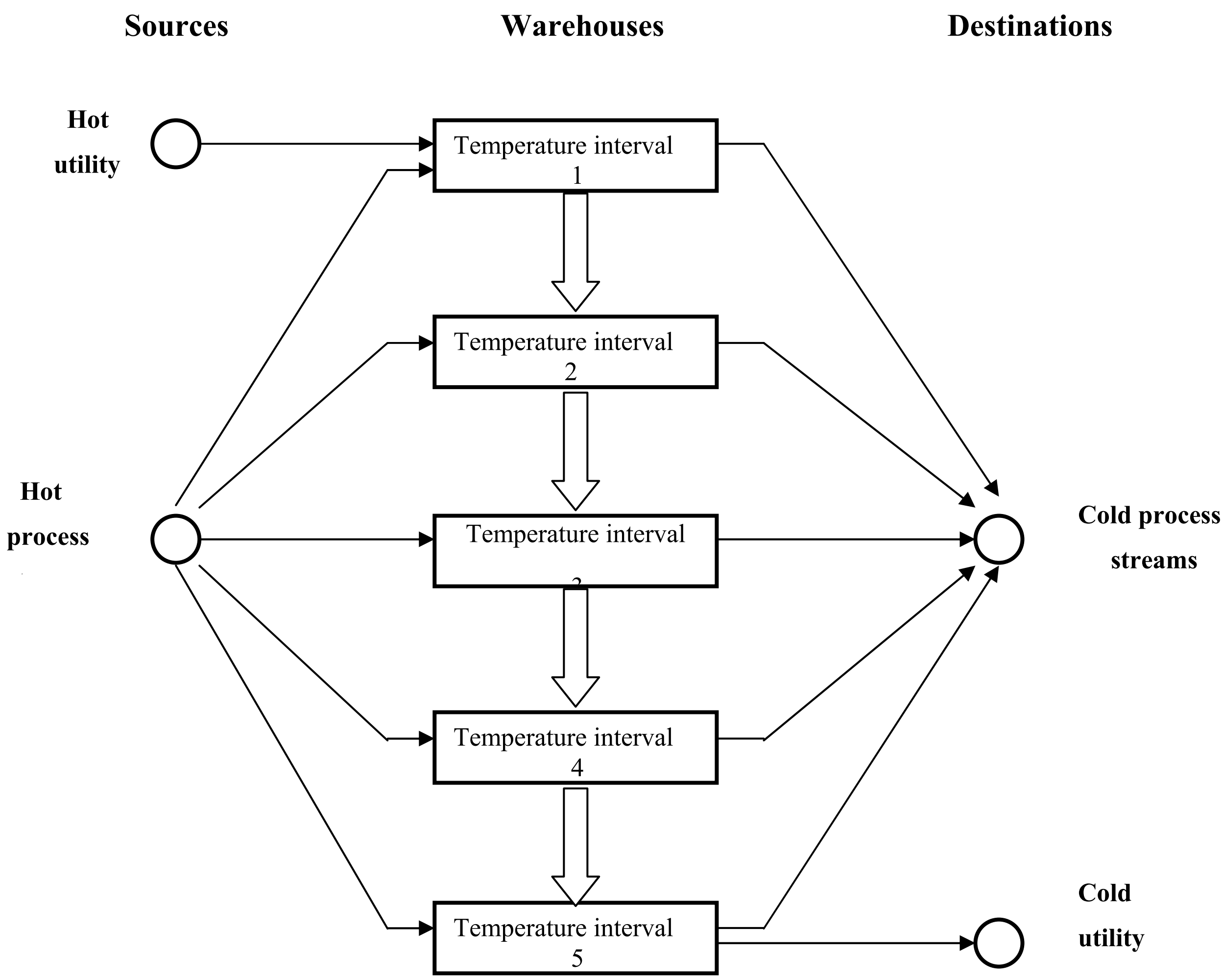

Figure 2.13: The transhipment model as applied to heat exchanger network synthesis, HENS (Floudas, 1995).

Figure 2.13 illustrates the transhipment model as applied to heat exchange process. The nodes on the left represent the heat sources (from hot process streams and utilities) which are transferred to the temperature intervals (depicted as warehouses), represented by the thin arrows. The heat stored in the warehouses (temperature intervals) can either be taken up by the cold process streams (and cold utilities) or shipped from one temperature interval to another, this is represented by the block arrows and it can only go in one direction. Also, no residual heat enters from the top temperature interval (except for the heat from the hot process streams and hot utilities) and none exits from the bottom temperature interval (except for that taken up by the cold process streams and cold utilities). The LP transhipment model is discussed next.

LP Transhipment Model

The LP transhipment model as applied to heat exchange networks can be used to identify the heat transfer pinch and hence target for the minimum utility requirement. The procedure entails first identifying the variables like, the heat flow (from the sources through each of the warehouses to the destinations) and then carrying out an overall heat balance around each warehouse. The heat balance serves as the constraint. Finally a mathematical model which aims to minimize the utility cost subject to the heat balance constraint is written.

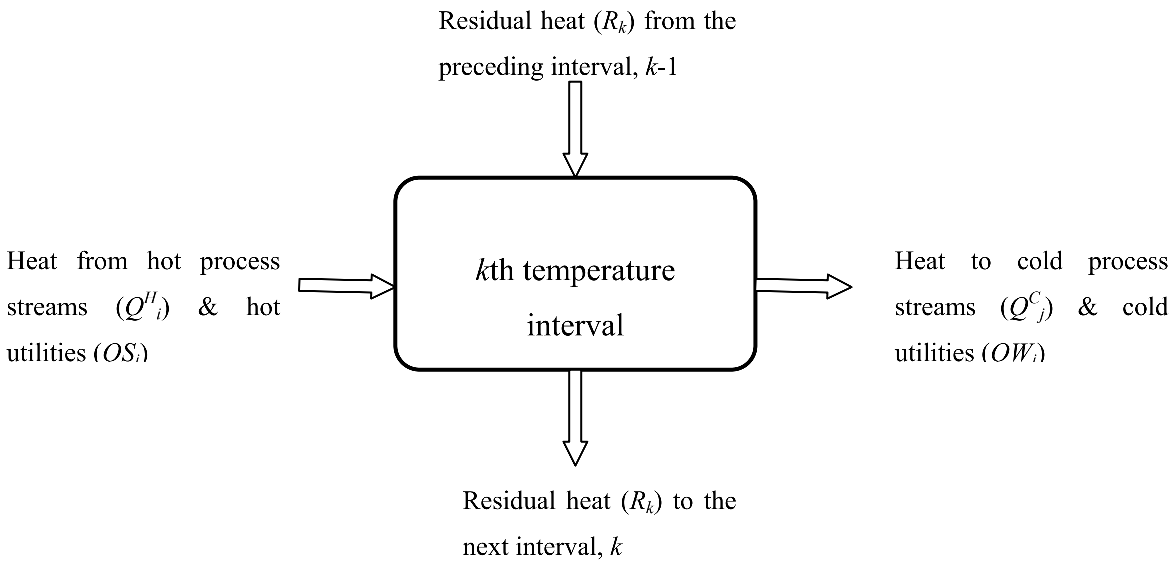

Figure 2.14: Heat flow representation for the kth temperature interval

Note that all the different heat flow loads which are represented as variables are nonnegative and so they are defined appropriately.

Overall heat balance around temperature interval k can be written as

$$R_k - R_{k-1} + \sum_{j \in CU_k} QW_{jk} - \sum_{i \in HU_k} QS_{ik} = \sum_{j \in HP_k} Q_{ik}{}^H - \sum_{j \in CP_k} Q_{jk}{}^C \qquad (2.18)$$

Equation 2.18 is a linear equality constraint.

The objective function which aims to minimize the utility requirement can be written as

$$\min \quad \sum_{i \in HU} C_i \sum_{k \in TI} QS_{ik} + \sum_{j \in CU} C_j \sum_{k \in TI} QW_{jk} \tag{2.19}$$

where C_i and C_j are the costs of the hot utility i and cold utility j

HP and *CP* are hot and cold process streams present in interval k

HU and *CU* are hot and cold utilities present in interval k

TI is the set of all temperature intervals

Equation 2.19 is linear in the variables QS_{ik} and QW_{jk} and the program is a linear programming problem since the objective function as well as the constraints are all linear. The pinch point is the location between k and k+1 interval where the heat residual R_k becomes zero. Simultaneously, the optimal values for the hot and cold utility loads are obtained as targets. See Floudas (1995) for extensive discussions and applications.

Minimum Number of Matches Target

The pinch divides the overall network into subnetworks which can be treated independently since it has been assumed that there would not be transfer of heat across the pinch. The minimum number of matches target is used to discriminate among all the networks that meet the minimum utility cost target (Floudas, 1995).

MILP Transhipment model

The solution from the LP transhipment model identifies the pinch thereby making for the treatment of each subnetwork independent from the other for the minimum number of matches target. Papoulias and Grossmann (1983) proposed the MILP transhipment model.

The MILP transhipment model aims to embed all possible heat exchange between all pairs of streams (this excludes hot utilities to cold utilities). The criteria used are

- Existence of each match, modelled using binary variables
- Amount of heat load of each match, modelled using continuous variables
- Amount of heat residual for each hot process stream/utility, also modelled using continuous variables.

Energy balances are carried out for the hot and cold process streams as well as the hot and cold utilities at each temperature interval k. The residual flows of each interval and the heat loads of each match are defined. The relationship between the heat loads and binary variables are established while the nonnegativity constraints on the continuous variables as well as the integrality conditions on the binary variables are imposed on the program.

The objective function which aims to minimize the number of matches is written as

$$\min \sum_{i \in HP \cup HU} \sum_{j \in CP \cup CU} y_{ij} \tag{2.20}$$

where y_{ij} represents a match between stream i and j.

Equation 2.20 is subject to constraints based on the criterion stated above. The resulting equations are all linear with binary variables and so the program is an MILP model. The solution to the resulting program gives the required minimum number of matches which according to Floudas et al. (1986) corresponds to the minimum number of units. Also the allocation of heat load for each match is given in the solution to the program for each of the subnetworks. The criterion of: no restrictions on matches, required matches, forbidden matches, restricted heat loads on matches, preferred matches etc as the case may be is further imposed as constraints so as to be able to calculate the lower and upper bounds of heat loads on each match (See Floudas, 1995 for further discussions and examples).

The above MILP transhipment model solution for minimum number of units will have different global solutions all meeting the criteria of the same minimum utility target as well as the minimum number of units targets. So Gundersen and Grossman (1990) proposed a technique with which to evaluate the different networks meeting the utility and number of units targets based on the degree to which each network transfers heat vertically between the composite curves. This is discussed below.

Minimum Area Target

The minimum area target discussed in section 2.2.1.2 under pinch technology is based on the assumption of vertical transfer of heat from the hot streams to the cold streams within each enthalpy intervals on the heat exchange composite curves. So networks that approach closely this vertical heat transfer concept within the exchangers would have the minimum area requirement. It is on this concept that Gundersen and Grossman (1990) based their vertical

MILP transhipment model. They partitioned the composite curves into enthalpy intervals and determined the various heat loads of each interval, such loads are ideal loads due to vertical heat transfer. The ideal heat loads were then compared to the respective heat loads of the various set of matches obtained from the MILP transhipment model. For situations in which the heat load of a match is larger than the maximum heat load due to vertical heat transfer, the objective function is penalized with a term which attempts to cut back the heat loads of those matches to the maximum possible in the enthalpy intervals. The penalty is as a result of non-vertical (criss-cross) heat transfer.

The objective function is written as

$$\min \sum_{i \in HP \cup HU} \sum_{j \in CP \cup CU} y_{ij} + \varepsilon \sum_{i \in HP \cup HU} \sum_{j \in CP \cup CU} S_{ij} \qquad (2.21)$$

where ε is the weight factor and y_{ij} represents the existence of a match between streams i and j.

Equation 2.21 is subject to the constraints of Equation 2.20 in addition to the following two constraints:

$$\left.\begin{array}{r} S_{ij} \geq Q_{ij} - Q_{ij}^{V} \\ S_{ij} \geq 0 \end{array}\right\} \begin{array}{l} i \in HP \cup HU \\ j \in CP \cup CU \end{array} \qquad (2.22)$$

The aim of the objective function, Equation 2.21 is to select the minimum number of matches and at the same time choose the set of matches whose heat loads most correspond to vertical heat transfer. See Floudas (1995) for detailed discussion on the partitioning of the enthalpy intervals.

The target for minimum utility cost as well minimum number of matches has been discussed, the next review is on techniques with which to generate a network configuration which would have a minimum investment cost and also meet the aforementioned targets.

Network Generation

The network generation technique of Floudas et al. (1986) will be reviewed. The authors argued that *HRAT* should be the only optimization variable while *EMAT* may be set equal to

HRAT or less than *HRAT*. For the minimum number of matches as well as the heat load of each of these matches, *HRAT* could be set equal to *TIAT*. There can also be $EMAT = TIAT <$ *HRAT* for each of the subnetworks as this may bring about fewer units, less total area as well as lower investment cost.

The basic idea of their network generation approach involves first establishing the fact that a match corresponds to a heat exchanger unit, then proposing each of the possible alternative HEN configurations (superstructure) using a graph-theoretical approach which meets the number of units target as well as their heat loads. The final stage entails optimizing the superstructure with the aim of getting the network with the minimum investment network cost. The optimisation solution results in the best stream interconnections, flow rates and temperatures as well best areas for the heat exchangers.

A superstructure is established for each stream and allocated an input and an output, also the number of matches with which the stream is involved are represented as heat exchangers. Further components of each stream superstructure are all the potential linkages from the inputs to the exchangers between each pair of exchangers and from the exchangers to the outputs. To accommodate the aforementioned, each stream is allocated a splitter and a mixer and each exchanger, a mixer at its inlet and a splitter at its outlet. Through the careful manipulation of the heat capacity flowrates of each of the streams, so many alternative structures could be verified. The procedure discussed above is applied to each of the subnetworks and the resulting networks are combined to give the overall network structure.

The mathematical formulation of the HEN superstructure involves defining variables such as the heat capacity flowrate of each stream, the temperature of each stream and also the areas of the heat exchangers. The constraints are: mass balances for the mixers and splitters, energy balances for the mixers and exchangers, feasibility constraints for heat exchange as well as the nonnegativity constraints. The objective function would aim to minimize the investment cost of the network in terms of the areas of the heat exchangers. The energy balances for the mixers and exchangers and the objective are non-linear and thus they make the model a non-linear program, (NLP).

The vertical MILP transhipment model of Gundersen and Grossman (1990) embedded in the HEN synthesis strategy of Floudas et al. (1986) is illustrated in the following algorithm.

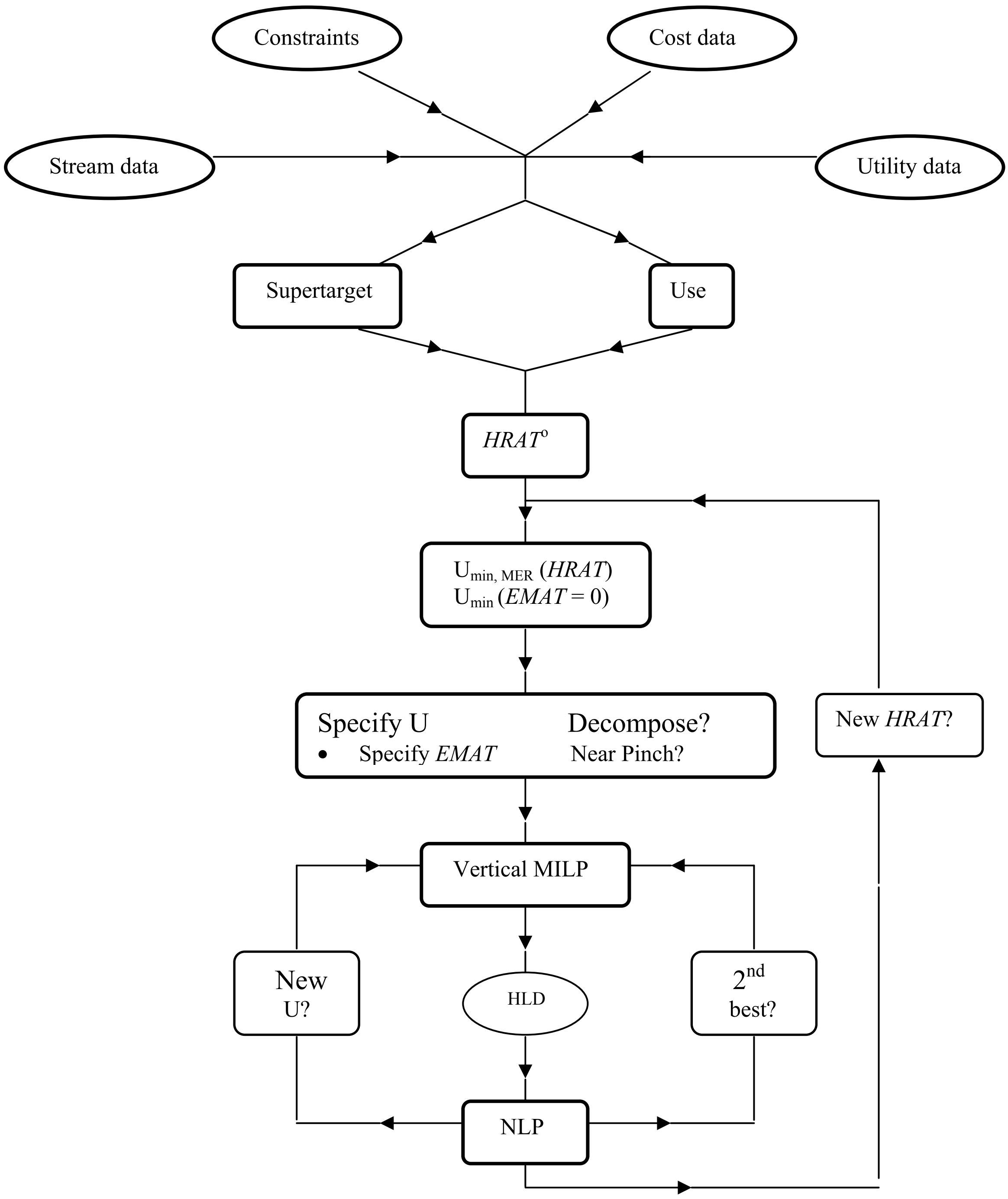

Figure 2.15: Sequential approach to HENS with the vertical MILP model embedded (*Gundersen & Grossman, 1990*).

An initial *HRAT* could be obtained either through supertargeting or from experience and then the engineer decides on a number of units as found suitable. The vertical MILP transhipment model is then used to determine the best heat load distribution which is then submitted to the NLP for subsequent network generation and optimization (Gundersen & Grossman, 1990).

2.2.2.2 Simultaneous Approach

As discussed earlier, the decomposition based approach to HENS does not trade-off simultaneously the different costs associated with the network cost, also time and effort is consumed in trying to obtain the optimal *HRAT* through iteration. These and other deficiencies of the decomposition based approach are what gave birth to the simultaneous technique.

The level to which the HEN synthesis is decomposed is another factor which comes to play in categorizing the simultaneous approach. The minimum number of matches and minimum investment cost network generation has been synthesized simultaneously as a single task subject to a minimum utility cost target and pinch location, this technique does not involve partitioning into subnetworks. A simultaneous synthesis which uses the *pseudo-pinch* concept has been developed too. Floudas (1995) has reviewed the two aforementioned approaches. He also discussed two other techniques, the first being one which does not decompose the task in any way but instead treats *HRAT* explicitly as an optimization variable and the second is similar to the first but it is simplified with the assumption of isothermal mixing. This assumption helps to restrict the nonlinearities to the objective function alone thereby reducing the complexity of the mathematical model but this assumption sidetracks potential optimal configurations from evaluation. What is common to each of the above simultaneous approaches is the fact that their objective functions and constraints are all mixed integer non linear programs. The fully simultaneous approach of Ciric and Floudas (1991) will be reviewed in the next section.

Simultaneous HENs Synthesis

This technique does not decompose the HEN synthesis task in any way. It trades-off simultaneously the operating cost and capital cost. The following solutions are generated simultaneously: hot and cold utility requirement, required matches, heat exchanger areas and network topology. Since *HRAT* is not specified, the utilities required are treated as unknown optimization variables. The pinch is also neglected by allowing heat to flow across the pinch. The technique also involves postulating a hyperstructure and finally writing out a mathematical model which has an objective function which aims to minimize the total annual cost. The resulting mathematical model is a mixed integer non linear program.

The objective function is written as

$$min\ \ TAC = \left[\sum_i \sum_j c_{ij} A_{ij}^{\ 0.6} . y_{ij}\right] + \left[\sum_{i \in HU} C_i Q_i^{\ H} + \sum_{j \in CU} C_j Q_j^{\ C}\right] \tag{2.23}$$

where A is the heat exchange area

c is the heat exchanger cost coefficient.

Note that the utility loads, $Q_i^{\ H}$ and $Q_j^{\ C}$ are unknowns.

The merits and demerits of each of the synthesis approaches for HENs discussed will be highlighted under the section for CHAMENS. This study proposes to harness the strength of each of these techniques in synthesizing CHAMENS, hence the word *hybrid*.

2.3 Mass Exchanger Network Synthesis, MENS

Mass exchanger network synthesis (MENS) unlike HENS has not received much attention. Much of the synthesis techniques for MENs arose as a result of the analogy which can be drawn from HENs. The synthesis of mass exchange networks started with the use of pinch technology (El-Halwagi and Manousiouthakis, 1989) and later mathematical programming found applications too (El-Halwagi and Manousiouthakis, 1990). Examples of mass exchange operations are: Absorption, stripping, adsorption, ion exchange, leaching and extraction.

The MENS problem statement can be stated as follows (El-Halwagi, 1997; Hallale, 1998):

> *Given a number N_R of rich streams (sources) and a number N_S of MSAs (lean streams), it is desired to synthesize a cost-effective network of mass exchangers that can preferentially transfer certain species from the rich streams to the MSAs. Given also are the flowrate of each rich stream, G_i, its supply (inlet) composition, y_i^s, its target (outlet) composition, y_i^t, where $i = 1,2,.....,N_R$. In addition, the supply and target compositions, x_j^s and x_j^t, are given for each MSA where $j = 1,2,.....,N_S$. The*

mass transfer equilibrium relations are also given for each MSA. The flowrate of each MSA is unknown and is to be determined as part of the synthesis task.

The candidate MSAs (lean streams) can be classified into N_{SP} process MSAs and N_{SE} external MSAs (where $N_{SP} + N_{SE} = N_S$). The process MSA already exists on the plant site and can be used for the removal of the species at a low cost (often virtually free). The flowrate of each process MSA, L_j, that can be used for mass exchange is bounded by it availability in the plant and may not exceed a value of L_j^c. On the other hand, the external MSAs can be purchased from the market and their flowrates are to be determined by economic considerations.

The design questions to be tackled are:

- Which mass exchange operations should be used?
- Which MSAs should be selected?
- What should be the optimal flowrate of each MSA?
- Which MSA should be matched with which process stream?
- What is the optimal system configuration (e.g. how should these mass exchangers be arranged? Is there any stream splitting and mixing?)?

Figure 2.16 below is a schematic representation of the MENS problem.

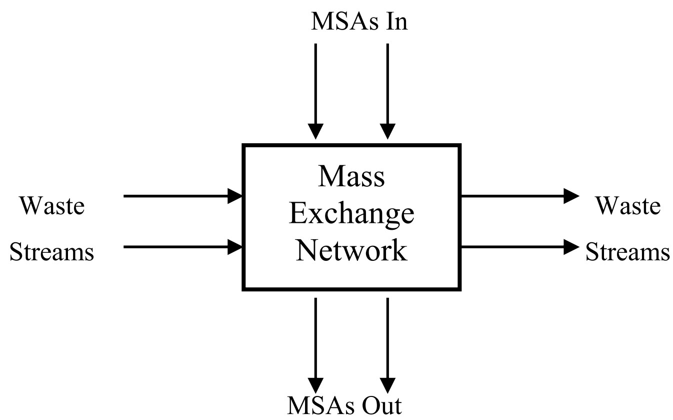

Figure 2.16: A schematic representation of the MEN synthesis problem (*El-Halwagi, 1997*).

Target composition of the MSA is not stated explicitly as an optimization variable in the problem statement because this is to be determined by the situation at hand which can be physical, technical, environmental, safety or economic. The physical and economic criteria could be capitalized upon to optimize the network; this will be explored in this study.

2.3.1 Pinch Technology as applied to MENS

Pinch technology application to MENS involves targeting before actual design. It started off just as it did for HENS in which the minimum mass separating agent (MSA) costs and minimum number of units corresponding to the minimum MSA cost target were the first targets to be established (El-Halwagi, 1997). The subsequent design was then tailored towards this minimum number of units which meets the MSA targets. Unlike in HENS, the network featuring the least number of units MENS is not always the optimal. Hallale & Fraser (1998, 2000a, & 2000b) drew analogues from the capital cost targeting techniques of Townsend & Linnhoff (1984), Ahmad (1985) and Ahmad & Smith (1989) for area and the minimum number of shells targeting. This they did so that the sizes of mass exchangers would be factored into the total annual cost targeting for MENS as well. Each of these targeting techniques is discussed in subsequent sections.

2.3.1.1 Mass Separating Agent Targets

The concept behind pinch technology as applied to mass exchange network synthesis is to maximize the use of the process MSAs before calling on external MSAs. The more the process MSAs are used, the less the external MSAs need to be purchased, therefore the constraint to maximum mass separating agent recovery lies with the process MSA`s thermodynamics which are: its available flowrate and process temperature on site. For a given process MSA flowrate and temperature, there is a limit to how much mass could be recovered, this limit is otherwise known as the pinch. It is worthwhile to point out here that this so called “pinch point” can be relocated so as to improve the mass recovery capacity of the process MSA. Identifying a means of relocating the pinch point and also analyzing its effect on the overall separation and heat subsystems is a major focus of this study.

The pinch targeting technique for the minimum MSA requirement discussed in the next paragraph will form the basis for the pinch technology technique to be developed in this research for CHAMENS. There are two methods, the graphical (pinch diagram) and algebraic approaches (El-Halwagi, 1997) just as for HENS (Linnhoff et al., 1982). The graphical approach will be reviewed in this study, for the algebraic approach, see El-Halwagi (1997).

Analogies are established between heat and mass pinch so as to target for the minimum MSA cost. But some of these analogies are not very direct, the major one being the fact that a one-to-one correspondence has to be established among the compositions of all streams for which mass exchange is thermodynamically feasible since equilibrium relations come to play in mass exchange unlike heat exchange. This, El-Halwagi and Manousiouthakis (1989) accomplished by establishing the concept of a "minimum allowable composition difference, ε" which is analogous to the minimum temperature difference, ΔT_{min}, in HENS. An illustration of this concept is as follows:

For a mass exchange operation involving a rich stream with composition y_i, whose equilibrium relation governing the transfer of its species to a lean stream j is given by

$$y_i = m_j x_j^* + b_j \tag{2.24}$$

In theory, x_j^* is the highest composition that the lean stream MSA can attain. In practice, exchangers do not operate at this maximum theoretical composition because it would result in infinitely tall absorbers. So a limit composition is set in the following relation:

$$x_j = x_j^* - \varepsilon_j \tag{2.25}$$

x_j must not exceed the above stated composition for feasible mass transfer. The role played by ε in Equation 2.25 is synonymous to that played by ΔT_{min} in HENS i.e. the driving force for mass and heat transfer respectively. But in HENS, it is simply the difference between any hot stream and any cold stream while in MENS, it is the difference between actual and equilibrium compositions and it is stream dependent. Combining Equations 2.24 and 2.25 gives the maximum composition for the lean stream based on a specified ε.

$$x_j = \frac{y_i - b_j}{m_j} - \varepsilon_j \tag{2.26}$$

Most systems, particularly environmental, involve low concentrations, and so their equilibrium relations can be assumed linear and also that species transfer from rich to lean stream is independent of the presence of other species. For cases that are strongly non-linear, linearization over discrete intervals could be employed. Another assumption is that stream flowrates are constant, this can be when very small composition changes occur or there is counterdiffusion (El-Halwagi and Manousiouthalis, 1989a). Inert flowrates and compositions (e.g. mass or molar ratios) should be used in cases with significant flowrates changes.

The Pinch Diagram

The pinch diagram approach for targeting the minimum external MSA requirement is similar to that of the HENS pinch. First, a composite of all the rich streams is established by plotting each rich streams mass to be exchanged against its supply and target compositions. This is illustrated in Figure 2.17 below.

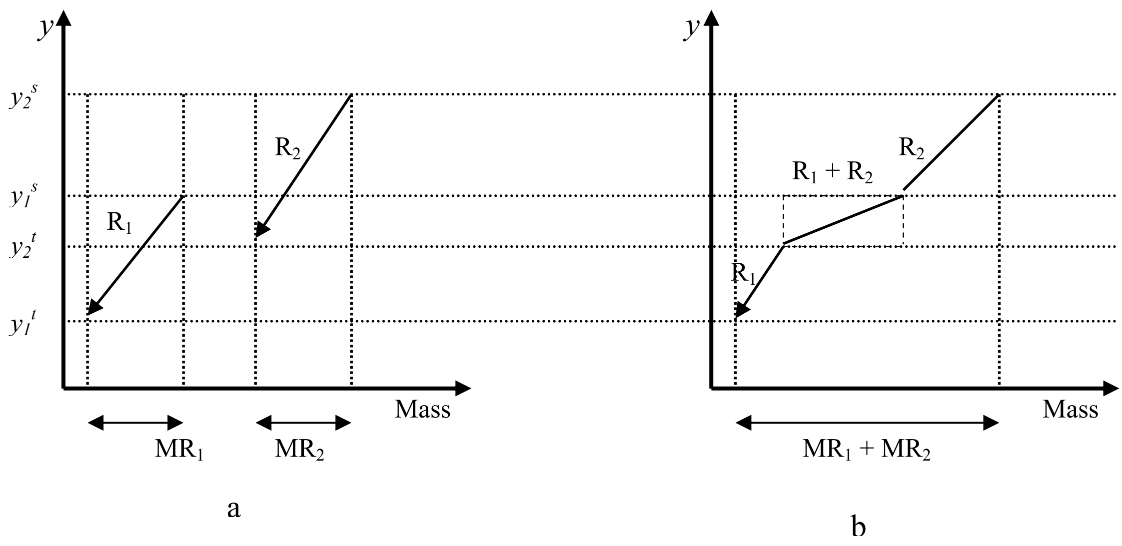

Figure 2.17: Forming a composite of the rich streams.

As illustrated in Figure 2.17a, the horizontal distances of MR_1 and MR_2 are the mass exchanged by streams R_1 and R_2 while the vertical distances of the two streams are the composition ranges. The slopes of R_1 and R_2 correspond to the flowrates of these streams respectively. The stream curves R_1 and R_2 could be slid either to the right or left while still maintaining the same composition ranges because the vertical scale is only relative. Sliding R_2 closer to R_1 and using the "diagonal rule", the masses of each stream within the highlighted box is added up to give the cumulative mass (El-Halwagi, 1997). This is illustrated in Figure 2.17b.

Forming a composite of the lean curve is not directly comparable to that of the cold curve in HENS because there is a direct relationship between every hot and every cold stream but this is not the case for the lean streams. Each MSA has its own relation with the rich stream: this relation is known as the equilibrium relation. El-Halwagi and Manousiouthakis (1989) established a means by which each of the MSAs would be related to the rich streams for which mass transfer is feasible thermodynamically on the same basis, the tool is known as the *corresponding composition scale*. Equation 2.26 is used to get the equivalent of each MSA composition on the rich stream composition scale: this makes all the MSAs to be represented on the same plot and a composite plot to be formed as well.

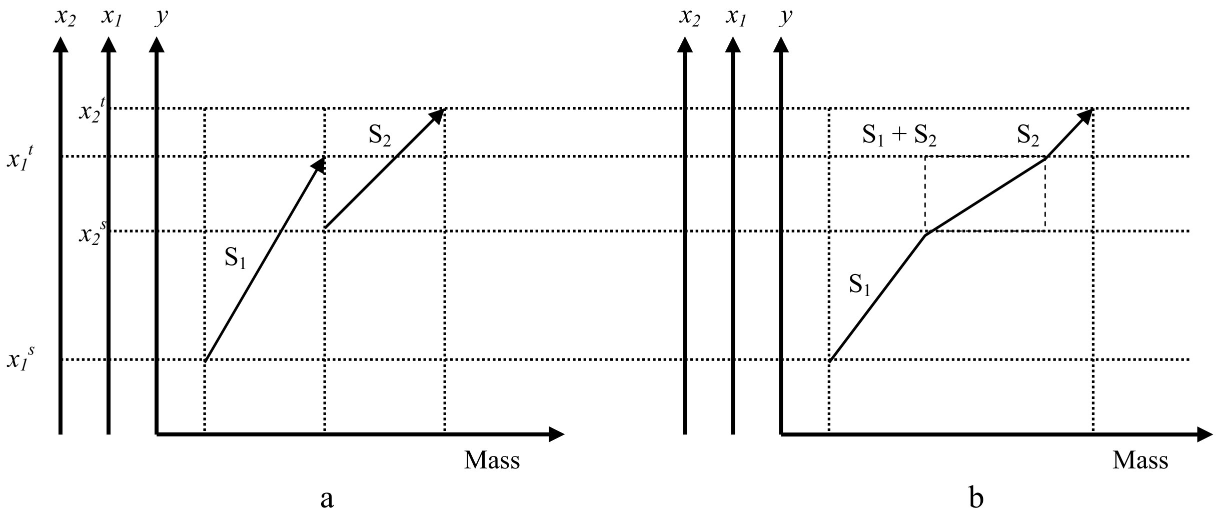

Figure 2.18: Forming a composite of the lean streams.

A composite of the lean streams is formed just as was done for the rich streams. The slope of MSAs, S_1 and S_2 corresponds to the maximum available flowrate on site of these process MSAs. The two curves are then plotted on the same axes. Shifting the lean composite curve horizontally towards the rich composite curve until it touches it locates the pinch point: this is illustrated in Figure 2.19 below.

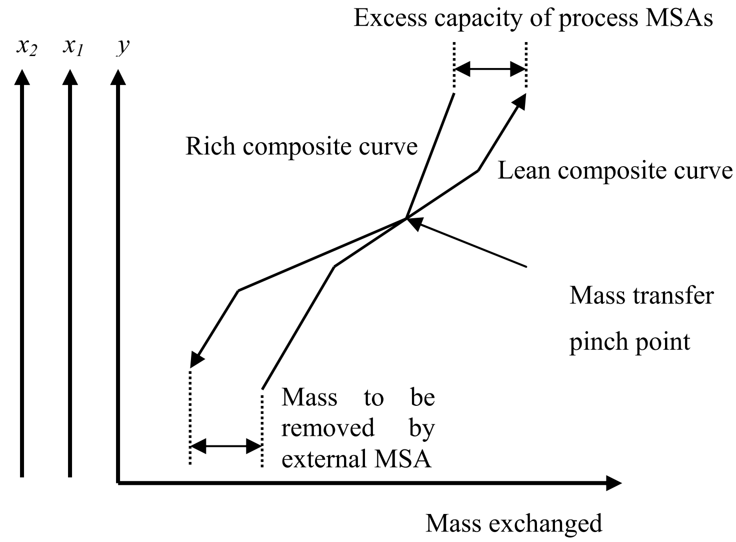

Figure 2.19: Construction of the rich and lean composite curves on the same axes locates the mass transfer pinch and MSA targets.

The point at which the rich and lean composite curves touch each other is known as the *mass transfer pinch.* This is the thermodynamic constraint to mass transfer within the process. Just as it applies in HENS, the region at which there is complete vertical overlap of the rich composite curve over the lean composite curve is known as the region of mass integration, it depicts the maximum amount of species that can be taken up by the process MSAs. The overshoot of the lean composite curve over the rich composite curve indicates the excess capacity of the process MSAs to remove mass, this is analogous to the minimum hot utility target in HENS. This capacity cannot be used because of thermodynamic infeasibility and this can be done away with by lowering either the target composition of the process MSA or its flowrate.

It is worth pointing out here that this excess capacity is dependent on the equilibrium constant of such process MSAs because for equilibrium relations that are temperature dependent, the equilibrium constant could take on some other values thereby affecting this excess capacity. This study aims to include this excess capacity in terms of equilibrium temperature as an optimization variable. On the other hand, the overshoot of the rich composite curve over the lean gives the mass to be taken up by the external MSA: this is analogous to the minimum cold utility target in HENS. This gives the MSA cost targets.

A distinction between Figures 2.1 and 2.19 as pointed out by Hallale (1998) is the fact that the hot and cold composite curves are separated by ΔT_{min} which is the heat transfer driving force, but in the case of mass transfer, the two curves touch at the pinch. This is because the mass transfer driving force, ε, was used in constructing the corresponding composition scale, so in essence, it is already built in.

Above the pinch in Figure 2.19 are streams (or part of streams) having compositions that are higher than that of the pinch while below the pinch are those streams (or parts of streams) with compositions lower than that at the pinch. Above the pinch, process MSAs only remove the masses from the rich streams while below the pinch both process MSAs and external MSAs remove the masses from the rich streams. No mass should be transferred across the pinch, just as it is in HENS because this will shift upwards the composite lean stream thereby requiring an excess of external MSA to remove this mass below the pinch. In essence minimizing the cost of external MSAs requires that no mass be transferred across the pinch.

The MENS Grand Composite Curve, GCC

The mass transfer grand composite curve, GCC, is reviewed in this study because it will be used to develop sequential synthesis techniques for CHAMENs based on pinch technology. Fraser and Shenoy (2005) developed techniques for selecting between alternative MSAs and the minimum flowrate requirement for such chosen MSAs. Prior to their study, MSA selection had been based on the one with the lowest cost per unit mass but they argued that this should not be so. The new selection criteria they proposed involves selection based on the MSA with the lowest overall cost of removal of the mass load and that this depends on both the cost of the MSA and its allowable concentration range.

2.3.1.2 Capital Costs Targets

The mass exchangers that will be focused on in this study are absorbers and strippers, the staged and continuous contact absorbers will be discussed. This is because extensive capital cost targeting techniques have been developed for these types of mass exchangers using pinch technology by Hallale (1998).

As already mentioned, many analogies exist between HENS and MENS, this is reflected in the capital cost targets which are to be reviewed in this section. In predicting the capital cost of a mass exchanger network, factors like, number of mass exchangers, size (or number of stages) of the exchangers, and material of construction have to be accounted for as these contribute to the capital cost of a mass exchange network. The number of units targets is reviewed next.

Number of Units targets

Designing towards a low number of mass exchange units is beneficial not only because it reduces cost but also makes for a simple plant layout for piping, foundations, maintenance, controllability, etc. El-Halwagi and Manousiouthakis (1989) designed towards the minimum number of units that meets the MSA cost targets so as to minimize the capital cost of the network since the cost of each mass exchanger is usually a concave function of the unit size. According to Hallale and Fraser (2000a) this was the synthesis procedure for HENS in which designs were geared towards the minimum number of units. But for MENS, minimizing the number of units is not always synonymous to the optimal network cost because the sizes of the mass exchangers should also be factored into the targeting procedure as later done for HENS by Townsend and Linnhoff (1984).

The minimum number of units targets is carried out for above and below the pinch separately so as to meet the MSA cost targets, both are then added for the minimum number of units for the overall network.

$$N_{\text{units, pinch}} = (S\text{-}1)_{\text{Above pinch}} + (S\text{-}1)_{\text{Below pinch}}$$

S is the total number of streams (rich, lean and external MSAs).

Mass Exchange Number of Stages and Height Targets

Targeting techniques have been developed for the factors that contribute to the capital cost of mass exchange networks (Hallale, 1998) apart from the number of units which has been discussed in the previous section. These factors (for both stagewise and continuous contact exchangers) are: total number of real stages (or total exchanger height), exchanger diameters, tray spacings, inactive heights, distribution of units between streams and distribution of stages and height between streams.

This study will review the very simplest cases of mass exchange networks capital cost targeting, namely problems involving one transferred component, exchangers of the same type, linear equilibrium relations and a single minimum composition difference for all streams. For the more complex cases, see Hallale (1998).

Hallale (1998) classified MENS problems into three different types: the first is a case in which there is only one MSA, the second has two MSAs which do not overlap i.e. each is restricted to one side of the network based on the pinch division, while the third is the more general case involving many MSAs which do overlap. For the second case, the inlet composition of the MSA causes the pinch therefore lies to one side of the pinch. It is necessary to review each of these types of MENS problems because combining the synthesis of any of them with HENs produces very different results.

Hallale (1998) addressed first the simplest case of MENS problem i.e. MENS with just one MSA, because this is easily built upon for the other two cases. There is no direct analogy between the heat transfer composite curve and the mass transfer composite curve (Figure 2.19) for the targeting of the number of trays or height requirements for columns. The heat transfer composite curve explicitly shows the driving force for heat transfer which is temperature differences between the hot and cold composite curves but this is not the case with mass transfer because the driving forces for mass transfer involve equilibrium relations and this is not shown explicitly on the mass transfer composite curves. He overcame this difficulty by constructing a tool known as the *y-x composite curve plot.* This curve like the heat transfer composite curve shows explicitly the difference between the operating and equilibrium lines of mass exchangers since the number of stages or height depends strongly on this difference. This difference is the minimum composition difference, ε of El-Halwagi and Manousiouthakis (1989) which Hallale (1998) regarded as the mass transfer driving force.

The procedure for the number of stages or height targeting entails forming a composite of the operating line and the mass transfer equilibrium line for each mass exchange operation. The composite operating line is formed by dividing the rich stream compositions into composition intervals. Material balances are then carried out for the transferred species in each interval so as to determine the different compositions that the MSA would assume at each point in the network.

The composition of the transferred species in the MSA starts off as x^s and increases within each interval *k,* by an amount Δx_k . Equation 2.27 is used to set up the material balance:

$$\Delta x_k = \Delta y_k \frac{\left(\sum G\right)_k}{\left(\sum L\right)_k} \tag{2.27}$$

where Δy_k is the change in y over the interval,

$\left(\sum G\right)_k$ is the total rich stream flowrate in interval *k,*

$\left(\sum L\right)_k$ is the total lean stream flowrate in interval *k* (for cases with more than one MSA).

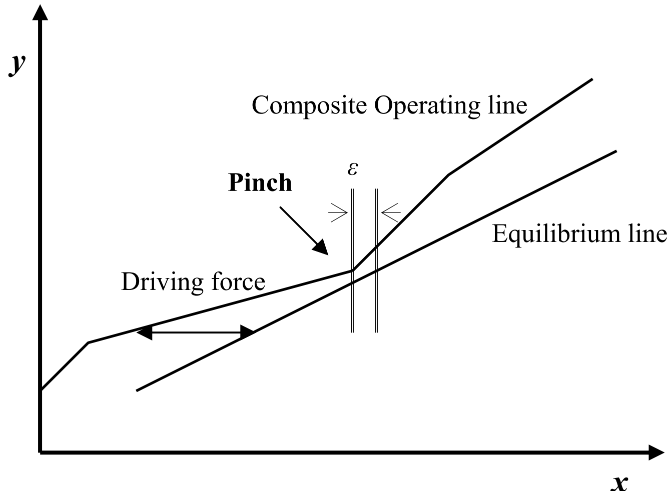

Figure 2.20: *y-x* Composite curve showing driving forces (Hallale, 1998).

Figure 2.20 is identical to the *y-x* diagram for sizing individual mass exchangers in which the compositions of the species to be transferred are plotted as an operating line and the equilibrium line also plotted on the same axes. The only difference is the fact that Figure 2.20 is a composite of more than one exchanger. For feasible mass exchange, the operating line must lie completely above and to the left of the equilibrium line so that the distance between these two curves either measured vertically or horizontally is the driving force for mass transfer, which is represented as *ε* in Figure 2.20. The key feature in this *y-x* composite curve is the fact that the importance of the pinch is depicted as being the point of closest approach between the composite operating line and the equilibrium line, in essence, the point of the least driving force. In the lean phase, it is exactly equal to ε. Also, the diagram shows the profile for perfect countercurrent or vertical mass transfer.

The *y-x* composite curve tool of Hallale (1998) is extensively reviewed in this study because it comes in handy for formulating as a mathematical model the verticality of mass transfer so as to aim to minimize the number of stages or height requirement of a mass exchange network, this would aid in discriminating among all potential networks meeting the same MSA target in an automated fashion.

The number of equilibrium stages requirements for a mass exchange network could be predicted from the diagram by the stepping off technique of McCabe or done analytically using the Kremser equation.

This new tool goes a long way in establishing analogies between HENS and MENS. It is similar to the problem table and composition interval of Linnhoff et al. (1982) and El-Halwagi and Manousiouthakis (1989) respectively. It can be demarcated into composition intervals and each interval treated as an imaginary exchanger for targeting purpose. The composition intervals could also be represented on a grid as is the case with HENS. This are illustrated in Figure 2.21 and 2.22 below:

Figure 2.22 illustrates the stream populations within the composition intervals, the rich streams run from right to left and the lean from left to right. Also the pinch is represented as dividing the network into two distinct regions: above and below the pinch.

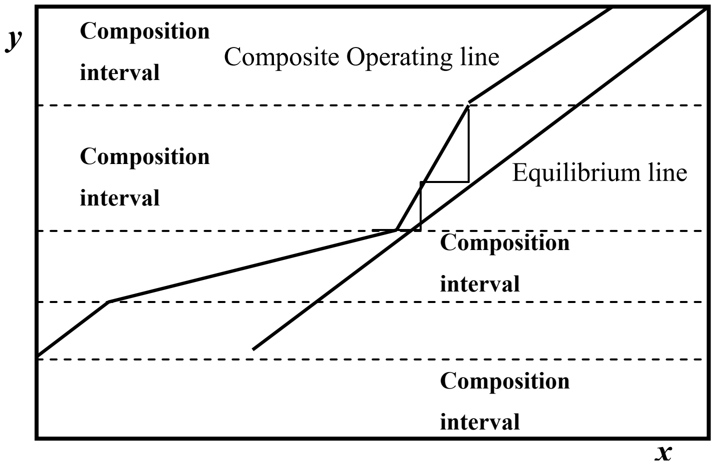

Figure 2.21: composition intervals represented on the *y-x* composite curve (*Hallale, 1998*).

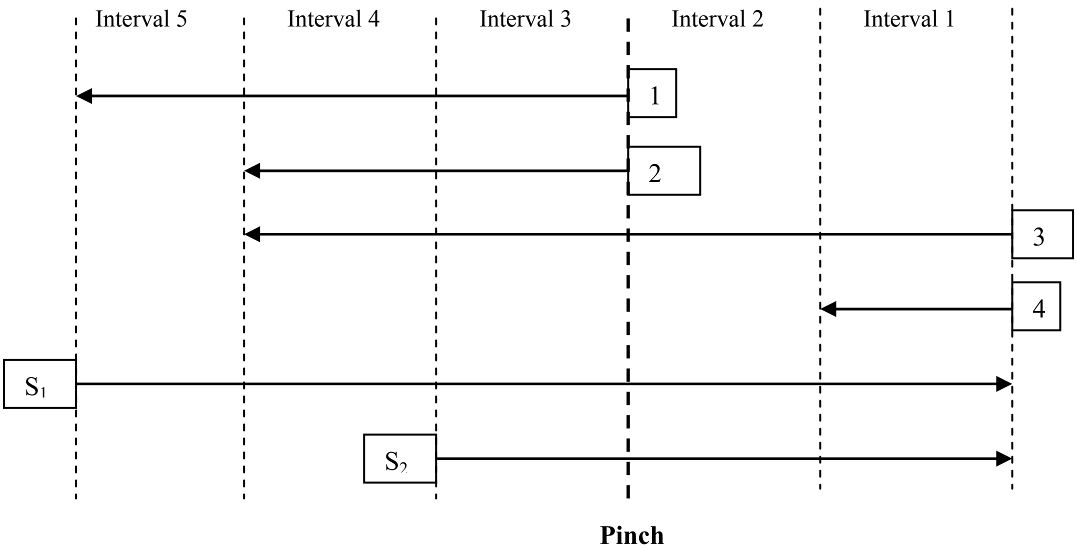

Figure 2.22: Grid representation of composition intervals (*Hallale, 1998*)

For stagewise columns, the contribution of each rich stream within each interval to the number of stages within that interval has to be accounted for, just as it is with shells targeting of Ahmad and Smith (1989) in HENS. Only the rich stream contribution is considered because there is only one MSA whose contribution is not used explicitly. The stage contribution by rich stream R_i is given as

$$N_i = \sum_{k=\alpha_i}^{\beta_i} N_k \tag{2.28}$$

Rich stream *i* starts in interval α_i and ends in interval β_i .

Equation 2.28 is the equilibrium number of stages: an overall column efficiency is used to convert it to the number of real stages. The number of real stages, N_{real}, is targeted for both above and below the pinch separately (so as to ensure consistency with the MSA target) and each rounded up. The total number of stages target for the overall network is the sum of the contributions from above and below the pinch which is given by:

$$N_{\text{real, total}} = \sum_{i}^{\substack{\text{Rich}\\\text{streams}}} \left[N_{\text{real},i}\right]_{\text{Above pinch}} + \sum_{i}^{\substack{\text{Rich}\\\text{streams}}} \left[N_{\text{real},i}\right]_{\text{Below pinch}} \tag{2.29}$$

The minimum number of units targets of El-Halwagi and Manousiouthakis (1989) is factored in for the capital cost target, it is assumed that the minimum number of trays is achieved in the minimum number of units. According to Hallale (1998), the column diameter and tray spacings also have to be predicted before actual design. For gas liquid MENS problems, the properties of each of the gas streams are used to target the tray spacings and column diameter and a unit distribution pattern set out for the gas steams.

Targeting for continuous contact columns requires accounting for all that were enumerated for stagewise exchangers as well as the total packed height, and distribution of packed height between streams. Hallale (1998) used the transfer unit approach for the height targeting and this is discussed based on MENS problems with one MSA. The rich stream properties are used for the calculation of the transfer units. The *y-x* and is equally used to target the minimum packed height requirement for the network. The intervals on the composite operating line are also considered as fictitious continuous contact exchangers. For a constant value of the rich phase mass transfer coefficient K_ya and column cross-sectional area S throughout the network, the minimum height target is given by:

$$H_{\min} = \frac{1}{K_y aS} \sum_{k}^{\text{Intervals}} \frac{W_k}{\Delta y_{\text{lm},k}} \tag{2.30}$$

where $H_{\min}$ is the minimum network height,

W_k is the mass transferred in interval k.

Equation 2.30 will only give a good prediction if mass transfer coefficient and column cross-sectional areas are constant all through the network but this is not usually the case because these properties are usually stream dependent. In overcoming this problem Hallale (1998) derived an equation analogous to the Bath formula which is expressed in terms of the rich streams:

$$H_{\min} = \sum_{k}^{\text{Intevals}} \frac{1}{\Delta y_{lm,k}} \left(\sum_{i}^{\text{Rich streams}} \frac{w_i}{K_y aS_i} \right)_k \tag{2.31}$$

where w_i is the mass load of stream i.

Equation 2.31 will predict to a good extent the minimum height requirement if $K_y aS$ do not vary too much. $K_y a$ accounts for the mass transfer resistances in both the rich and lean streams and so the lean steams do not have to be included explicitly in the equation.

Equation 2.31 could also be written as:

$$H_{\min} = \sum_{k}^{\text{Intervals}} \text{NTU}_k \left(\sum_{i}^{\text{Rich streams}} \text{HTU}_i \right)_k = \sum_{k}^{\text{Intervals}} H_k \tag{2.32}$$

The column diameter and $K_y a$ are also estimated based on the gas streams: the distribution of units between streams is the same as it is for stagewise exchangers. Equation 2.32 can still be stated in terms of the streams so as to be able to distribute the total packed height among the streams.

$$H_{\min} = \sum_{i}^{\text{Rich streams}} \text{HTU}_i \sum_{k=\alpha_i}^{\beta_i} \text{NTU}_k = \sum_{i}^{\text{Rich streams}} H_i \qquad (2.33)$$

where R_i starts in the interval α_i and ends in β_i.

In keeping with the pinch division, each rich stream's contribution above the pinch is added to that below the pinch to give the total target which is:

$$H_{\min} = \sum_{i}^{\text{Rich streams}} \left(H_{i,\text{ above pinch}} + H_{i,\text{ below pinch}} \right) \qquad (2.34)$$

The second class of MENS problem according to Hallale (1998) classification are those in which the problem is divided into two independent regions, this is because the pinch is caused by the entry of the only process MSA in the process and so all the previously discussed targeting techniques can be applied to each of the regions separately as if it were a whole problem. The overall result is obtained by adding the results from the two independent subproblems.

The difficulty with the third class of MENS problem is how to represent the driving forces because more than one MSA may be present in each region of the pinch. Each MSA has its own equilibrium relation and the *y-x* composite plot cannot handle multiple equilibrium relations. Hallale overcame this problem by developing a new tool known as the *y-y* composite curve plot*. This is a tool that represents the *x* composition of each of the MSA as the rich stream composition with which it is in equilibrium, y^*, this brings all the MSAs to the same basis. Since the minimum composition difference, ε, is normally expressed in terms of the lean stream, Hallale (1998) instead, expressed it in terms of the rich stream through the following relation:

$$\Delta y = m_j \Delta x \qquad (2.35)$$

where Δx is the composition difference with ε being the minimum, it then follows that:

$$\Delta y_{\min} = m_j \varepsilon \qquad (2.36)$$

With the new minimum composition difference, Δy_{min}, expressed in terms of the rich stream, the lean composite curve of the mass transfer curve of El-Halwagi and Manousiouthakis (1989) was reconstructed in terms of y^*. The resulting mass transfer composite curve this time depicts the mass transfer pinch as the point of closest approach between the rich and lean composite curves, just as it is with the heat transfer composite curves. This is illustrated by Figure 2.23 below:

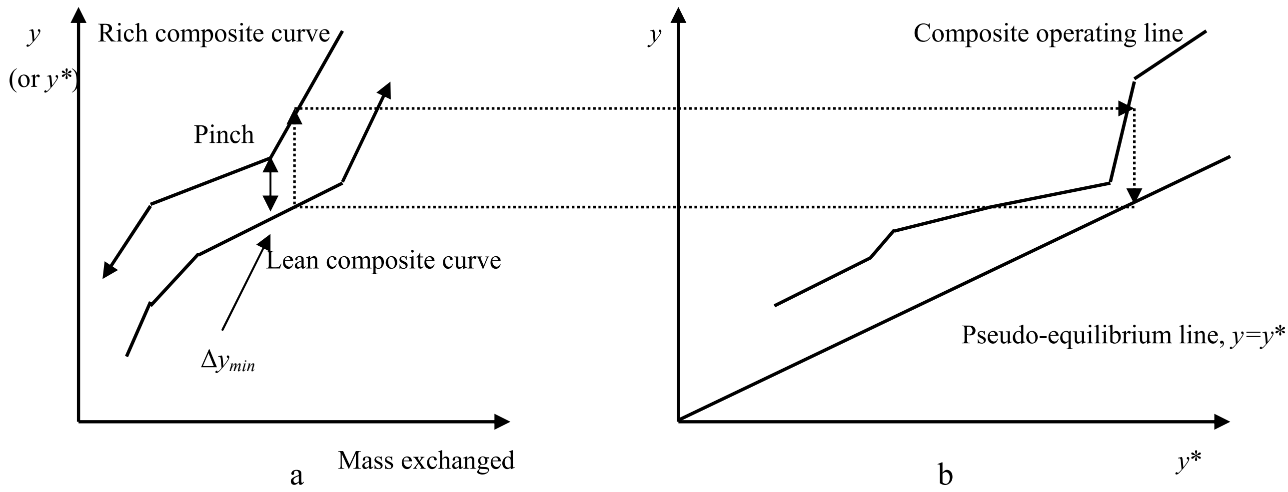

Figure 2.23: Construction of the y-y^* composite curve plot form the balanced mass transfer composite curve plots (*Hallale, 1998*).

Figure 2.23a & b illustrate the construction of the *y-y* composite curve plot* from the modified *mass transfer composite curve plot.* The *y-y* composite curve plot* can be used for stages and height targeting just as has been explained for the *y-x composite curve plot*. It can also be used for the first two classes of MENS.

Capital Cost Estimation

The procedure for estimating the capital cost is just as it applies to HENS, the capital cost correlation is applied to each of the imaginary units. For both stagewise and continuous contact columns, the capital cost correlation is applied to each of the fictitious units taking note of the contributions of each rich stream to the units, diameters, height, and stages. Rich streams which cross the pinch are accounted for twice.

Vertical transfer predicts the minimum or near-minimum area requirements in HENS, so it was presumed that it will also predict well the number of stages and height requirements in MENS. But this was found not to be so all the time. The reasons are that: the number of trays targeting does not always predict the actual minimum, exchanger diameter are not usually known before actual design and this can affect the accuracy of the targets, this is more pronounced in continuous contact exchangers because exchanger height strongly depends on the column diameter. Lastly, the rich streams were used for the targeting with the assumption that they would not be split, this assumption does not always hold in designs for MENS problems with overlapping MSAs (Hallale, 1998).

Hallale (1998) in trying to overcome the aforementioned problems developed techniques for the capital cost targeting of mass exchange networks based on the mass or volume of the exchangers rather than on the number of stages, height or diameter. This targeting approach still employs the verticality of mass transfer as well as the aforementioned *y-x* and *y-y** targeting tools. The author states that exchanger mass or volume and not diameter is the appropriate analogy to heat exchanger area. These target techniques will be reviewed briefly in this study because one of the aims of this research is to formulate the pinch capital cost targeting procedure for MENs as a mathematical model.

Capital Cost Targets Based on Exchanger Mass or Volume

Due to the shortcomings associated with capital cost targets based on mass exchanger stages or height, techniques were developed by Hallale (1998) for targets based on exchanger mass or volume, these are discussed below.

a Continuous contact exchangers

Hallale, 1998 (as mentioned previously) states that continuous contact mass exchangers are better analogues of heat exchangers. But the targeting based on exchanger height does not fully reflect this analogue so he established an equation based on exchanger mass because shell cost is dominant in the capital cost of such exchangers. Since Equation 2.4 gives the rigorous minimum area for constant overall heat transfer coefficient, *U*, Hallale, (1998) argues that vertical transfer in a network of continuous-contact exchangers would also minimize the sum below:

$$\sum_{k}^{\text{Intervals}} \frac{W_k}{\Delta y_{lm,k}} \tag{2.37}$$

where W_k is the mass transferred in interval k.

Costing an exchanger in terms of the shell mass gives:

$$\text{Cost (Shell, installed)} = a + BM^c \tag{2.38}$$

Hallale (1998) then expressed the mass of an exchanger as:

$$M = \frac{W}{K_\mathrm{W}\ \Delta y_{lm}} \tag{2.39}$$

where K_W is a lumped coefficient and it is defined as:

$$K_\mathrm{W} = \frac{K_y a\left(2Jf - P_\mathrm{i}\right)}{4\,P_\mathrm{i}\rho_\mathrm{m}\left(1+f_i\right)\left(1+f_e\right)\left(1+f_c\right)} \tag{2.40}$$

where: J is the welded joint factor

f is the design stress for the construction material at the design temperature

P_i is the internal design pressure

ρ_m is the density of the construction material

f_i is the fractional allowance for inactive height

f_e is the fractional allowance for extras such as skirts, nozzles, manholes, etc.

f_c is the fractional allowance for corrosion.

For cases in which K_W is constant, then the rigorous minimum would be given by:

$$M_{\min} = \frac{1}{K_\mathrm{W}} \sum_{k}^{\text{Intervals}} \frac{W_k}{\Delta y_{lm,k}} \tag{2.41}$$

Equation 2.41 is analogous to Equation 2.4 for HENS.

For stream dependent K_{W}, an equation which is related to the HENS Bath formula is:

$$M_{\min} = \sum_{k}^{\text{Intrevals}} \frac{1}{\Delta y_{lm,k}} \left(\sum_{i}^{\substack{\text{Rich}\\ \text{streams}}} \frac{w_i}{K_{\mathrm{W}\,i}} \right)_k \tag{2.42}$$

Equation 2.42, just as it is with the Bath formula would predict the minimum mass to a close approximation provided the K_{W} values do not differ by more than an order of magnitude (Hallale, 1998).

Converting Equations 2.41 and 2.42 to a capital cost requires the assumption that the total targeted mass would be distributed evenly among all the streams, just as it is assumed for HENS. This gives equation 2.43 below:

$$\text{Capital cost target (Shell)} = N_{\text{units}} \left[a + b \left(\frac{M_{\min}}{N_{\text{units}}} \right)^{c} \right] \tag{2.43}$$

b Stagewise Exchangers

The problems encountered in the targets based on height for continuous-contact exchangers as discussed above are also present in stagewise exchangers. Hallale (1998) explains that the reason for which the number of shells target of Ahmad and Smith (1989) is beaten by the number of shells in design also applies to MENS in which the number of stages in design beats the number of stages targeted. This discrepancy as explained by Ahmad and Smith (1989) is as a result of the conversion of real to integer number of shells (or stages for stagewise columns). Hallale (1998) argues however that this is not the main cause based on the analogy he was able to draw from Equation 2.41 for continuous-contact exchangers. Number of stages should be targeted using $G \times N_{Stages}$ (rich stream flowrate multiplied by equilibrium number of stages) instead of the total number of stages, and for HENS, it should be number of shells multiplied by heat capacity flowrate. Vertical transfer according to Halalle (1998) still would not give a strict minimum for this term because an equilibrium stage is not the same as a transfer unit but will minimize it better than the number of stages.

Hallale (1998) derived the following expressions for gas-liquid and liquid-liquid operations based on exchanger mass (shell) since the capital cost is dominated by it.

Gas-liquid (rich stream is the gas stream):

$$M = \frac{GN_{stages}}{K_{\mathrm{Wg}}} \tag{2.44}$$

where K_{Wg} is a lumped coefficient and it is defined as:

$$K_{\mathrm{Wg}} = \frac{E_0 \rho_v u_v (2Jf - P_{\mathrm{i}})}{4s\, P_{\mathrm{i}} \rho_{\mathrm{m}} (1 + f_i)(1 + f_e)(1 + f_c)} \tag{2.45}$$

where: E_0 is the overall efficiency

ρ_{v} is the gas stream density

u_{v} is the superficial gas velocity and

s is the tray spacing

All other parameters are as defined for continuous-contact exchangers.

For cases in which K_{Wg} is constant, then the rigorous minimum would be given by:

$$M_{\min} = \frac{1}{K_{\mathrm{Wg}}} \sum_{k}^{\text{Intervals}} G_k \; N_{\text{stages},\,k} \tag{2.46}$$

where G_k is the total rich stream flowrate in interval k.

For stream dependent K_{Wg}, an equation which is related to the HENS Bath formula is:

$$M_{\min} = \sum_{k}^{\text{Intrevals}} N_{\text{stages},\,k} \left(\sum_{i}^{\substack{\text{Rich} \\ \text{streams}}} \frac{G_i}{K_{\mathrm{Wg},\,i}} \right)_k \tag{2.47}$$

Equation 2.47, just as it is with the Bath formula, predicts the minimum mass to a close approximation provided the K_{Wg} values do not differ by more than an order of magnitude (Hallale, 1998).

Gas-liquid (lean stream is the gas stream):

The model equations for gas-liquid operations in which lean stream is the gas stream are as given for cases for which rich stream is the gas stream except that G_k is replaced by L_k, which is now the total lean stream flowrate.

Liquid-liquid (rich stream is the dispersed phase):

$$M = \frac{GN_{stages}}{K_{W1}} \tag{2.48}$$

where K_{W1} is a lumped coefficient and is defined as:

$$K_{W1} = \frac{\rho_d d_0{}^2 v_0 h E_0 \left(2Jf - P_i\right)}{26.7\ p^2 s P_i \rho_m \left(1+f_i\right)\left(1+f_e\right)\left(1+f_c\right)} \tag{2.49}$$

where: ρ_d is the dispersed phase density,

d_0 is the holes diameter in the tray,

v_0 is the dispersed phase velocity through a hole,

p is the pitch of the hole and

h = 3.62 for holes set on a triangular pitch; 3.14 for holes set on a square pitch.

All other parameters are as defined earlier for K_{Wg}.

For cases in which K_{W1} is constant, then the rigorous minimum would be given by:

$$M_{\min} = \frac{1}{K_{W1}} \sum_{k}^{\text{Intervals}} G_k\ N_{\text{stages},k} \tag{2.50}$$

where G_k is the total rich stream flowrate in interval k.

For stream dependent $K_{W1,}$ the minimum mass can be obtained by the following equation:

$$M_{\min} = \sum_{k}^{\text{Intrevals}} N_{\text{stages},\,k} \left(\sum_{i}^{\substack{\text{Rich}\\ \text{streams}}} \frac{G_i}{K_{W1,\,i}} \right)_k \tag{2.51}$$

Equation 2.51 will give a close estimate of the actual minimum if K_{W1} do not differ by more than an order of magnitude.

Liquid-liquid (lean stream is the dispersed phase):
The model equations for liquid-liquid operations in which lean stream is the dispersed phase are as given for cases for which rich stream is the dispersed phase except that G_k is replaced by L_k, which is now the total lean stream flowrate.

The equations for the minimum masses are converted into capital costs just as was done for continuous-contact exchangers in Equation 2.43.

2.3.1.3 Supertargeting

The traditional optimization procedure which characterized the early days of HENS as discussed in the section under HENS also applies to MENS. This procedure entailed repeated design and costing at different ε values so as to identify the minimum total annual cost (El-Halwagi and Manousiouthakis, 1989) and it was tedious. Formulating the MENs problem as an MINLP has also been used as an optimization approach by Papalexandri et al. (1994) and this method also has its shortcomings (El-Halwagi, 1997), which are the problem of presence of non-convexities in the mathematical model equations which will make locating the global optimum a difficult task. Another limitation of the MINLP technique is the fact that the designer has to be clever enough to be able to include within the parent hyperstructure, all the potential network configurations that the MENs problem could have.

With the development of capital cost targeting techniques for MENs, optimization can now be carried out prior to actual design since the capital cost requirement corresponding to an annual operating cost target can be obtained at a specified ε or $\Delta y_{\min}$. This is accomplished by first annualizing the capital cost target by multiplying the capital cost by the annualization factor; the MSA cost is also annualized by multiplying the MSA flowrate targets by their respective costs and annual operating time, summing up the annualized capital cost target and annual operating cost targets results in the total annual cost targets. The second phase entails varying the ε or Δy_{min} because as the ε or Δy_{min} increases, the stages or height requirements decreases and vice versa meaning that the TAC varies with ε or Δy_{min}. The ε or Δy_{min} that corresponds to the least TAC is the optimal value and this is used to initialize the design. Designs initialized with such ε or Δy_{min} usually require very little evolution before meeting the targets (Hallale, 1998).

The new supertargeting procedure by Hallale (1998) is illustrated by Figure 2.24 below which is analogues to Figure 2.8 above for HENS:

This new supertargeting procedure is less tedious since the repeated design aspect has been eliminated. Also the area of search for the optimum has been expanded because there is no restriction imposed on the basis of a specified number of units. It also eliminates the sequential trade-off procedure of operating versus capital cost inherent in the previous optimization procedure; instead, it trades-off simultaneously operating versus capital cost. The supertargeting diagram is illustrated by Figure 2.25 below:

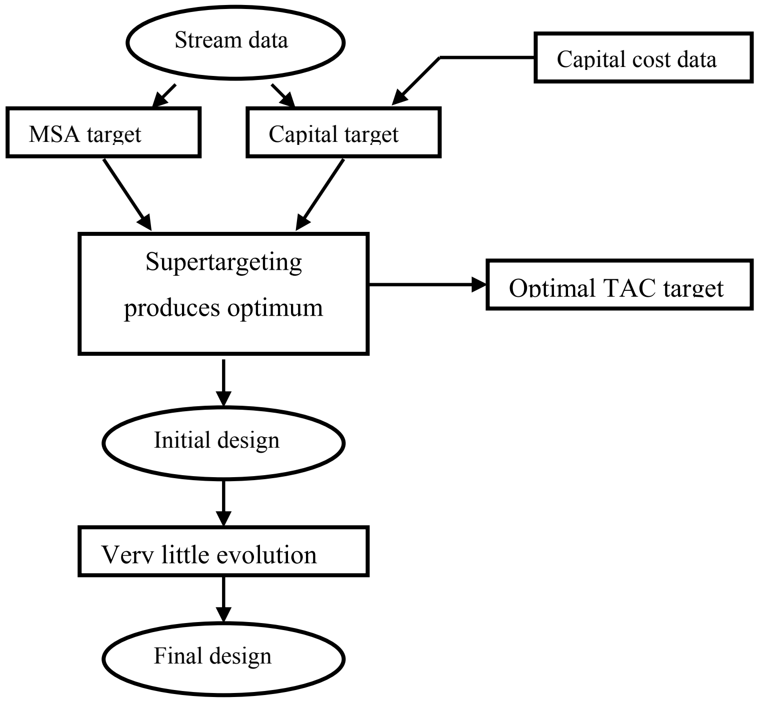

Figure 2.24: Improved pinch technique for mass exchange network optimization, Supertargeting (Hallale, 1998)

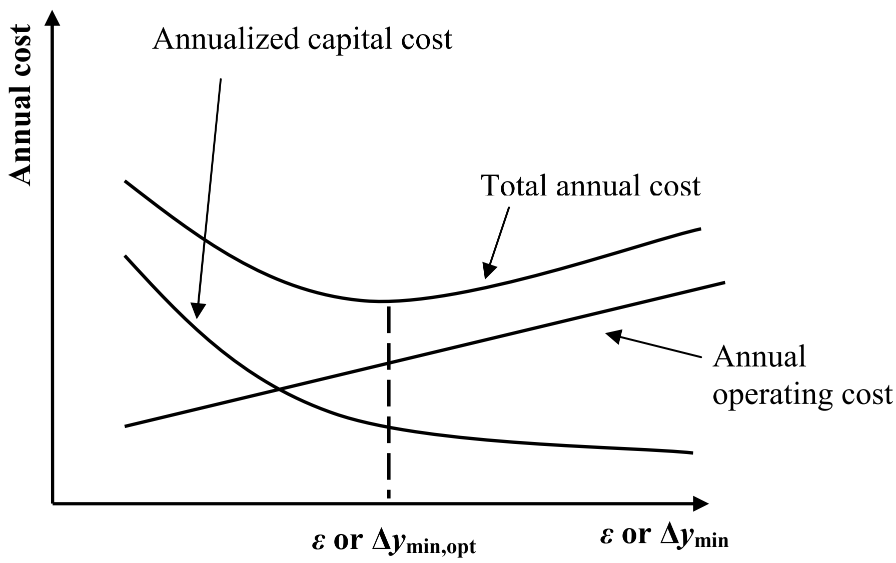

Figure 2.25: The supertargeting curve for MENS optimization (Hallale, 1998).

2.3.1.4 Retrofit Targeting

Retrofitting may be necessary in mass exchanger networks due to changes in operating conditions or as a result of desire to maximize the use of MSA and minimize operating cost. The retrofitting should be carried out with the aim to maximize the use of the existing units and minimize the cost of new units that might need to be added (Alfadala and El-Halwagi, 2001).

Fraser and Hallale (2000) approached the retrofitting of MENs in a manner similar to the Tjoe and Linnhoff (1986) approach for HENs which entails three steps. The first stage involves developing the stages/height versus MSA (size-load) plot which is analogous to the area versus energy plot of Tjoe and Linnhoff (1986) for HENs retrofit. The stages/height target versus MSA target diagram is constructed by targeting for MSAs and the corresponding number of stages or height requirements at different values of the minimum composition difference ε. The MSA consumption of the existing plant based on the mass exchangers installed is then located relative to the size-load curve. Cost information is used to translate the different MSA and stages/height targets to savings and investment respectively, this is the second step. Moving to the left along the curve in Figure 2.26 below so as to reduce MSA consumption results in incurring extra stages/height with which to accomplish this MSA savings.

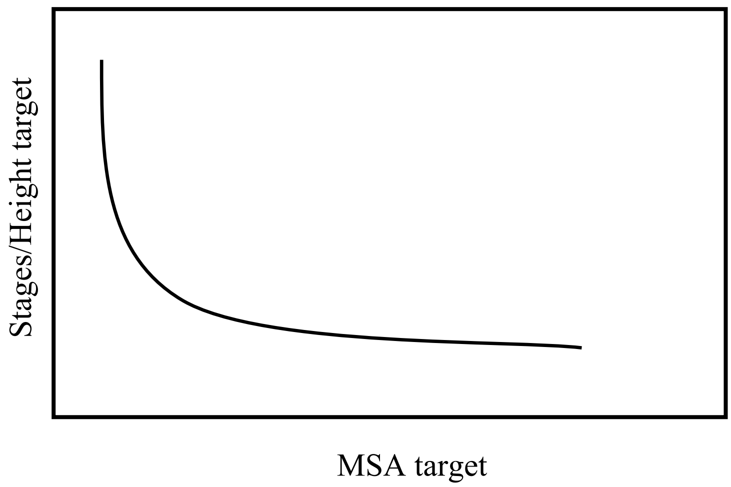

Figure 2.26: The size-load plot (Fraser and Hallale, 2000).

The savings-investment curve diagram below (Figure 2.27) illustrates how much MSA cost could be saved for a given capital investment and at what payback period (this is depicted by the different lines).

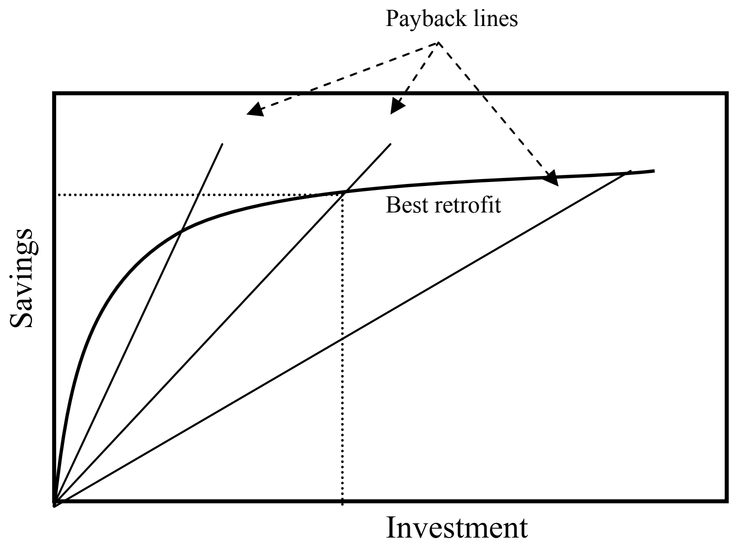

Figure 2.27: The savings-investment plot (Fraser and Hallale, 2000).

In Figure 2.27 above, the point at which the payback line intersects the retrofit curve gives the target and the corresponding ε can be obtained from the size-load plot. The third step is the design stage. The retrofit design starts off with the grid diagram of the existing plant so as to identify and do away with the cross-pinch and criss-cross exchangers, also an adjustment is done for the targeted flowrate. The design process is completed by making use of the grassroots design techniques of El-halwagi and Manousiouthakis (1989) and Hallale (1998) with the aim of reusing as many of the existing exchangers as possible.

Alfadala and El-Halwagi (2001) addressed the issue of mass exchange networks retrofit by the identification of alternative structural configurations of interest making use of heuristics. The structures could be in series or in parallel. Two approaches were used: that in which capital is readily available and the other does not have capital. The aim in the first case is to minimize the total annual cost of the network and have a proper trade-off between operating and capital cost. The aim in the second approach is to increase MSA flowrate without the addition of new equipments or carry out a solvent substitution. The effects of the size of retrofitted networks are also taken into consideration alongside the usual thermodynamic limitations in identifying maximum performance.

2.3.1.5 Network Design

The grid diagram (El-Halwagi and Manousiouthakis, 1989) is also used for the design of MENs. Figure 2.28 below illustrates this diagram: rich streams are shown running from the right to the left while lean streams run the other way. The flowrates as well as the equilibrium constants of the streams are indicated on the right: this is similar to the HENS grid in which the *FCP* of streams are also stated on the right. Matches are depicted on the grid as a line connecting two streams, the exchanger number is indicated in the circles while the exchanger load is indicated below each exchanger. The pinch is depicted as broken lines with the different pinch compositions placed next to it. Supply and target compositions of each stream are placed on the starting point and end point of each stream.

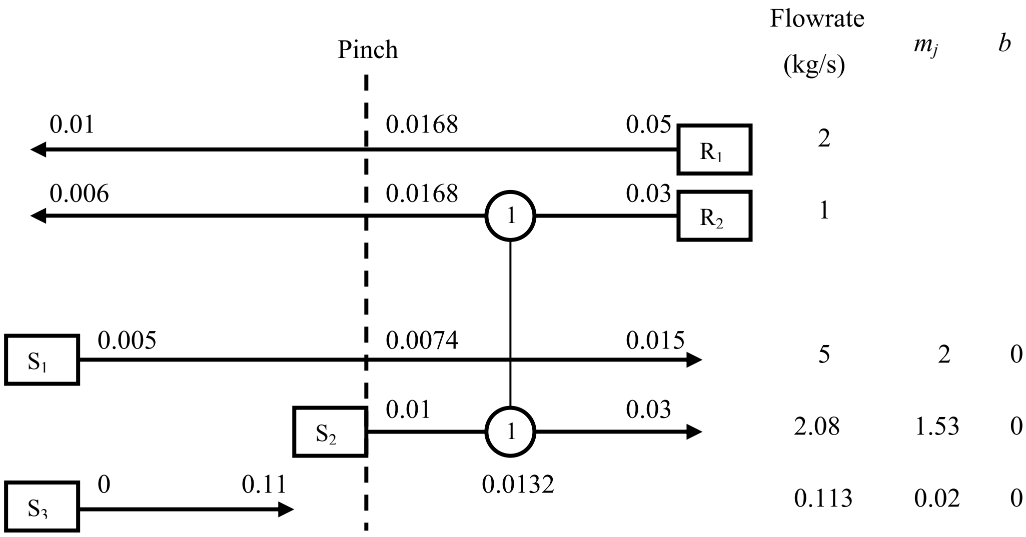

Figure 2.28: Grid representation of matches.

El-Halwagi and Manousiouthakis (1989) identified some design rules which needs to be adhered to so as to meet the MSA target in design. Hallale (1998) also developed some design procedures which ensure that the capital cost targets are met in design. El-Halwagi and Manousiouthakis (1989) guidelines require that the design starts at the pinch and move away from it to either side because this is the most constrained part of the process while Hallale (1998) recommends that a low number of units should be used to approach as closely as possible the ideal profile (as depicted by the *y-x* composite curve) so as to avoid the spaghetti design as it is in HENS (Ahmad and Linnhoff, 1990). The first two feasibility criteria of El-Halwagi and Manousiouthakis (1989) are first discussed followed by those of Hallale (1998):

Stream Population

At the rich end of the pinch, i.e. immediately above the pinch the following stream population inequality must hold,

$$N_{\text{R, above pinch}} \leq N_{\text{S, above pinch}} \tag{2.52}$$

and at the lean end i.e. immediately below the pinch the following must hold,

$$N_{\text{R, below pinch}} \geq N_{\text{S, below pinch}} \tag{2.53}$$

Stream splitting may be required to meet these inequalities.

Operating line versus equilibrium line

At the rich end of the pinch, i.e. immediately above the pinch the slope of the operating line must be greater than or equal to the slope of the equilibrium line:

$$\frac{L_j}{m_j} \geq G_i \tag{2.54}$$

Immediately below the pinch the following must hold:

$$\frac{L_j}{m_j} \leq G_i \tag{2.55}$$

Stream splitting may be necessary here as well in order to meet the above stated inequalities. These two design rules according to El-Halwagi and Manousiouthakis (1989) apply to pinch matches. For subsequent matches away from the pinch, the driving force gives the main restriction for the matching criteria. The *tick-off* rule can be used so as to meet the minimum number of units target. Hallale (1998) agues that this is not always compatible with achieving the minimum capital cost.

The next set of design guidelines discussed below are those set out by Hallale (1998) for achieving the capital cost targets in design, they have analogues in HENS as usual but the presence of equilibrium relations brings in some differences.

The driving force plot

The driving force plot for MENS is constructed from the *y-x* composite curve plot of Hallale (1998) and it serves more or less the same purpose as the driving force plot of Ahmad and Smith (1990) for HENS. The goodness of selected matches is evaluated on the *y-x* composite curve by comparing the operating line of each potential match with the composite operating line. Matches which use driving forces exactly as it is on the *y-x* composite curve are the ideal matches, the good matches use close to the driving forces available while the poor matches driving force use is very different from that available on the composite curve. Matches that use too little driving forces compared with that on the *y-x* curve would require a higher number of stages/height and this will result in designs exceeding the target while matches which use driving forces more than is available on the *y-x* curve will require low number of stages/height but this would result in forcing the remaining matches to make do with the lower driving forces remaining and the net result is an increase in the stages/height requirement beyond the target. This method makes for a quick screening of potential matches and is illustrated by Figure 2.29 below.

See Hallale (1998) for an in depth discussion of how the driving force plot blends with meeting the MSA target.

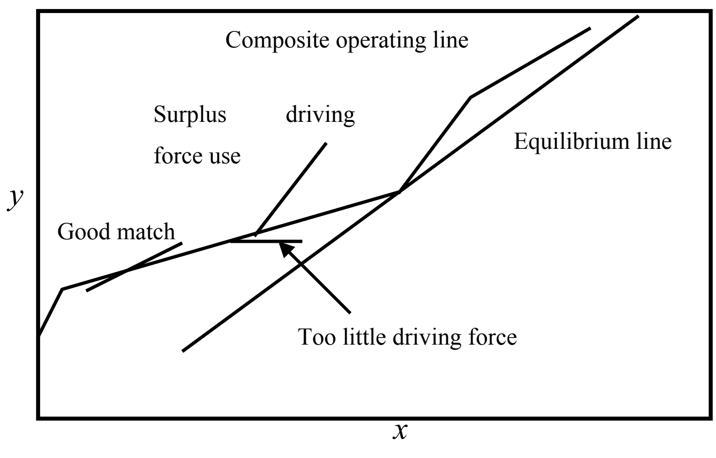

Figure 2.29: Evaluation of the goodness of matches based on the composite operating line (Hallale, 1998).

The remaining problem analysis

The concept behind the remaining problem analysis (RPA) is exactly as it applies to HENS RPA.

Pinch technology has successfully been applied to the synthesis of MENs, this was made possible through establishing analogies between heat and mass exchange networks. But how much of these analogies have been tackled using mathematical programming? This is reviewed in the next section because the present study aims to bridge the gap between mathematical programming as applied to both HENS and MENS by capitalizing on the analogies identified with the use of pinch technology.

2.3.2 Mathematical Programming as Applied to MENS

The philosophy of sequential and simultaneous approaches as discussed for heat exchanger network synthesis in the previous section also applies to mass exchanger network synthesis. The difference lies in the fact that not much analogy has been established between the two operations. The problem of mass exchange network synthesis is also combinatorial in nature, this and other reasons is what informed the decomposition of the task into simpler subtasks. The problem of inadequate trade-offs between the competing costs inherent in the decomposition approach gave birth to the simultaneous technique. Each of these approaches will be reviewed broadly.

Pinch technology as applied to HENS, designs all the heat exchangers based on a single minimum temperature approach but this is not the case in reality. For this reason different temperature approaches were defined for HENS (these are discussed in section 2.2.2) (Floudas, 1995). This trend that characterizes pinch technology application to HENS is also the case with MENS in which the mass exchange network is generated with a global minimum composition difference. The present study would address this situation by defining some other minimum composition differences just as is done for HENS.

2.3.2.1 Sequential Approach

The problem of mass exchange network synthesis has been tackled through the decomposition method just as has been done for HENS. The sequential approach entails:

i. Minimum MSA cost
ii. Minimum number of matches
iii. Minimum investment cost network configurations

In addition to the above is a technique in which the outlet composition of each MSA is optimized.

El-Halwagi and Manousiouthakis (1990) established analogies between the transhipment model and the mass exchanger network problem just as was done by Papoulias and Grossmann (1983) for the heat exchanger network synthesis problem. These analogies are illustrated by Table 2.2 below:

Table 2.2: Analogies between the transhipment model and the mass exchanger network synthesis problem.

Transhipment model		**MEN**
Commodity	=	Mass
Intermediate nodes (i.e. warehouses)	=	Composition intervals
Sources	=	Rich streams
Destinations	=	Lean (MSA) process and external streams

They formulated as a mathematical optimization model the problem of determining the mass exchange pinch point and hence the minimum MSA cost requirement using linear programming. These authors went on to use MILP to determine the set of matches that meet this minimum MSA cost.

Linear Programming Model

The linear programming model of El-Halwagi and Manousiouthakis (1990) aims to minimize the MSA cost and determine the mass transfer pinch. This they accomplished by using a single minimum composition difference value and subsequently generating composition intervals using the supply and target composition of each stream to partition the intervals.

The objective function is stated as follows:

$$min \sum_{j=1}^{N_S} C_j L_j \tag{2.56}$$

where C_j is the unit cost of the j^{th} MSA

L_j is the flowrate of the j^{th} MSA

The flow of mass within interval k can be represented as:

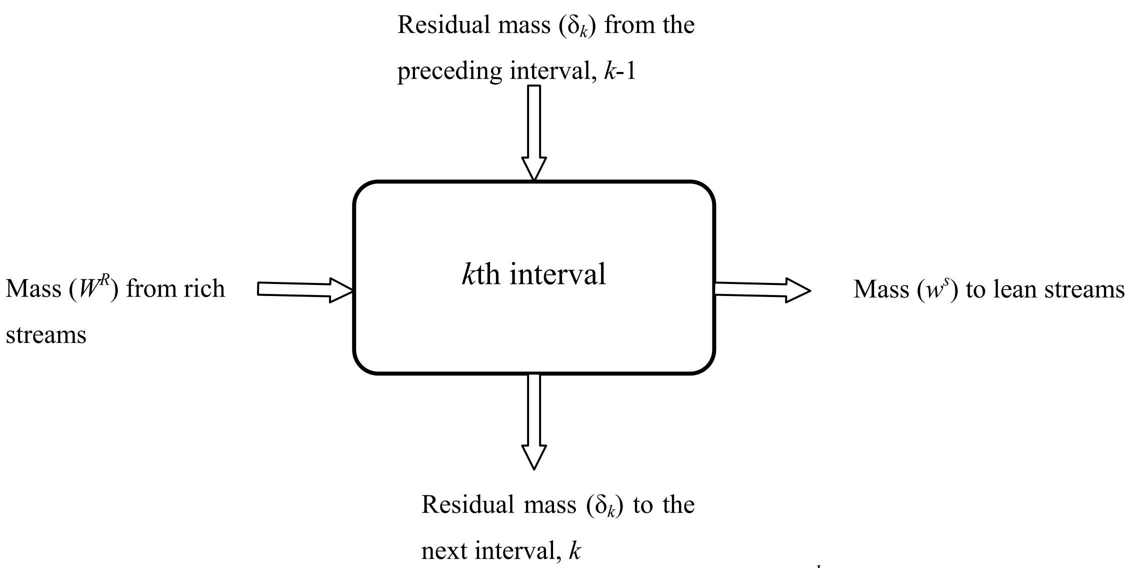

Figure 2.30: Mass flow representation for the k^{th} interval.

Figure 2.30 is a composition interval, carrying out a material balance over this interval gives the residual masses entering and leaving each interval,

$$\delta_k - \delta_{k-1} + \sum_{j \text{ through interval } k} L_j w^s{}_{j,k} = W_k{}^R \tag{2.57}$$

where $W_k{}^R = G_i\left(y_{k-1} - y_k\right)$ and $w_{j,k}{}^S = x_{j,k-1} - x_{j,k}$

G is the flowrate of the i^{th} waste stream

$$L_j \geq 0 \tag{2.58}$$

$$L_j \leq L^c{}_j \tag{2.59}$$

where $L^c{}_j$ is the upper bound on the available flowrate of the j^{th} MSA

Equations 2.58 is the non-negativity constraint while 2.59 places an upper limit on the MSA flowrate based on the amount available on site.

The constraints $\delta_0 = 0$ and $\delta_{N_{\text{int}}} = 0$ keeps track of the overall material balance and $\delta_k \geq 0$ ensure thermodynamic feasibility.

The point between any two consecutive intervals, k and $k + 1$, at which the residual mass load, δ_k being transferred equals zero is the mass transfer pinch. The driving force at this point equals the minimum composition difference. The solution to the objective function is the optimal flowrates for the MSAs, L_j.

El-Halwagi and Manousiouthakis (1990) regarded the target compositions of the leans streams as just upper bounds on the outlet compositions: they set up techniques with which to optimize this target composition by decomposing the parent lean streams into substreams with each substream having the same supply composition, x^s, as the parent stream but a target composition, x^t that is equal to or less than that of the parent lean stream.

MILP Transhipment Model

El-Halwagi and Manousiouthakis (1990) formulated the stream matching problem for mass exchange network synthesis as a mixed integer linear program (MILP) which aims to minimize the number of mass exchangers for the minimum MSA cost determined using the LP model. The pinch point divides the synthesis problem into two subnetworks, above and below the pinch respectively.

Constraints were imposed by these authors on the mathematical model, one of them being a binary integer variable, $E_{i,j,m}$, which takes on the value of 0 when there is no match between streams i and j, and takes on the value of 1 when there is a match between these streams.

Another of the constraint sets limits matches between streams i and j to the smaller of the mass load/capacity of the two steams, i.e.

$$\sum_{k \in SN_m} W_{i,j,k} - U_{i,j,m}\, E_{i,j,m} \leq 0 \qquad i \in R_m,\, j \in S_m \tag{2.60}$$

where $U_{i,j,m}$ is the upper bound on exchangeable mass between i and j in subnetwork m.

The other set of constraints are the material balances for each rich and lean stream around each composition interval, the non-negative residuals and mass loads.

The objective function is then stated as:

$$Minimize \sum_{m=1,2} \sum_{i \in R_m} \sum_{j \in S_m} E_{i,j,m} \tag{2.61}$$

The solution to the above objective function gives the stream matching and the load of each match. The solution is generated for each of the subnetworks which are then added to arrive at the solution for the overall network.

Non-Linear Programming

Lee and Park (1996) generated a composite structure, known as the maximal structure. This structure is a fusion of all possible network structures and it is generated by converting all the rich/lean stream data into the material set of the P-graph theory while those of the mass exchange units are converted into the operating unit set. The authors went on to formulate each of the generated structures as a non-linear programming model which is subsequently optimized so as to provide the operating conditions of the structure.

The variables of the NLP model of Lee and Park (1996) are stated in terms of the flow of rich stream i and lean stream j relative to splitter, mixer and mass exchanger. Also bypass, mass exchanged, composition of rich (and lean) streams before and after mass exchangers, number of theoretical plates and height for columns are also stated as variables. Mass balances are carried out for rich and lean raw material nodes and the transferable component is considered too. Some other mass balances are carried out for the operating units nodes, splitters, mixers and mass exchangers. The objective function is stated as follows:

$$\text{TAC} = \sum_{LR_j \in M} CL_j L_j + \sum_{O_{ij} \in O'} \Phi(O_{ij}) \tag{2.62}$$

where O' is operating unit set and O_{ij} is the mass exchanger connecting streams i and j.

2.3.2.2 Simultaneous Approach

Papalexandri et al. (1994) used a mixed integer non-linear program to tackle the problem of mass exchange network synthesis. They formulated the mass exchange network problem as a mathematical optimization model which solves simultaneously the operating and capital cost requirements. This, the authors claimed, trades-off appropriately the competing costs unlike the sequential approach which decomposes the MENS problem into subtasks.

The authors set up a hyperstructure which is believed to embed all the potential network configurations (in terms of structural and operating conditions) possible and subsequently optimizes it for the best network in terms of total annual cost (TAC).

The objective function is a composite made up of the annualized operating cost and annualized capital cost. This is stated as:

$$min\ \text{TAC} = \sum_{j \in L} (AC_j)(L_j) + \sum_{(i,j) \in M_{p,s}} (AC_{st})(N_{st,ijs}) + \sum_{(i,j) \in M_{t,s}} (AC_h)(H_{ijs}) \tag{2.63}$$

where N_{st} and H are the number of stages of staged and height of continuous contact columns respectively.

The objective function is subject to a set of constraints which are:

- Overall mass balances at the initial splitter for each stream
- Overall mass balances at the mixer preceding each mass exchanger for each stream
- Overall mass balances at the splitter after each exchanger for each stream
- Mass balances for the transferable component at the mixer preceding each exchanger for each stream

- Mass balance for the transferable component at the final mixer of each stream
- Mass balances for the transferable component at each potential exchanger or each stream
- Feasibility constraints which ensures that the driving force is greater than zero
- Logical constraints
- Sizing equations for the mass transfer units and
- Bounds on the variables.

The MINLP as applied to MENS though being simultaneous still has some limitations in terms of solver environment, guarantee of global optimum and ability to include all possible configurations in the hyperstructure. Later in this review, mathematical programming will be compared with pinch technology.

Mass exchange network synthesis using mathematical programming is yet to receive much attention unlike its heat exchange network counterpart. A key synthesis technique missing in the array of methods is an analogue of Gundersen and Grossmann (1990) vertical MILP model which not only targets for the minimum (or a specified number of units) but also has the ability to discriminate among these units in terms of their ability to transfer heat vertically on the composite curve. Section four of this study would establish this analogue for MENS i.e. a vertical MILP model that has the ability to target for the minimum (or specified) number of units and at the same time discriminate between all the networks featuring the same number of units and also meeting the same MSA cost targets in terms of how much each approaches vertical mass transfer.

2.4 Combined Heat and Mass Exchanger Network Synthesis (CHAMENS)

Just as it was in the early days of HENS in which networks that featured the minimum number of units that corresponds to an energy target was taken as being the optimal in terms of the total annual cost, so it was with MENS. CHAMENS has been treated in the same way too. The studies of Townsend & Linnhoff (1984) brought forth the notion of targeting for the minimum area that corresponds to a specific utility target at a specific minimum temperature approach which leads to the optimization technique known as supertargeting. Hallale & Fraser (1998, 2000a and 2000b) were able to establish analogues for MENS in which the minimum absorber size that corresponds to a particular mass separating agent target at a specific minimum composition difference, ε, was obtained. They also developed the corresponding supertargeting technique in MENS. This study aims to use these established frameworks for CHAMENS because previous studies on CHAMENS which used the sequential approach failed to factor into the synthesis the size requirements of the heat and mass exchangers. Synthesizing combined heat and mass exchange networks with the sole aim of minimizing the heating/cooling and mass separating agents cost will fail to exploit to the fullest the potentials in combining the synthesis. Also the resulting networks will be non-optimal.

The few studies that have been done on CHAMENS using both pinch and mathematical programming techniques are discussed in the following sections while the development for CHAMENS by the present study is discussed in section three. Figure 2.31 below gives a schematic representation of the CHAMENS problem.

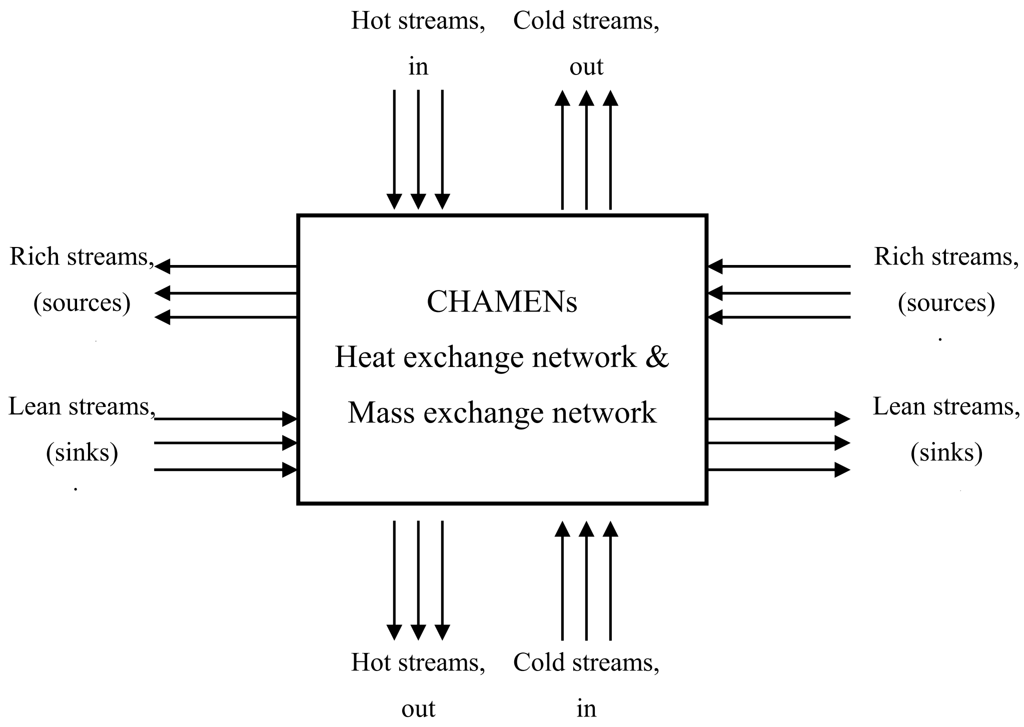

Figure 2.31: Schematic representation of the combined heat and mass exchange network synthesis problem.

2.4.1 Pinch Technology as applied to CHAMENS

El-Halwagi (1992/1993) tackled the problem of synthesizing CHAMENs by making use of mass exchange temperatures which fall within the working temperature range of the rich and lean streams. Edgar and Huang (1993) on the other hand decomposed the problem into two subtasks, the first task entails fixing the mass exchange temperature with which a MEN is synthesized. The heat requirements of the synthesized MEN in the first subtask are then synthesized as the second subtask. Srinivas and El-Halwagi (1994) argued that this approaches are helpful only when the optimal mass exchange temperature is known ahead of design or when the permissible variation in the temperature of each MSA is small (e.g. 10-20K). It is worth stating at this point that the optimal mass exchange temperatures can be known ahead of design due to the fact that the operating and capital cost implications (in terms of the MSA/utilities and mass/heat exchanger requirements) of varying the mass exchange temperatures can be identified before design. This is possible through the use of the well established pinch technology targeting tools for HENs (Linnhoff and Ahmad, 1990; Ahmad and Smith, 1989; Townsend and Linnhoff, 1984) as well as those for MENs (Hallale, 1998). Section three of this study discusses a sequential procedure for tackling the problem of CHAMENS.

2.4.2 Mathematical Programming as applied to CHAMENS

Srinivas and El-Halwagi (1994) addressed the problem of combined heat and reactive mass exchanger networks, they argued that since the two economic objectives of mass exchange and heat recovery are incompatible, the problem has to be addressed simultaneously. Their approach is in two stages: the first entails identifying the minimum operating cost requirements of the network through a mixed-integer nonlinear program (MINLP) which naturally decomposes the problem into two independent subproblems. These subproblems were solved to identify the minimum number of heat and reactive mass exchangers. Srinivas and El-Halwagi (1994) applied the developed technique to an example but it was not clear what procedure they used to identify the optimal minimum approach temperature as well as the minimum composition difference, if these parameters were optimized. This means that there is no assurance of the optimality of the operating cost target. Also they did not account for the capital cost requirements of the units explicitly.

Another shortcoming of this approach is that the philosophy of gearing designs towards the minimum number of units that meets the operating cost target does not always produce optimal networks (Hallale, 1998), this is because there is restriction of the designer towards a particular topology so there is no way to account for the variations in the size requirements of the units.

Papalexandri and Pistikopoulos (1994) are another set of workers that tackled the problem of combined heat and mass exchange network synthesis using mathematical programming techniques. These authors used the simultaneous approach which has been applied to the synthesis of HENs (Floudas and Ciric, 1989) and MENs (Papalexandri et al., 1994) separately by establishing analogues as usual. Papalexandri and Pistikopoulos (1994) set up hyperstructures which is a multiperiod representation of all the potential configuration and operational options for the rich, lean, regenerating, hot and cold process streams. Initial splitting, mixing of inlet and outlet streams into exchangers (heat or mass), bypassing of exchangers (heat or mass) either individually or overall, all account for a means of obtaining the optimal network. All the possible network structural options (in terms of stream matches, piping connecting splitters, mixers, and exchangers) are set out by representing them as a “1” if any of these units or connections exists. The operational alternatives such as stream flows, compositions, temperatures, mass and heat loads of each exchanger are defined as continuous variables for each period of operation. Also set out as continuous variables are the capital cost requirements such as heat exchanger areas, number of equilibrium stages and height of mass exchangers for all periods of operation.

The constraints to the model to be optimized are very similar to those imposed by Papalexandri et al. (1994) on the objective of mass exchange network synthesis and these have been highlighted in section 2.3.2.2. The objective function aims to minimise the sum of the operating cost (for the hot and cold utilities as well as mass separating agents) and annual capital cost (sum of the heat and mass exchangers).

2.5 Comparison of Techniques

The present study aims to combine the synthesis of two subsystems of the chemical process i.e. heat and mass exchange subsystems. Also the technique with which to accomplish this synthesis is a combination of methods i.e. pinch technology and mathematical programming techniques. Previous sections in this study have reviewed extensively each of these techniques as applied to both heat and mass exchanger network synthesis.

Msiza and Fraser (2003) introduced the concept of hybrid synthesis method for MENs. The approach is basically in five steps: the first step entails using the established pinch techniques (El-Halwagi and Manousiouthakis, 1989; Hallale, 1998) to set targets for the TAC of the expected flowsheet. The second step involves using an MINLP superstructure similar to that of Papalexandri et al. (1994) to model the synthesis problem. A flowsheet is then initialised, this is the third step. The next step is the optimisation of the hybrid model and comparison of the generated output with the targeted TAC of step 1 to see if it lies within 10% of the target. If the output is out of the expected range, then the last step which is the driving force analysis is carried out. The analysis is done by evaluating the selected matches on the driving force plot of Hallale (1998) and the degree to which theses matches deviate from ideality (which the driving force plot depicts) dictates the next flowsheet to be generated and subsequently used to initialise the MINLP model. This approach can help in speeding up the network generation process, especially for large industrial problems which by the use of pinch technology would be tedious since the established pinch design techniques do not give the order in which selection of matches would be carried out. But a main shortcoming of this hybrid method is the fact that it still suffers form the problem of getting trapped in a local optima.

Table 2.3 below compares the two methods which make up the hybrid synthesis method, i.e. pinch technology and mathematical programming.

Table 2.3: Comparison of Methods

Pinch technology	**Mathematical programming**
• Targeting ahead of design	• Cannot target ahead of design
• Involvement of the designer	• Designer is not involved
• Cannot handle multiple variables	• Can handle multiple variables
• Can provide initial solution hence guide for MINLP	• Needs an initial solution
• Provides test for optimum	• Cannot guarantee global optimum
• Can help reduce region of search	• Realistic trade-offs
	• Can have numerical problems

Each of the techniques has strengths and weaknesses: the aim of this study is to combine the best of both in a hybrid method.

3 PROBLEMS IN WHICH ENERGY UTILITIES ARE USED TO ENHANCE WATER USE OR MASS EXCHANGE

For key design objectives such as cost, energy efficiency, yield enhancement and pollution avoidance to be met, a conceptual understanding of the interaction among the various unit operations in a chemical process is essential. Energy and mass transfer are two key subsystems of chemical processes whose interaction with one another should not be overlooked, this is because some processes may require streams to operate at different temperature levels; also, phase equilibrium is improved at lower temperatures for absorption and at higher temperatures for stripping, combining the synthesis of heat and mass exchangers becomes beneficial. Improved phase equilibrium results not only in reduced operating costs for the mass exchange networks, but also in reduced operating and capital costs for both the mass and heat exchange networks. This section presents the use of pinch technology for the synthesis of combined heat and mass exchange networks

3.1 Introduction

The conversion of raw materials to chemical products passes through many steps such as reaction, separation, mixing, heating, cooling, etc. These steps are individual transformation steps which have to be interconnected so as to form a complete process that meets the desired overall transformation.

3.1.1 Synthesis of Subsystems and Combination of Sub-Systems

The traditional design approach of focussing attention on the design of individual items of equipments which starts from the centre of the “onion diagram” (Smith, 2005) has evolved with time to the level of identifying subsystems. The integration of the items of equipments within these subsystems has been accomplished using various techniques, with heuristics, physical and thermodynamic insights and mathematical programming being the most common of them. The heat exchanger network synthesis (HENS) has received most attention (Gundersen & Naess, 1988; Linnhoff, 1993) while mass exchanger network synthesis (MENS) is following suit (El-Halwagi, 1997; Hallale & Fraser, 1998). Reactor networks synthesis is gaining ground too (Smith, 2005) while heat induced separation systems (such as distillation columns) and heat and power systems are being integrated into site’s heat exchange operations (Shenoy, 1995).

The identification and subsequent synthesis of subsystems has gone a long way in helping to attain optimal overall design, but this is restricted to such subsystems as there are still interactions among different subsystems such as energy and mass (because some streams may require heating/cooling). So in order to meet desired criteria such as economics, yield improvement, pollution abatement, flexibility etc, in the design and operation of chemical processes, efforts should be focused not only on design of individual items of equipments (Hallale, 1998) or the synthesis of subsystems but also on the techniques with which to select and connect such equipment from more than one layer of the chemical process.

There are so many process alternatives in the light of the different process variables (such as temperatures, pressures, flowrates, compositions etc) as well as performance criteria at the disposal of the design engineer. This calls for a conceptual understanding of the interaction among these process variables (as each applies within the layers) so as to be able to establish design and synthesis techniques that would tackle the problem systematically in achieving the aforementioned desired goals.

3.1.2 The Pinch Concept

Ability to locate the pinch not only in heat exchanger networks but in some other networks of interest such as mass exchangers, reactors, distillation columns, combined heat and mass exchangers and so many other chemical-based, and non-chemical-based processes as well, has gone a long way in helping the designer to achieve cost efficient networks/operations. The designer knows the best that is possible before actual design through targeting. Also, the designer is confident, because there are design techniques that would meet the targets. The pinch is the constraint (or bottleneck) to further recovery of energy, matter or the key component that is of interest. In the case of chemical processes, this constraint is thermodynamic.

For mass exchanger network synthesis, El-Halwagi and Manousiouthakis (1989) identified the process mass separating agent's (MSA) thermodynamic properties as being the criterion for the pinch location. They limited these properties to the process MSA`s flowrate and temperature on site. With this, a "pinch" is identified. One of the main tasks of this research is to explore some of the conditions surrounding the thermodynamic properties of the process MSA at the so called pinch, e.g. its process temperature. A change of the mass exchange temperature of any of the streams will reposition the pinch; this will give either a higher or lower mass recovery capacity to the process MSA based on its availability on site. A change in the pinch position would have a resonating effect on other network requirements depending on what unit operation (e.g. heating or cooling) is used to explore the thermodynamic properties of the process MSA. This brings to the fore the first reason for which the research is being done.

3.1.3 Classification of Combined Heat and Mass Exchange Networks Synthesis (CHAMENS) Problems

Before going on to classify CHAMENS problems, MENS will first of all be classified using the classification of Hallale and Fraser (2000a). The authors classified MENS because they are more complex to deal with due to the presence of equilibrium relations.

The different MENS classes are:

- MENS with only one MSA
- MENS with non-overlapping MSAs
- MENS with overlapping MSAs

As will be explained later, the cooling/heating of external MSAs (or process MSAs) in each of these classes of MENS produces different effects on the network cost. Each of these needs to be investigated.

We propose that CHAMENS systems should be classified as follows

- Type 1: Problems in which energy utilities are used to enhance water use or mass exchange.
- Type 2: Problems in which process energy streams are used to enhance water use or mass exchange.

The above classification is done in the light of the fact that utility heating or cooling may be used to enhance a mass exchange operation for the first type, as well as utility water use or mass separating agents may be used to reduce/increase requirements for heat exchange operation. In the second type we have both heat and mass exchange systems together, and they interact and both can be used to enhance the other.

This part of the report addresses the first type of problem while the second type will be discussed in Section 4 of this report.

3.1.4 Current State of the Art

Pinch technology has been applied extensively to the synthesis of HENs and to a less extent for MENs. Combined heat and mass exchanger network synthesis using pinch technology has not received much attention. Any attempt to apply pinch technology to the synthesis of CHAMENs will fail if a proper trade-off is not established among the competing costs. Hallale (1998) established capital cost targeting techniques for the synthesis of MENs. This completes the chain as far as targeting techniques are concerned for HENs and MENs because targeting methods have already been established for the annual operating costs requirements for HENs and MENs (Linnhoff et al., 1982 and El-Halwagi & Manousiouthakis 1989 respectively) and for the annual capital cost requirement for HENs (Linnhoff and Ahmad, 1990).

The research which has been carried out on mass exchanger network synthesis (El-Halwagi, 1997; Halalle, 1998) has been limited to the rich and lean streams operating at their supply temperatures throughout the network (Srinivas and El-Halwagi, 1994). However, this might not be the best because specific streams in some processes would be better off economically or technically if they flow at some other temperatures other than their supply temperatures within networks. Deliberately cooling and heating of streams (for absorption and stripping respectively) would enhance their phase-equilibrium relations which will turn out to improve mass exchange (Seader and Henley, 1998; Srinivas and El-Halwagi, 1994). The effect of this has been known to be that either flowrate reduces and absorber size requirements increases or vice versa, but not both reducing or increasing simultaneously. For this reason, trade-offs among the competing costs has been established because the cooling/heating could be accomplished by heat exchangers which will in turn require heating/cooling utilities.

With the classification of MENS problems (as outlined above) and the subsequent development of capital cost targeting tools for these networks by Hallale and Fraser (1998, 2000a & 2000b), a study needs to be carried out on the effect of cooling/heating (of not only the external MSAs as done by Srinivas and El-Halwagi, 1994, but also on the process MSAs) on both the annual operating and annual capital costs of mass and heat exchangers when their synthesis is combined. Simultaneous reductions in MSA flowrate requirements, absorber size as well as the total annual costs of heat exchange could be achieved especially for MENS problems having process MSAs with excess capacities on site. So there should be a systematic way of combining the synthesis of heat and mass exchangers so as to harness the potentials for these simultaneous reductions in costs for the different types of MENS problems, these are addressed in this report using the established pinch techniques.

3.1.5 Motivation

Process MSAs are usually available on site at a very low cost, or virtually free. The more the amount of the process MSAs used, the less the amount of external MSAs (with their associate costs) that would need to be used. Apart from the supply/target composition, another limiting factor to the amount of process MSA that can be used in a process is determined by its pinch composition and this is in turn dependent on the process MSA temperature.

Going by the pinch technology approach to mass exchanger network synthesis (MENS), the pinch composition corresponds to the point at which there is the highest negative mass transfer in a mass cascading process within composition intervals, this negative mass transfer is corrected for (since this is not feasible thermodynamically) by either reducing the flowrate of the process MSA or its outlet composition (El-Halwagi and Manousiouthakis, 1989). After the correction, the interval previously transferring the highest negative mass load will now be transferring zero mass load. Reducing the mass load to be removed by the process MSA means that some mass has to be rejected below the pinch for an external MSA to absorb. This implies that, in most cases of process MSA operating temperature, there is usually an excess capacity which goes unutilized so as to avoid thermodynamic infeasibility.

Foo et al. (2004), in addressing the problem of mass exchange network synthesis for batch processes, developed the time-dependent composition interval table (TDCIT). Their technique involves the philosophy of mass storage (as first introduced by Kemp and Macdonald, 1987, 1988, for HENS). The mass that could be stored is that which is rejected below a local pinch in a single batch. The local pinch corresponds to a given time interval. This mass, instead of it being rejected to an external MSA, can be stored and later supplied above the pinch at a later time interval. The advantage of this procedure is that less external MSA would be required overall because more of the capacity of the process MSA is being put to use. However, this is only applicable to batch processes at no cost other than the cost of storing the mass rejected below each local pinch for use in a later time interval.

Based on the aforementioned mass storage and reuse philosophy, the question which arises for continuous processes is: how can more of the capacity of the process MSA be utilized so as to reduce the amount of external MSA (and its associated capital cost in terms of absorbers and strippers) that would be needed and at the same time generate a simple plant layout.

A systematic approach in tackling this synthesis question is developed in this study; the technique involves the cooling/heating of the process/external MSA. The approach that will be used entails the investigation of the improvements which could be achieved through the combination of the synthesis of heat exchanger networks with the different types of MENS problems using purely pinch technology. This will lead to the outlining of a set of heuristics for the synthesis of combined heat and mass exchange networks. The established pinch technology approaches for the synthesis of heat and mass exchanger networks (Townsend and Linnhoff, 1984; Ahmad and Smith, 1989 and Hallale and Fraser, 1998; Hallale and Fraser 2000a; Hallale and Fraser 2000b) is employed in the synthesis, and it is illustrated below for different types of MENS problems.

3.2 Problem Statement

In combining the synthesis of heat and mass exchange operations, this study will regard CHAMENS problems as being of the following nature:

Given a number N_R of rich streams, a number N_S of lean streams, a number N_H of hot streams and a number N_C of cold streams, it is desired to synthesize a cost-effective network of combined heat and mass exchangers which can transfer certain species from the rich streams to the lean streams and also perform the required heating and cooling duties of the respective streams. Given also are the flowrate of each rich stream, its supply (inlet) composition, y_i^s and target (outlet) composition, y_i^t and the supply and target compositions, x_j^s and x_j^t for each lean stream, the supply and target temperatures for the hot, cold and MSA/lean streams are also given and the heat capacity flowrates (for the hot/cold streams as well as the lean streams). Equilibrium information for exchanged species in each MSA is given (and its dependence on temperature). The flow rate of each lean stream is unknown and is to be determined so as to minimize the network cost. The candidate lean streams can be classified into N_{SP} process MSAs and N_{SE} external MSAs (where $N_{SP} + N_{SE} = N_S$). The process MSAs already exist on plant site and can be used for the removal of the species at a very low cost *(virtually free). The flowrate of each process MSA that can be used for mass exchange is bounded by its availability in the plant i.e.* $L_J \leq L_J^{\,C}$ *j = 1, 2,…,* N_{SP}*, where* $L_J^{\,C}$ *is the flowrate of the* j^{th} *MSA that is available in the plant. The cost of the external MSAs is also specified. In addition, available for service are hot and cold utilities with given properties, supply and target temperatures (and costs) that can be used to optimize the temperatures of the lean streams (and hence the mass exchange temperatures) and also perform the required heating and cooling duties of the hot and cold streams. Cost data for the heat and mass exchangers are also specified.*

The task is to synthesize the combined cost optimal network of heat and mass exchangers, by determining flowrates and temperatures of all streams to meet required target specifications. Optimization will be in terms of total annual cost (this is the sum of annualized capital cost and annual operating cost).

Along with the questions posed under HENS and MENS problem statements (El-Halwagi, 1997) some other questions which the designer should aim to answer for the combined HENS and MENS are:

- What will be the optimal temperature profile for each stream all through the network?
- Which of the MSAs should be cooled or heated and to what temperature?
- What should be the supply and target compositions of each MSA?

3.3 Example problems

3.3.1 Problem with only one MSA (Example 3.1)

The first MENS problem to be examined in this report is adapted from Hallale and Fraser, (1998). It is a case involving four rich gaseous streams from which SO_2 has to be absorbed using water, which is the only available MSA at a temperature of 20°C. The concentrations of SO_2 in the gas and liquid streams are expressed as molar ratios *Y* and *X*. The gas streams are assumed to take on the temperature of the liquid stream, also, each absorber operates isothermally. Two mass exchange scenarios are going to be considered, the first is SO_2 absorption by water without subsequently regenerating the water while the second situation investigates the regeneration of the water. Discrete temperatures over a range which includes the supply temperature for the MSA for mass exchange are going to be considered using established pinch techniques. Stream and cost data for this example problem and all the other example problems can be found in Appendix A.

3.3.1.1 No regeneration

3.3.1.1.1 Mass exchange network

Table 3.1 below presents the annual operating and capital costs targets for the MEN at the above mentioned mass exchange temperatures while Table 3.2 illustrates the annual operating and capital cost targets for the heat exchange as well as the CHAMENS total annual costs.

Table 3.1: Total annual cost targets for different mass exchange temperatures

Options (°C)	***Optimal*** **$\varepsilon \times 10^{-5}$**	**Final x comps $\times 10^{-4}$**	**Costs (\$/yr)$\times 10^3$**		
			AOC	**ACC**	**TAC**
30	*2.9*	*5.45*	*498*	*94.0*	*592*
20	*3.8*	*7.17*	*378.8*	*93.8*	*472.6*
10	*8.3*	*11.28*	*240.8*	*85.9*	*326.7*

The total annual cost required at 10°C operating temperature is 44.8% lower than that required at 30°C. As the mass exchange temperature reduces, the optimal ε (from supertargeting) for the total annual cost increases. The annual operating and capital costs both reduce with temperature, the reason for this is that at lower equilibrium constants, the final x composition with which there can be a feasible mass exchange with the highest supply composition of y is greater at lower temperatures (48% higher) than what obtains at higher temperatures (i.e. higher equilibrium constants). In essence, the flowrate of the lean stream needed at the lower equilibrium constants will be lower, and the absorber size required to accomplish such separations will also be smaller for the same mass load, hence the trend observed on Table 3.1 above.

Operating at lower mass exchange temperatures is beneficial for situations in which there is no restriction on the permissible outlet composition of the MSA due to environmental reasons i.e. if the MSA would be used on a "once-through" basis and then discharged and hence, no need for regeneration of the now SO_2 rich MSA stream. But for economic reasons in which the MSA has to be regenerated (regenerable MSAs), the benefits of these lower mass exchange temperatures has to be weighed against the stripping and heat exchange costs as well as the increased MSA outlet compositions observed at lower MSA temperatures. In doing this, the effect of higher outlet lean stream compositions from the absorbers on the annual operating and capital cost requirements of the stripping process has to be investigated because these compositions could be treated as optimization variables (Hallale, 1998). The results of the investigation are presented in the stripping section below.

3.3.1.1.2 ***Heat Exchange Network***

For the external MSA (water) to be used to accomplish the absorption of SO_2 from the gaseous streams at 20°C and 10°C respectively, it has to be cooled to these temperatures from the supply temperature of 30°C, hence incurring cooling costs. These costs are presented on Table 3.2 below and compared with the Option of using the MSA at the temperature at which it is available, 30°C, which does not require any cooling.

Table 3.2: CHAMENS total annual costs

Options (°C)	Costs ($/yr)$\times 10^3$				
	HENS			MENS	CHAMENS
	AOC	ACC	TAC	TAC	TAC
30	-	-	-	*590.4*	*590.4*
20	*4*	*39.3*	*43.3*	*473.1*	*516.4*
10	*15.1*	*27.7*	*42.8*	*328.8*	*371.6*

The total annual cost requirement for cooling the external MSA from 30°C to 20°C and 10°C respectively is more or less the same. The annual capital cost required for the cooling to 10°C is 29.2% lower than that for cooling to 20°C. This is because the heat capacity flowrate of the MSA is lower at 10°C temperature option than at 20°C, also there is a higher driving force for cooling to 10^{o}C. But overall, the CHAMENS total annual cost requirement for operating the mass exchange at 10°C is 37% lower than that required for operating it at the supply temperature of the MSA. So it is more beneficial to operate at 10^{o}C mass exchange temperature than the supply temperature of 30^{o}C.

3.3.1.2 Regeneration

3.3.1.2.1 ***Mass Exchange Network***

As stated above, in order to obtain the minimum annual operating and capital costs of the absorption and regeneration processes, the x^s and x^t both have to be treated as optimization variables along side ε, this is because different combinations of x^s and x^t both require different lean stream flowrates and hence different mass exchanger sizes. The supply (z^s) and target (z^t) compositions of the regenerative MSA (in this case steam) are given and these would be used to determine the regenerative MSA flowrate required based on the mass load to be taken up by it, this load is the same as that taken up by the primary MSA. This brings to three the degrees of freedom in simultaneous mass exchange and regeneration networks. However for combined heat and mass exchange networks synthesis, the $\Delta T_{\min}$ as well as the mass exchange temperatures equally have to be optimized alongside the aforementioned variables. The reason for this is that at different mass exchange temperatures, different primary MSA flowrates are required and since the MSA flowrate (and hence its heat capacity flowrate) determines the amount of heat to be exchanged as well as the heat exchange equipment sizes; hence the need to find the $\Delta T_{\min}$ that minimizes the competing costs. So in all, there are five degrees of freedom at the disposal of the design engineer.

The network involving the absorption of SO_2 from the gas streams by the primary MSA (water) will be regarded as the primary mass exchange network while that involving the regeneration of the SO_2 from the water stream will be called the secondary mass exchange network (El-Halwagi and Manousiouthakis, 1990).

Due to the large number of variables, the trade-offs cannot be easily represented graphically. A sequential approach involving the discretisation of the mass exchange temperatures and subsequent analysis of the mass exchange/regeneration and thermal cost requirements of each of these temperatures is used. An exhaustive numerical search was carried out for the combined mass exchange and regeneration operation over each of the mass exchange temperature options and the results obtained are presented on Table 3.3 below. Note that the primary MSA (water) now becomes the rich stream in the stripping (regeneration) process while the steam (secondary MSA) is the lean stream. So the supply and target compositions of the primary MSA in the primary network are now reversed for the secondary network.

Table 3.3: Total annual cost for the primary and secondary networks (Costs in $\$/yr \times 10^3$)

Options (°C)	**Optimal ε $\times 10^{-5}$**	**Primary Network**			**Secondary Network Costs**		**Combined Costs**
		MSA opt comps.$\times 10^{-5}$		**Costs**			
		x^s	x^t	**ACC**	**AOC**	**ACC**	
30	*4.7*	*0.18*	*51.5*	*78.7*	*74.3*	*9.3*	*162.3*
20	*4.7*	*0.26*	*701*	*87.8*	*74.3*	*8.7*	*170.8*
10	*9*	*0.5*	*111*	*85*	*74.3*	*7.9*	*167.2*

The secondary MSA flowrate and hence the annual operating cost is fixed since its supply and target compositions as well as the mass load to be removed by it are all fixed. Illustrated on Table 3.3 above, are the different supplies and target compositions for the primary MSA which are different from those of the case in which there is no regeneration. Operating at 30°C mass exchange temperature is 2.9% lower than that of 10°C, with the 20°C operating temperature needing the highest cost. But this still has to be weighed against the cost of heating/cooling for the stripping process and it is discussed next.

3.3.1.2.2 ***Heat Exchange Network***

The use of stripping as a regeneration option requires heating up the stream to be regenerated (the external MSA) to a high temperature (since stripping is enhanced at higher temperatures than the corresponding absorption temperature) and subsequently cooling it back to the absorption temperature. This heating/cooling is carried out using heat exchangers and a systematic way of synthesizing the network of heat exchangers in the light of the mass exchange operation has to be established. Figure 3.1 below illustrates the heating/cooling requirements for the primary MSA in other to enhance the stripping of the SO_2 from the primary MSA.

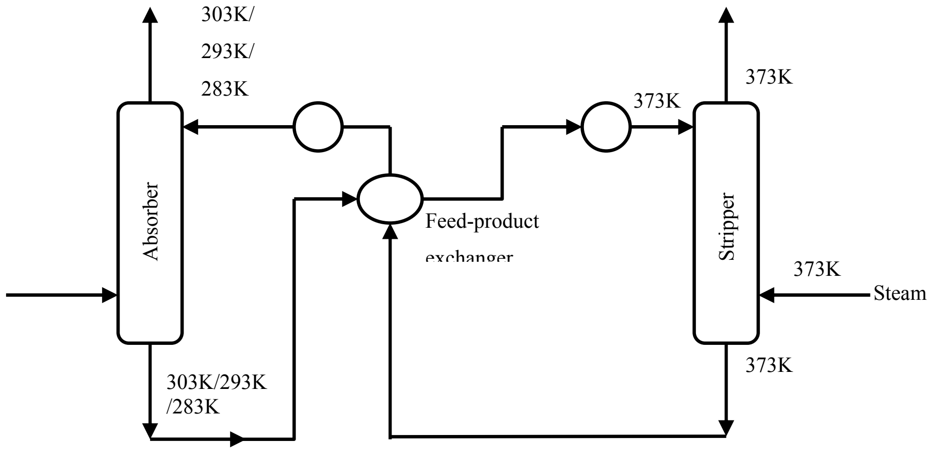

Figure 3.1: Flowsheet representation for the use of the primary MSA, water at 303, 293 & 283K respectively.

Table 3.4 below presents the annual operating and capital cost requirements for the heating/cooling of the SO_2 rich MSA.

Table 3.4: Annual operating and capital costs for heat exchange

Options (°C)	$\Delta T_{min,opt}$ **(°C)**	**Costs (\$/yr)× 10^3**		
		AOC	**ACC**	**TAC**
30	*13*	*79.0*	*143.4*	*222.4*
20	*15*	*67.0*	*132.4*	*199.4*
10	*15*	*49.8*	*98.2*	*148*

The total annual cost of operating at 10°C is 33.45% lower than that at 30°C, this reduction can be observed in both annual operating and capital costs respectively on Table 3.4 above. The reason for such a trend is that the heat capacity flowrates at lower temperatures are lower than what obtains at higher temperatures (this can be seen in the annual operating cost trend in Table 3.1); hence the lower annual operating and capital cost targets.

The CHAMENS total annual cost of operating the removal of SO_2 from gaseous streams at 10°C and the subsequent regeneration of the absorbing stream is 18% and 15% lower than carrying out the operation at 30°C and 20°C respectively, as is shown on Table 3.5 below.

Table 3.5: CHAMENS total annual costs for the case with regeneration

Options (°C)	**MENS ($/yr)× 10^3**			**HENS ($/yr)× 10^3**		**CHAMENS TAC ($/yr)× 10^3**
	Absorption	**Stripping**				
	ACC	**AOC**	**ACC**	**AOC**	**ACC**	
30	*78.7*	*74.3*	*9.3*	*79.0*	*143.4*	*384.7*
20	*87.8*	*74.3*	*8.7*	*67.0*	*132.4*	*370*
10	*85*	*74.3*	*7.7*	*49.8*	*98.2*	*315*

There is no significant difference in the combined costs of the respective mass exchange and regeneration networks (Table 3.3 above); this is because the previous value for the annual operating cost of the absorption process was not added to the total cost, but the cost for the primary MSA to be regenerated is added instead. The reduced CHAMENS total annual cost at 10°C stems from the HENS total annual cost, this is due to the fact that at lower absorption temperatures a reduced MSA flow is required to accomplish the SO_2 absorption and this translates to a reduced heat capacity flowrate for the heat exchanger network synthesis, hence the lower CHAMENS total annual costs. In all, it pays to operate at 10°C mass exchange temperature; this is 18% lower than the cost of operating at the supply temperature of the primary MSA, i.e. 30°C.

The two scenarios investigated above could serve as one of the criteria for choosing whether to use the primary MSA on a “once-through” basis and then discharge or to regenerate it.

3.3.2 Problem with one process MSA and one or two external MSA (non-overlapping MSAs, Example 3.2)

The proposed CHAMENS techniques for problems of this nature will be illustrated by Example 3.2, which is adapted from Srinivas & El-Halwagi, (1994). This is a case involving two rich gaseous streams from which hydrogen sulphide has to be absorbed, available for the absorption is white liquor (a process MSA) and two external MSAs (15 wt% *N*-methyl-2-pyrrolidone and 15 wt% methyldiethanolamine). Srinivas and El-Halwagi (1994) tackled this problem using mixed-integer non-linear programming but did not factor into the synthesis procedure the capital costs of the heat and mass exchangers. The present report will include in the optimization approach both the annual operating and capital costs of the heat exchangers and mass exchangers. The equilibrium constant of the process MSA is strongly dependent on temperature (this is the case with many other equilibrium relations) with a very high process temperature (368K). The capital cost of a column will be assumed to be \$4552 per year per stage as used by Papalexandri et al. (1994). This correlation will be used because the respective costs of the capital items (heat and mass exchangers) are not included in the study of Srinivas and El-Halwagi (1994). Also, the simple cost correlation is suitable for comparison purposes. The stream and cost data for this problem are presented in Appendix.

The synthesis problem is tackled in the conventional way of pinch technology at the supply temperatures of the lean streams, and this is labeled as Option 1a. Subsequent Options (1b and 2) still employ the pinch approach but investigate the effect of cooling the process/external MSA on the pinch, and the resulting annual operating and capital costs of the networks. Each of the generated networks will be costed and the respective costs compared. Also to be used as a criterion with which to evaluate the two approaches is the simplicity of the resulting networks. The mixed integer non linear programming method of Srinivas and El-Halwagi (1994) will also be considered in the comparison.

In developing a synthesis approach for tackling CHAMENS problems of this nature, two mass exchange temperature options for the process MSA are going to be considered, but within these options are sub options to also be investigated, the reason for this will be explained later.

Options

1a: Process MSA, S_1 at 368K and external MSA, S_3 at 298K

1b: Process MSA, S_1 at 368K and external MSA, S_3 at 280K

2: Process MSA, S_1 at 297K

Note that the reason for which S_1 is used at 297K in Option 2 is explained under the mass exchange network section for the no-regeneration case. Just as was done in Example 3.1, two scenarios requiring regeneration and no-regeneration are going to be investigated for each of these options.

3.3.2.1 No-Regeneration

3.3.2.1.1 Mass Exchange Network

Table 3.6 below presents the flowrate targets for the MSAs using the different mass exchange options.

Table 3.6: Flowrate targets

Options	Pinch Composition $\times 10^{-5}$	Excess Capacity Kg/s	Flowrate target For S_1 Kg/s			Load by S_1, kg/s	Mass Load by either S_2 or S_3	
			S_1	S_2	S_3		S_2	S_3
1a	*2.63*	*1.1903*	*9.8112*	*1 295*	*1.296*	*0.38684*	*.01166*	*.01166*
1b	*2.63*	*1.1903*	*9.8112*	*1 295*	*1.296*	*0.38684*	*.01166*	*.01166*
2	-		*10.107*	-	-	*0.3985*	-	-

For Options 1a and b, carrying out the cascading process and correcting for the excess capacity of the process MSA, S_1, gives the flowrate target, the mass load taken up by S_1 and the loads to be rejected to either S_2 or S_3. Note that each of the above mentioned targets and loads are the same for Options 1a and b, this is because the only difference between these two options involves the external MSA, which is the only MSA below the pinch (non-overlapping MSA problem). Instances in which there are differences in targets for these two options will be discussed later.

For Option 2, after cascading the mass loads, a different flowrate target is obtained for the process MSA which is higher than that gotten in Options 1a and b. The difference stems from the fact that operating at a sufficiently low mass exchange temperature (297K downwards) results in a lower equilibrium constant which in essence produces a corresponding *y* composition with which there can be a feasible mass exchange which is lower than the target compositions of R_1 and R_2, this is possible because S_1 still has an excess capacity on site. This is why S_1 is able to take up the entire mass load. Networks of this nature do not have a pinch composition, i.e. only one sub network. This is illustrated in the discussion under annual capital cost target.

From the MSA targets, it can be deduced that, for MENS problems having just one process MSA, effort should be made to make the process MSA supply composition create the final interval as this would result in no need for an external MSA since there will be no pinch composition, but this applies only to problems whose process MSA site flowrate availability is high enough to accommodate this.

Annual Capital Cost Targets

This type of MENS problem as discussed by Hallale and Fraser (1998) and Hallale and Fraser (2000 a & b) does not involve overlapping MSAs since there is just one process MSA whose inlet composition creates the pinch. So the required absorber sizes could be determined separately for above and below the pinch, and these are illustrated by Figure 3.2 below. Note that S_3 was chosen due to the lack of reliable equilibrium data for the solubility of H_2S in 15 wt% *N*-methyl-2-pyrrolidone.

Grid diagram

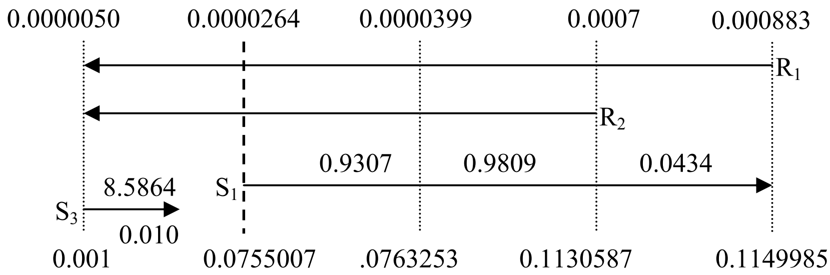

Figure 3.2a: Grid representation of the composition intervals for Option 1a and b.

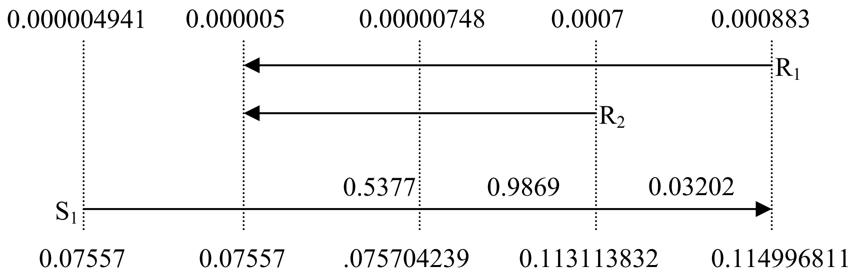

Figure 3.2b: Grid representation of the composition intervals for Option 2.

Table 3.7 below presents the number of stages targets as well as the annual capital costs targets for each of these mass exchange temperature options.

Table 3.7: Tray contributions from streams.

<table>
<tr><th rowspan="2">Options</th><th rowspan="2">Streams</th><th colspan="2">Stages Target</th><th rowspan="2">Total Stages</th><th colspan="3">ACC Targets×10^3 ($/yr)</th></tr>
<tr><th>Above</th><th>Below</th><th>Above</th><th>Below</th><th>Total</th></tr>
<tr><td rowspan="2">1a</td><td>R_1</td><td>10</td><td>43</td><td rowspan="2">106</td><td>45.5</td><td>195.7</td><td rowspan="2">482.4</td></tr>
<tr><td>R_2</td><td>10</td><td>43</td><td>45.5</td><td>195.7</td></tr>
<tr><td rowspan="2">1b</td><td>R_1</td><td>10</td><td>8</td><td rowspan="2">36</td><td>45.5</td><td>36.4</td><td rowspan="2">163.8</td></tr>
<tr><td>R_2</td><td>10</td><td>8</td><td>45.5</td><td>36.4</td></tr>
<tr><td rowspan="2">2</td><td>R_1</td><td>8</td><td>0</td><td rowspan="2">16</td><td>36.4</td><td>0</td><td rowspan="2">72.8</td></tr>
<tr><td>R_2</td><td>8</td><td>0</td><td>36.4</td><td>0</td></tr>
</table>

In Figure 3.2a above, S_1 is operating at 368K above the pinch while S_3 could be used at either 298K or 280K below the pinch. This Figure illustrates that the MENS problem has non-overlapping MSAs. Most of the stages requirement is concentrated in the only interval below the pinch; this is despite the smaller load to be taken up by S_3 below the pinch, compared with that taken up by S_1 above the pinch. This is due to the close approach between the operating line and the equilibrium line. Since the target composition of S_3 cannot be increased, an approach with which to reduce or do away with entirely the number of stages required below the pinch needs to be developed.

Figure 3.2b on the other hand illustrates just one subnetwork involving the use of S1 at 297K. Note that S1 now creates an interval with a *y* composition (0.000049) lower than the final target composition of the gas streams (0.000005). It should be noted that operating at some temperature higher than 297K for S1 will fail to produce a corresponding y composition which is lower than the final target composition for the gaseous streams.

Operating S_3 at 280K results in 16 real stages below the pinch, which is an 81.4% reduction compared with the 86 real stages predicted at a mass exchange temperature of 298K for S_3. But the implication of this might be revealed in the heat exchanger annual operating and capital cost requirements which are discussed in the heat exchanger network synthesis section. This reduction is only obtained in the absorber size requirement for the mass exchange and not in the flowrate of the external MSA to be purchased. It should be noted here that a target composition is imposed on S_3 unlike in the case of the only MSA in

Example 3.1. This is the reason for which there is no flowrate reduction (as illustrated on Table 3.6) but only absorber size reduction for the same mass load which is to be absorbed. In essence, the annual operating cost of problems of this nature i.e. non-overlapping MSAs in which there is a target composition for the external MSA, is not dependent on its temperature (its equilibrium constant) but only on the mass load to be taken up by it, so cooling it does not reduce the annual operating cost requirement, since it has to take up the same mass load at both choices of mass exchange temperatures with the same flowrate.

For cases in which there is no target composition imposed on S_3, the trend observed in Example 3.1 (Table 3.2) will be the case here as well in which there is a simultaneous reduction in the MSA flowrate and absorber size as the mass exchange temperature reduces, but with an increment in the outlet composition.

The predicted number of stages for above the pinch division are the same for the two operating temperature options of 298K and 280K, so also is the units targets, this is also because the MSAs are non-overlapping, so there is no way the cooling of S_3 which is the only MSA below the pinch can alter the pinch and hence, the absorber size required above the pinch. For MENS problems in which the MSAs are overlapping, this is not the case, as will be illustrated by the problem with two or more process MSAs to be presented as Example 3.

Operating the process MSA, S_1 at 297K results in a drastic reduction in the number of stages for the absorbers, 92.5% reduction compared with Option 1a and 77.8% for Option 1b. Also, the need for an external MSA is done away with entirely. The expectation for the number of stages required for the use of S_1 alone would have been an increased number of stages because it is taking up all the mass load, but this is not the case since S_1 has an excess capacity which is able to take care of the increased flowrate requirement, (hence the 10.1074 kg/s targeted on Table 3.6). Therefore the column size required for the H_2S absorption reduces. Thus, with S_1 at 297K, the problem becomes a threshold one. Another benefit of operating S_1 at 297K is that since there is no need for an external MSA, it means that there would also not be a need for regeneration of such external MSA, this in essence takes away the need for the heating/cooling of the MSA to the stripping/absorption temperature and this makes for a simple plant layout.

The cooling of S_1 to 297K would be accomplished with cold utility and heat exchangers, so the costs of these additional operations have to be accounted for. The heat exchanger network synthesis for this option is discussed below.

3.3.2.1.2 ***Heat Exchange Network***

Cooling/Heat requirements for the options,

1a: Use S_1 at 368K and cool S_3 from supply temperature of 310K to 298K

1b: Use S_1 at 368K and cool S_3 from supply temperature of 310K to 280K

2: Use S_1 at 297K by cooling it from 368K and heating it back to this temperature.

Figure 3.3 below is a flowsheet representation of Option 2.

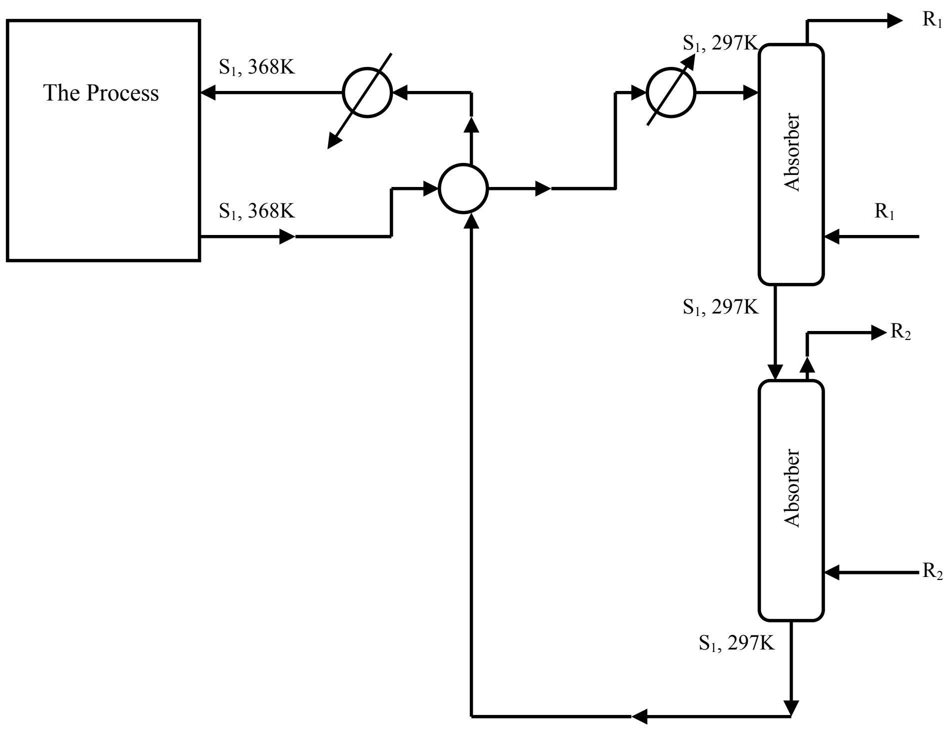

Figure 3.3: Flowsheet representation for the use of S_1 at 297K.

The heating/cooling costs needed for each of these temperature options are presented in Table 3.8 below.

Table 3.8: Heat Exchange Costs

Options	Costs $\times 10^3$ (\$/yr)		
	AO	AC	TA
1a	*0.4*	*8.6*	*9*
1b	*2.8*	*10.4*	*13.2*
2	*38.9*	*85.6*	*124.5*

From Table 3.8, it can be seen that it costs more to cool S_3 from 310K to 280K than it is costs to cool it to 298K, this is due to the fact that the heat capacity flowrates of S_3 at these two operating temperatures stays the same since the mass load to be taken up by S_3 below the pinch is fixed, its composition ranges are also fixed, therefore its flowrate will remain the same (as explained previously), the slight difference in costs stems from the fact that Option 1b involves cooling over a wider temperature range than is required for Option 1a.

The costs needed for Option 2 is 93% and 89% higher than those needed for Option 1a and b respectively. This is because the heat capacity flowrate for S_1 at 297K is very high, also, the temperature range over which the cooling/heating is carried out is very wide unlike Options 1a and b in which only cooling is done without having to heat back to the mass exchange temperature of S_3 since S_3 is not being regenerated. But how do these increased cooling costs in Options 1b and 2 compare with the benefits obtained from the reduced mass absorber sizes presented in Table 3.7 above. These are presented in Table 3.9 below.

Table 3.9: CHAMENS total annual costs (\$/yr $\times 10^3$)

Options	MENS		HENS		CHAMENS
	AOC	ACC	AOC	ACC	TAC
1a	*40.1*	*482.4*	*0.4*	*8.6*	*531.5*
1b	*40.1*	*163.8*	*2.8*	*10.4*	*217.1*
2	*0*	*72.8*	*38.9*	*85.6*	*197.3*

From Table 3.9 above, the cheapest option is 2; this is 10% cheaper than Option 1b and 63% cheaper than Option 1a. Option 1b is 59% lower in cost compared with Option 1a. This problem is one in which most of the stages requirements is concentrated below the pinch and since it is a MENS problem with non-overlapping MSAs, cooling the external MSA (which is below the pinch) enhances the absorption of H_2S by S_3 from the gas stream with a reduced mass exchanger size but without a corresponding reduction in MSA flowrate. This trend can be observed on Table 3.9 above. Option 2 apart from being the cheapest will also produce a simple plant layout since it requires fewer units.

3.3.2.2 Regeneration

3.3.2.2.1 ***Mass Exchange Network***

For MENS problems in which the MSA has to be regenerated due to environmental and or economic reasons, the cost of regeneration should be included explicitly in the targeting process. For this case study, Srinivas and El-Halwagi (1994) only mentioned the annual operating cost of the regeneration without the annual capital cost for the absorbers as well as the regenerating units.

The regeneration costs are only discussed for Options 1a and 1b because Option 2 does not require the use of an external MSA since the only process MSA, S_1, takes up the entire mass load. However, the costs of operation for Option 2 will be included in the CHAMENS TAC table just for the purpose of comparing the options.

Just as was the case for Example 3.1 in which the optimum primary MSA target composition has to be determined because of the interaction with the stripping column, i.e. the secondary network, so it is in this case. An exhaustive numerical search was carried out and the results obtained are illustrated on Table 3.10 below.

Table 3.10: Total annual Costs for the Primary and Secondary Networks ($\times 10^3$ \$/yr)

Options	Primary Network			Secondary Network Costs		Combined Costs
	MSA opt comps.		Costs			
	x^s	x^t	ACC	AOC	ACC	
1a	*0.001*	*0.0032*	*63.7*	*56.4*	*9.1*	*129.2*
1b	*0.001*	*0.005*	*45.5*	*56.4*	*13.7*	*115.6*

It should be noted that the annual capital cost obtained for above the pinch number of stages on Table 3.7 is \$391,400/yr (\$195,700/yr for each of the two units at 298K mass exchange temperature), this is different from that obtained when the S_3 is being regenerated i.e. on Table 3.10 (\$63,700/yr). The reason for this difference is due to the fact that the S_3 composition ranges differs in these two scenarios, 0.001 – 0.01 for the case without regeneration and 0.001 – 0.0032 for the case with regeneration. For 280K mass exchange temperature, the opposite is the case, i.e. the annual capital cost of operation for the no-regeneration case is lower than that of regeneration. Carrying out the mass exchange below the pinch at 280K i.e. Option 2, is 11% lower in costs than at 298K. However these costs do have not have the heating/cooling costs added to them, the resulting effects of the heating/cooling costs are discussed in the next section.

3.3.2.2.2 ***Heat Exchange Network***

Cooling/Heating requirements for the options

1a: Use S_1 at 368K, cool S_3 to 298K from 373K for absorption and heat back to 373K for Stripping.

1b: Use S_1 at 368K, cool S_3 to 280K from 373K for absorption and heat back to 373K for Stripping.

Table 3.11 below illustrates the annual operating and annual costs requirements for the heating/cooling for Options 1a and b.

Table 3.11: Heat Exchange Costs

Options	$\Delta T_{\text{min, opt}}$	Costs $\times 10^3$ (\$/yr)		
		AO	AC	TA
1a	16	22.4	55.2	77.6
1b	19	17.3	44.8	62.1

The total annual cost (for heat exchange) of operating S_3 mass exchange at 280K is 20% lower than that needed to operate it at 298K, this is due to the fact that at 280K, the heat capacity flowrate of S_3 is lower than at 298K, hence a smaller heat exchange area is needed, as well as the lower utilities cost.

Table 3.12 below presents the overall CHAMENS total annual cost which comprises of the costs of the mass absorbers both above and below the pinch, the cost of the regeneration (operating and capital) and the cost of the heat exchange (operating and capital).

Table 3.12: CHAMENS total annual costs (\$/yr $\times 10^3$)

Options	MENS		HENS		CHAMENS
	AOC	ACC	AOC	ACC	TAC
1a	56.4	163.8	22.4	55.2	297.8
1b	56.4	150.2	17.3	44.8	268.7
2	0	72.8	38.9	85.6	197.3

The annual operating costs for regeneration are the same for Options 1a and b but the total cost of both the absorbers and strippers is 8.3% lower for Option 1b than it is for Option 1a. Option 2 still comes out cheapest when compared with the cases requiring regeneration for Options 1a and 1b.

Srinivas and El-Halwagi (1994), as mentioned earlier, did not include the cost data for the heat and mass exchangers so these have been assumed using the simple cost correlation of Papalexandri et al. (1994) for the mass exchangers and also an assumed cost correlation for the heat exchangers (this is presented in Appendix A).

The solution generated by Srinivas and El-Halwagi (1994) CHARMEN MINLP model is more or less the same as presented in Option 1a of this example; it cannot be explicitly compared with the solution generated by this new approach because they did not include explicitly the type of regeneration process carried out for S_3 as well as its costs. The optimum TAC (which is just an AOC) reported by the authors is $94,094/yr. This is just the costs of S_3, regeneration operating cost, hot and cold utilities. It does not include the capital costs of the absorbers, strippers and heat exchangers. They reported 298K as the optimum temperature for S_3, but carrying out a detailed synthesis as well as costing of all the capital equipments, this is not the case. It is cheaper to operate at 280K for the case in which S_3 is being regenerated and that in which it is not being regenerated.

The benefit of operating S_3 at the lowest allowable working temperature of 280K in terms of the required absorber size and the amount of S_3 to be purchased could only be appreciated with an explicit capital cost targeting approach for mass exchange networks as well as for the heat exchange network. Also demonstrated in this problem, is the benefit of cooling the process MSA, this goes a long way in reducing the absorber annual capital cost requirements as well as the annual operating cost for mass exchange (which was eliminated entirely in Option 2).

3.3.3 Problem with two Process MSA and one external MSA (overlapping MSAs, Example 3.3)

The pinch technology approach for CHAMENS being developed in this study will be illustrated by Example 3.3, which is different from Example 3.2 in that it involves two process MSAs which overlap. Also, the equilibrium relations are linear within the range of compositions being considered. The benefits of cooling the only process MSA has been investigated in Example 3.2, so the question which arises is: for MENS problems in which there are more than one process MSA, which or what combination of process streams should be cooled and to what temperature, so as to minimize cost. Stream and cost data for this example can be found in Appendix A.

All the MSAs in this problem are water based streams. S_1 operates at 70°C while S_2, the second process MSA is at 55°C. The external MSA, S_3, is available at 30°C. This problem will be tackled just as was done for Example 3.2 (non-overlapping MSA). In establishing the benefits of combining the synthesis of heat and mass exchanger networks, different scenarios (options) of heating/cooling of the mass exchange streams are going to be compared in terms of costs and the simplicity of the resulting designs. In each of the options, two scenarios are going to be investigated, these are, the use of the external MSA, S_3 on a "once-through" basis and the regeneration of the external MSA through stripping with steam. Presented on Table 3.13 below are the different temperature options investigated.

Table 3.13: Mass Exchange Temperature Options

Options	**Mass Exchange Temperatures for MSAs (^oC)**		
	Process		**External**
	S_1	**S_2**	**S_3**
1	*70*	*55*	*30*
2	*70*	*55*	*10*
3	*70*	*10*	*30*
4	*70*	*10*	*10*
5	*25*	*55*	*25*
6	*25*	*25*	*25*

3.3.3.1 No Regeneration

*3.3.3.1.1 **Mass Exchange Network***

Table 3.14 below presents the effects on the network of applying different degrees of cooling to the MSA streams. The effects are reflected in the respective loads to be taken up by each of the MSAs, the excess capacities of the process MSA and the target flowrates. Note that the targets for Options 4 and 6 are not included on the table; the reasons for this will be explained later in this report.

Table 3.14: MSA targets

Option	Δy_{min} $\times 10^{-3}$	**Stream**	**Equilibrium constant**	**Load (kg/s)**	**Flowrate (kg/s)**	**Excess capacities (kg/s)**	**AOC** $\times 10^{3}$ (\$/yr)	**% diff**
1	*4.85*	S_1	*5.3331*	*0.135*	*25*	*0*		
		S_2	*3.6726*	*0.07928*	*13.214*	*0.1607*		
		S_3	*1.3371*	*0.03822*	*2.2481*	-	*329.8*	*99.9*
2	*0.37*	S_1	*5.3331*	*0.135*	*25*	*0*		
		S_2	*3.6726*	*0.10178*	*16.964*	*0.1382*		
		S_3	*0.5361*	*0.01572*	*0.9245*	-	*135.6*	*99.7*
3	*4.7*	S_1	*5.3331*	*0.135*	*25*	*0*		
		S_2	*0.5361*	*0.11735*	*19.560*	*0.1225*		
		S_3	*1.3371*	*0.00014*	*0.0083*	-	*1.2*	*66.7*
5	*4.25*	S_1	*1.0377*	*0.135*	*25*	*0*		
		S_2	*3.6726*	*0.117451*	*19.575*	*0.1225*		
		S_3	*1.0377*	*0.000049*	*0.00290*	-	*0.4*	

For Option 1, S_1 creates the pinch and its available flowrate on site is 25 kg s^{-1} while that of S_2 is 40 kg s^{-1}. The whole of the available flow of S_1 is used up while at 55°C operating temperature for S_2, only 13.214 kg $s^{-1}$of its site flowrate is used. The remaining load to be absorbed is rejected to the external MSA, S_3.

The use of S_3 at a lower temperature, 10°C in Option 2, results in the reduction of the mass load to be taken up by this MSA as illustrated in Tables 14, in essence, the amount of S_3 that has to be purchased reduces. But the question which arises is what happens to the mass load which S_3 is supposed to absorb? The answer to this is explained in the section for the annual capital cost requirements for the mass exchange network.

For Option 3, cooling S_2 to 10°C from 55°C, results in the use of more of its capacity and a reduction in the mass load to be absorbed by S_3, the external MSA, hence a reduction in operating cost. This is highly beneficial because the regeneration cost will also be greatly reduced.

Option 5 has the lowest annual operating cost, \$ 425/yr. Despite reducing the equilibrium constant of S_1, the mass load to be taken up by S_1, and hence its flowrate, still remains as it is in the previous options where its equilibrium constant is 5.3331, but the mass load to be rejected to S_3, changes. The reason for this is similar to that observed in Option 3, which has to do with the fact that a lower equilibrium constant for S_1 results in the creation of a *y* composition with which there can be a feasible mass transfer being very close to the target composition of R_1. Therefore, S_1 is responsible for the creation of the pinch; this is illustrated in the grid diagrams in the next section.

The *y-y** capital cost targeting tool for MENS problems with overlapping MSAs of Hallale (1998) has been used for the stages targeting and the grid diagrams, Figure 3.4, which illustrates the participation of each stream in the composition intervals are shown below, Table 3.15 presents the annual capital cost targets.

Table 3.15: Tray contribution from streams in each of the options

Options	**Streams**	**Targets**				**Total**		**ACC $\times 10^3$ (\$/yr)**		
		Stages		**Units**				**A**	**B**	**T**
		A	**B**	**A**	**B**	**Stages**	**Units**			
1	R_1	*7*	*3*	*2*	*1*	*20*	*6*	*63.7*	*27.3*	*91*
	R_2	*7*	*3*	*2*	*1*					
2	R_1	*8*	*3*	*2*	*1*	*21*	*6*	*68.3*	*27.3*	*95.6*
	R_2	*7*	*3*	*2*	*1*					
3	R_1	*3*	*0*	*2*	*0*	*6*	*3*	*27.3*	*0*	*27.3*
	R_2	*3*	*0*	*1*	*0*					
5	R_1	*3*	*0*	*2*	*0*	*5*	*3*	*22.8*	*0*	*22.8*
	R_2	*2*	*0*	*1*	*0*					

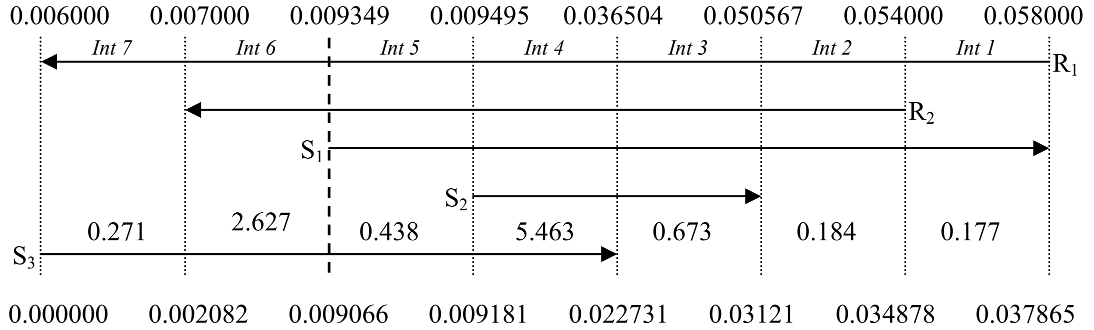

Figure 3.4a: Grid representation of the composition intervals for Option 1.

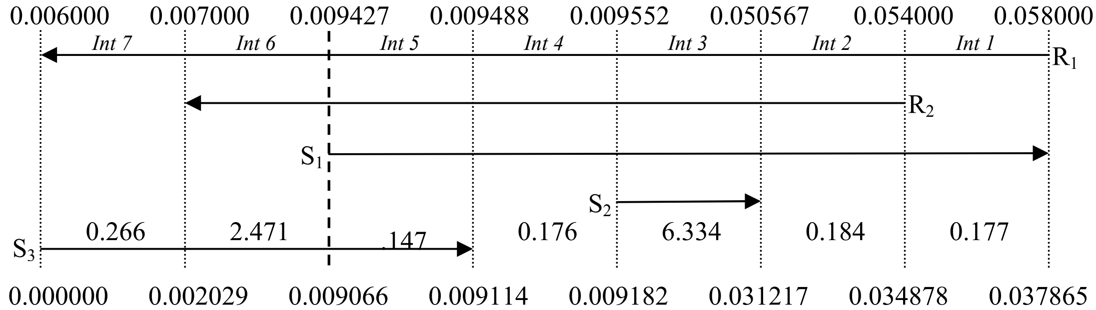

Figure 3.4b: Grid representation of the composition intervals for Option 2.

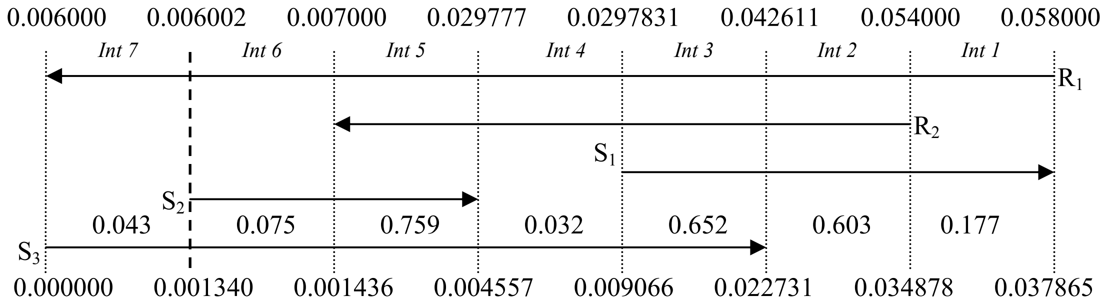

Figure 3.4c: Grid representation of the composition intervals for Option 3.

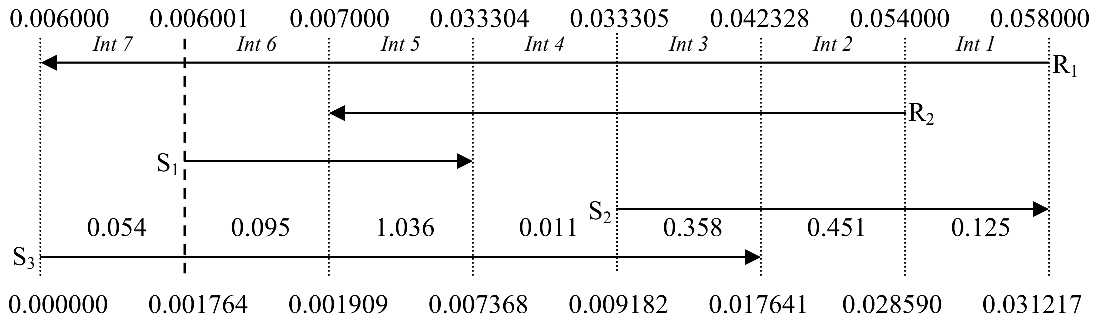

Figure 3.4d: Grid representation of the composition intervals for Option 5.

In Figure 3.4a above for Option 1, S_2 is entirely above the pinch, while S_3, the external MSA, crosses the pinch. Most of the stages above the pinch are concentrated in interval 4 which is the stage in which S_2 starts, while interval 6, which is immediately below the pinch, bears the next highest number of stages.

Comparing Option 2 with 1, there is a 4.8% increase in the annual capital cost requirements for the absorption process. Since there is a 60% reduction in the annual operating cost requirement (i.e. comparing Option 2 with 1), the expectation would have been a somewhat equal degree of increase in the annual capital cost that would be needed but just a slight increased is observed. The explanation for this is that reducing the mass exchange temperature of S_3, i.e. its equilibrium constant, leads to a reduction in the number of intervals within which S_3 participates (from 4 to 3 in Figure 3.4b), this is because its target composition is reduced, also, S_2 participates in one interval less. The amount of mass load that can be taken up by S_3 reduces at a lower equilibrium constant, so also is the flowrate and absorber size required. Since S_1 is fully used up, the extra load not taken up by S_3 is absorbed by S_2 (which has excess capacity on site, 40 kg/s), more of its flowrate is now used up (i.e. 16.964 kg/s) unlike in Option 1 (in which only 13.214 kg/s was used), so a reduced absorber size would be required, hence the not too high annual capital cost requirement in Option 2 compared with Option 1.

It is worth stating at this point that, in Example 3.2 which has just one process MSA which creates the pinch, operating the external MSA at the two temperatures of 280K and 298K (but the same target compositions) requires the same MSA flowrate which is 1,295.54 kg/s but different capital costs. This is not the case for overlapping MSAs (as illustrated by Example 3.3) because one of the process MSAs crosses the pinch. So changing the operating parameters of the external MSA which is below the pinch is reflected above the pinch where the process MSA that causes the pinch resides. In essence, in this Option, the operating cost is reduced, while the mass exchange annual capital cost increases slightly.

The cooling of S_2 (in Option 3) reduces the y composition with which there can be a feasible mass exchange to S_2, i.e. from 0.009427 to 0.006002, which is very close to the target composition of R_1. Since S_2 has excess capacity available on site, it is able to take up more load than it absorbed in Options 1 & 2; this therefore leads to reductions in the absorber size required for S_2, the mass load to be taken up by the external MSA, S_3, and hence the stages requirement for S_3, this are illustrated on Tables 14 & 15 above.

The mass exchange annual capital cost requirement in Option 3 is 70% lower than that of Option 1 and 71.4% lower than that of Option 2. The absorber size required below the pinch is very small since very little mass load is to be removed within the only interval existing in this region of the pinch, also the required MSA flowrate, S_3, is low. The reasons for this have been explained above. For Option 5, the trend which obtains in terms of absorber size requirement for S_1, S_2 and S_3 is just as it is in Option 3, but Option 5 is 16.5% lower than that required in Option 3.

*3.3.3.1.2 **Heat Exchange Network***

The mass exchange temperature options have been described on Table 3.13 above. For this scenario in which there is no regeneration of the external MSA, the cooling/heating needed are, cooling the process MSAs to the desired mass exchange temperatures indicated on Table 3.13 and subsequently heating them back to their respective process temperatures while for the external MSA, it is just cooled to the indicated mass exchange temperatures on Table 3.13. The external MSAs don't have to be heated back to their supply temperatures since they are just to be used on "once through basis"; this applies to all the options.

Table 3.16: CHAMENS Total Annual Costs ($\times 10^3$, \$/yr)

Options	**Costs**	**MENS**	**HENS**		**CHAMENS**
			$\Delta T_{min, opt}$ (^oC)	**Cost**	
1	**AOC**	*329.8*		-	*420.8*
	ACC	*91*		-	
2	**AOC**	*135.6*		*2.3*	*258.6*
	ACC	*95.6*		*25.1*	
3	**AOC**	*1.2*	*10*	*106.8*	*308.9*
	ACC	*27.3*		*173.6*	
5	**AOC**	*0.4*	*10*	*115.5*	*337.4*
	ACC	*22.8*		*198.7*	

Table 3.16 above presents the needed heat exchange costs; the mass exchange costs presented earlier as well as the final CHAMENS costs are also presented. Note that there is no heat exchange needed for Option 1 since the process MSAs, S_1 and S_2 are being use at their process temperatures while the external MSA, S_3 is being used at its supply temperature for the mass exchange.

The CHAMENS TAC needed in Option 2 is 38.5% lower that needed in Option 1. This is because the MENS AOC for Option 2 is very low at 10°C (59% lower) and the cost of cooling is not very high, hence the lower CHAMENS cost. The heat exchange cost in Option 3 is 90% higher than that needed for Option 2. This is due to the high heat capacity flowrate of S_2 in Option 3 unlike what obtains for S_3 in Option 2 which is far lower. The CHAMENS TAC for Option 3 is 16.2% higher than that needed in Option 2 but 27% lower than that of Option 1.

For Option 5, the CHAMENS TAC is 8.4% higher than that needed in Option 3 and 23% higher than that of Option 2. This is because the cost of cooling/heating S_1 from its process temperature of 70°C is higher than that needed to cool/heat S_2 from its own process temperature, also a higher number of heat exchange units are needed since S_1 has to be cooled and subsequently heated back to its process temperature. So for the no regeneration case, Option 2 is the best.

3.3.3.2 Regeneration

*3.3.3.2.1 **Mass Exchange Network***

The scenario involving regeneration is going to be investigated in this section. Note that the situation encountered in Examples 3.1 and 3.2 applies here as well in which the supply and target compositions of the MSA to be regenerated are treated as optimization variables, along with the mass exchange temperature, minimum composition difference as well as $\Delta T_{\min}$ for the heat exchange process. The optimal x^s and x^t after an exhaustive numerical search along with the annual operating and capital costs of the stripping process are presented in Table 3.17.

Table 3.17: Annual Operating and Capital Costs for the Combined Absorption and Regeneration Process ($/yr × 10^3)

Options	Δy_{min}	Primary Network			Secondary Network Costs		Combined Costs
		MSA opt comps.		Costs			
		x^s	x^t	ACC	AOC	ACC	
1	*0.005*	*0.0001*	*0.017*	*91*	*271.2*	*58.6*	*420.8*
2	*0.0004*	*.001*	*0.017*	*91*	*114.2*	*45.5*	*250.7*
3	*0.0047*	*.01*	*.017*	*27.3*	*1*	*22.8*	*51.1*
5	*0.0043*	*.01*	*.017*	*22.8*	*.3*	*22.8*	*45.9*

Note that the annual capital costs presented on Table 3.17 above are the capital costs of the whole of the absorption network, while the x^s and x^t represent the optimal compositions for the external MSA, S_3. Also, the annual operating cost for the primary network is not included on Table 3.17 above because S_3 is being regenerated. The heat exchange operations with which to accomplish this stripping are investigated in the next section.

3.3.3.2.2 ***Heat Exchange Network***

The process MSAs are cooled to the mass exchange temperature options indicated on Table 3.13 above and subsequently heated back to their process temperatures while the external MSA, S_3, is cooled to the indicated temperatures on Table 3.13 but heated back to the stripping temperatures, 100°C, unlike in the no-regeneration scenario in which no heating back was carried out on S_3. The heating to 100°C is done because steam stripping is used; this high temperature enhances the stripping of the ammonia from the MSA. The CHAMENS TAC which comprises of the annual operating costs of the stripping, heat exchange and the annual capital costs of the absorption, stripping and heat exchange are presented on Table 3.18 below.

In Table 3.18, Option 2 is 39% lower than Option 1; this is due to the high stripping annual operating cost needed in Option 1 which is as a result of the higher mass load being taken up by S_3 unlike in Option 2. So the stripping cost is a dominant cost in this example.

Table 3.18: CHAMENS TAC

<table>
<tr><th rowspan="3">Options</th><th rowspan="3">Costs</th><th colspan="5">Costs $\times 10^3$ ($/yr)</th></tr>
<tr><th colspan="2">MENS</th><th colspan="2">HENS</th><th rowspan="2">CHAMENS</th></tr>
<tr><th>Absorption</th><th>Stripping</th><th>$\Delta T_{min, opt}$(^oC)</th><th>Cost</th></tr>
<tr><td rowspan="2">1</td><td>AOC</td><td>-</td><td>271.2</td><td rowspan="2">15</td><td>15.9</td><td rowspan="2">482.6</td></tr>
<tr><td>ACC</td><td>91</td><td>58.6</td><td>45.9</td></tr>
<tr><td rowspan="2">2</td><td>AOC</td><td>-</td><td>114.2</td><td rowspan="2">17</td><td>9.5</td><td rowspan="2">295.8</td></tr>
<tr><td>ACC</td><td>91</td><td>45.5</td><td>35.6</td></tr>
<tr><td rowspan="2">3</td><td>AOC</td><td>-</td><td>1</td><td rowspan="2">11</td><td>117.5</td><td rowspan="2">366.5</td></tr>
<tr><td>ACC</td><td>27.3</td><td>22.8</td><td>197.9</td></tr>
<tr><td rowspan="2">5</td><td>AOC</td><td>-</td><td>.3</td><td rowspan="2">11</td><td>138.6</td><td rowspan="2">404.1</td></tr>
<tr><td>ACC</td><td>22.8</td><td>22.8</td><td>219.6</td></tr>
</table>

For Option 3, the total annual cost requirement for the cooling/heating of S_2 and S_3 is $315,400/yr; this is 80% and 86% higher than those needed in Options 1 and 2 respectively. The reasons for this increased cost are: S_3 is not the only stream that is undergoing heating/cooling as it is in Options 1 and 2 but S_2 as well, also the heat capacity flowrate of S_2 is high (82.16 $kJs^{-1}K^{-1}$). The required size of heat exchangers with which to accomplish this cooling/heating therefore will be very large, this translates to a high annual capital cost requirement which is the dominant cost item in the CHAMENS network. The CHAMENS TAC for Option 3 is 24% lower than that needed in Option 1 and 19.3% higher than that of Option 2. Note that the HENS TAC for the no-regeneration case is 11% lower than the regeneration case. The same explanation applies to Option 5 as it does to Option 3, hence the very high CHAMENS cost which is 9.3% higher than that needed in Option 3. So it could be said that Option 2 is the best with Options 3 and 5 following suit.

From this example, it can be seen that cooling the process MSA over the external MSA is not always beneficial, but it is difficult establishing a technique with which to narrow down on the MSA to cool without going through the cooling of all the MSAs as has been done in this example, hence the need for a mathematical programming approach.

Note that the results of operating at Option 4 mass exchange temperatures are very similar to what obtains for Option 3, this is due to the fact that the use of S_2 at 10°C mass absorption temperature reduces drastically the work to be done by S_3 (as indicated in Table 3.14 in which the mass load it needs to remove is just 0.00014 kg/s with a flowrate as low as 0.0083 kg/s). This therefore makes insignificant the benefits of cooling S_3 alongside S_2. So for Example 3.3, Option 3 sets a limit for the level to which S_2 and S_3 can be cooled because, it gives the lowest total annual cost of operation.

One of the factors which need to be considered in cooling a process MSA is the annual capital cost of the MENS, this is because if the annual capital cost of the MENS is not significant compared with the heat exchange cost (the determinant of the heat exchange cost is the heat capacity and the flowrate of the process MSA) whatever percentage reduction is obtained in the annual capital cost of the absorbers will be overwhelmed by the heat exchange cost. This can be observed in Option 3 of Example 3.3. The percentage reduction in equilibrium constant (due to cooling) is somewhat synonymous to the reduction in cost that would be observed for the annual capital cost of the MENS.

By virtue of the nature of this problem, there isn't much benefit in going from Option 5 to 6. This is because, even at Option 5, a very low cost has been obtained (for the no-regeneration case) because the need for S_3 is already done away with and the number of stages obtained is very low. For the case requiring regeneration, far higher costs would be obtained than what is gotten for Option 5. Option 5 sets a limit of mass exchange temperature combination for this problem (i.e. for the no-regeneration scenario) since the highest capacity of S_2 which could be used has been used up in Option 5, which involves the cooling of S_1 alone. Cooling S_2 alongside S_1 does not improve the situation any longer because very low costs have already been obtained in Option 5, also, the sizing of the mass exchangers would no longer be feasible. The required heat exchange cost would be higher as well.

Each mass exchange temperature (or temperature combinations as the case may be), i.e. the options, could be described as topologies. The ε and $\Delta T_{\min}$ of each topology can be optimized so as to obtain the optimum CHAMEN cost of such a topology, this is then compared with those of other topologies and the least is taken as the optimum total annual cost of the CHAMENS problem. Going from one topology to the other requires changing the supply/target temperature of the lean stream of interest, in essence, the stream temperatures are not fixed, this results in additional degree of freedom for such problems, but the approach used in this report eliminates the multidimensional nature of the problem by analyzing individually, the annual operating and annual capital costs requirement for the heat and mass exchanger networks.

3.3.4 Summary

Based on the three different CHAMENS problems considered above, a synthesis algorithm for achieving optimal designs can be described as follows;

3.3.4.1 MENS problems with one MSA

- Identify the most dominant variable and discretise (each being a topology), in this case, the mass exchange temperature is the most dominant of the variables and is not influenced by other variables. The search for the optimum is carried out within each of these temperature options (topologies) with the supply temperature for the only available MSA being the first topology while the lowest working temperature for the MSA is the last.
- Within each topology, the optimum ε is identified and for each optimum ε the $\Delta T_{\min}$ is optimized. The best $\Delta T_{\min}$ is noted so that it can then be compared with the best $\Delta T_{\min}$ from other ε. The least combination in terms of cost of ε - $\Delta T_{\min}$ is taken as the best for the concerned topology.
- The second step is repeated for all the temperature topologies and the least ε - $\Delta T_{\min}$ combination is taken as the optimum solution.

Note however that this is beneficial in situations in which the HENS cost is not dominant. However this approach is still good in that it helps to identify the dominant network in terms of costs between the HENS and MENS since a thorough search is carried out at all the variables that affect the costs of each of these networks so that the least combination of HENS and MENS can be easily compared with the MENS base problem (i.e. at the supply conditions with no option of introducing HENS).

3.3.4.2 MENS problems with non-overlapping MSAs

Each of the MSAs in this type of MENS problem is restricted to each side of the pinch, the process MSA being above while the external is below. The procedure highlighted above for

MENS problems with one MSA is followed for each side of the pinch division here as well. But for cases in which the process MSA at a low mass exchange temperature is not able to take away alone the entire mass load, the following steps should be followed.

- Identify temperature topologies for both process and external MSAs, i.e. above and below the pinch.
- Carry out a one-one mapping of the two temperature topologies at each mass exchange temperature and then follow the procedure stated for the MENS problem with just one MSA.

3.3.4.3 MENS problems with overlapping MSAs

The procedure for the MENS problems with non-overlapping MSAs is also followed here, the difference lies in the fact that the mapping of the temperature topologies would result in a matrix which will be somewhat difficult to handle manually since within each topology there still exists variables which need to be optimized.

3.3.5 Future work

For Example 3.1, which is a very simple problem with just one MSA, it is easy to know that the least working temperature of the concerned lean stream produces the best topology for mass exchange and so this reduces the region of search. For more complex problems in which there are many streams, this will not always be the case, also, for MSAs which have to be regenerated, their supply/target compositions become additional degrees of freedom which would be difficult to handle manually as has been done above, hence the need for a more automated search approach which is able to predict the optimum total annual cost before design for complex cases. Such a technique would be developed in future work.

Also, the examples considered in this report are such that the MENS problem is the foundation problem, HENS was only brought in so as to improve the equilibrium relations of the species to be removed from the rich streams in the lean streams. For problems in which both MENS and HENS are foundation problems, a more conceptual technique which is still an extension of the traditional pinch technology is being proposed; this will be presented in the next section of this report.

3.3.6 Conclusions

The benefits of combining the synthesis of heat and mass exchange networks have been demonstrated through the above combinations of networks, results obtained in the examples have indicated that just operating the lean streams at their supply temperatures might not be the best in terms of cost and simplicity of design.

The synthesis has been achieved using purely pinch approach of heat and mass exchange networks, this technique however is sequential, hence requires much time, also it is difficult identifying the order to proceed in cooling the lean streams. But this approach is advantageous in that it presents in a simple fashion, the benefits of combining the synthesis of heat and mass exchange networks. Also demonstrated in this report for MENS problems with either non-overlapping or overlapping MSAs, is that the combination of heat and mass exchange networks becomes beneficial in situations in which the process MSA which has an excess capacity to remove mass is cooled. Cooling the process MSA helps in reducing the flowrate of the external MSA that would be needed (and in some cases, it even does away entirely with the need for an external MSA) and hence, the attendant annual capital cost requirement of the external MSA, the absorber size required for this process MSA will reduce as well since there is an increased flowrate usage (Example 3.2). Also, regeneration cost is reduced since less MSA needs to be regenerated. So, a limit to the use of the available capacity of process MSAs is their mass exchange temperature.

The cooling/heating described above for the MSAs is achieved through incurring cooling/heating costs, but this has been demonstrated as not being capital intensive compared with the benefit that results in the annual capital/operating costs of the MENs.

4 PROBLEMS IN WHICH PROCESS ENERGY STREAMS ARE USED TO ENHANCE WATER USE OR MASS EXCHANGE

4.1 Introduction

This section builds on the findings in Section 3 but applies to CHAMENS problems in which we have both heat and mass exchange systems present, and they can interact with each other. The objective here is generally to use the process energy streams to enhance the water use or mass exchange.

4.2 Motivation

The motivation for this section stems from the opportunity available for integrating heat engine exhaust as well as a heat pump into a heat exchange process using the GCC. Here the heat engine exhaust instead of rejecting it to the environment is treated as a utility. The right positioning for a heat engine is entirely above or below the pinch. Above the pinch, heat is input to the boiler of the heat engine which produces power and can reject the remaining heat to the process so as to satisfy the hot utility demand of that process above the pinch. On the other hand, placing the heat engine entirely below the pinch helps to avoid a situation in which instead of sending the rejected heat from the process straight to cold utilities, it is first sent to the boiler of the heat engine and the remaining heat is then rejected to cold utilities, hence reducing the amount of cold utilities to be purchased. It is not profitable to position the heat engine across the pinch as this result in increments in both hot and cold utility requirements.

The heat pump on the other hand is best positioned across the pinch because this results in a reduction in both the hot and cold utilities needed simultaneously. This is possible due to the fact that heat is extracted from below the pinch (heat source) and rejected above the pinch (heat sink). All these are best investigated with the aid of the GCC in which the temperature levels at which the exhaust heat can be used is easily identified and so in all, aids utilities selection (Seider *et al.,* 2004).

A second motivation for the proposed approach in this section is the benefit obtained in shifting streams from below to above the pinch or vice versa as a result of process modification. The guiding principle in accomplishing this is the "plus-minus" principle (Smith 2005). Linnhoff et al. (1990) investigated the conflicts which could arise in carrying out optimisation between energy-capital trade-off, utility selection and process modification. The authors then went on to present techniques with which to establish a minimum total annual cost among such competing variables. This approach enables the designer to have a feel of the relevant topologies and hence be able to move from one topology to another which would be difficult to accomplish in a continuous mathematical optimisation environment. The method to be developed in this section is also a conceptual approach; it will as well give the designer a feel of the important topologies and go a step further by enabling the designer to easily set up a CHAMENS problem in a continuous mathematical optimisation environment so as to be able to handle more complex CHAMENS problems.

Applying the plus-minus principle in other to reduce utility targets results in an increase in capital costs of the heat exchangers because there is usually a reduction in temperature driving forces (Smith, 2005). This will not always be the case for the technique to be developed in this study for combining the synthesis of heat and mass exchange networks as would be demonstrated using some example problems.

Presented in Section three is the benefit of introducing heating/cooling on MENs, Section four on the hand examines the benefits on the HEN as well. Also, the previous section has investigated the interactions between process modifications and capital-MSA, there was no need for utility selection to be investigated since the CHAMENS problem is mass exchange networks dominated. But for a more complex situation in which there are streams which need to be stripped of their solutes and there also exists hot and cold streams which need to be heated/cooled, for the cost of such an operation to be minimised, there has to be a combination of the synthesis of the heat and mass exchangers. Optimising the combined system would require modifying the process conditions such as the mass exchange temperature/pressure, such modifications would result in a shift in the pinch position of the heat exchange network which will in turn alter the type of utility that could be used, hence the need to include utility selection in the optimisation.

4.3 Example Problems

4.3.1 MEN problem with four rich streams and one MSA, HEN with two hot streams and two cold streams (Example 4.1)

The potential interaction between HEN and MEN will be demonstrated in this section by integrating a MEN problem with a HEN problem. The MEN problem to be used is Example 3.1. in Section 3 while a HEN problem presented by Shenoy (1995) will be integrated with this MEN. The streams and cost data can be found in Appendix A. Two approaches of combination are going to be compared; the first is a situation in which the MSA streams of the mass exchange needing to be heated/cooled due to the need for stripping will simply be integrated into the heat exchange network in the traditional way (i.e. by treating the MSA streams as process streams) and the minimum utility and capital costs requirements would be determined using pinch technology. For the second approach, instead of integrating the MSA streams as process streams into the heat exchange network, one of them would be integrated as a hot or cold utility into the heat exchange network depending on the pinch temperature.

4.3.1.1 Integration by treating the MSA streams as HENS process stream

Presented on Table 4.1 below is the CHAMENS TAC of the use of the MSA stream at 30°C, 20°C and 10°C mass exchange temperatures respectively.

Table 4.1: Results for treating MSA streams as HENS process streams for different MSA stream temperatures

Options (^{o}C)	**MENS**	**HENS**				**CHAMENS TAC**
		ΔT_{min}	**Pinch Temp**	**AOC**	**ACC**	
30	*162.3*	*24*	*88*	*209.1*	*219.4*	*590.8*
20	*170.8*	*24*	*88*	*170.5*	*227.2*	*568.5*
10	*167.2*	*24*	*88*	*143.5*	*200.3*	*511*

Looking at Table 4.1 above, as the mass exchange temperature reduces the MENS TAC does not show much variation (the reason for this has been explained in Section three). Using a predetermined value of 24°C for the ΔT_{min}, it can be seen that the pinch temperature does not change for each of the mass exchange temperatures, but the AOC and ACC of the HEN reduces. This is because at lower mass exchange temperatures, lower flowrate of the MSA is needed to accomplish the separations; hence a reduced heat capacity flowrate in the heat exchange network which translates to a lower operating cost as well as smaller heat exchange areas.

4.3.1.2 Integration by treating the MSA stream as a HENS hot utility stream

For the HENS base case on Table 4.1, the pinch temperature is 88°C hence the MSA stream needing to be heated up from the respective mass exchange temperatures of choice to 100°C can be used as a cold utility in the heat exchange network, however the degree of the benefit of this depends on if the MSA streams which are mirror images of each other overlap the pinch or not i.e. if these streams both cross the pinch from above to below or vice versa.

Considering a situation in which MSA streams which are mirror images of one another are to be integrated into a low-temperature distillation heat exchange network problem. The MSA streams are to be heated from 30°C to 100°C and subsequently cooled back to 30°C. Analysing the operating and capital cost needs of the resulting heat exchange network problem using pinch technology with a 17°C as the $\Delta T_{\min}$ results in a network with a pinch at 7.5°C. The MSA stream would not cross the pinch in such a situation, since its supply temperature (for the cold stream) and target temperature (for the hot streams) are both 30°C. The heat duty of the hot MSA twin stream is 3,630.9 kW while the hot utility requirement of the network is 5880.9 kW, subtracting 3,630.9 kW from 5880.9 kW gives 2250 kW; this is still the same hot utility need of the case of using the MSA as a process stream. The reason for this is; the two streams lie entirely on one side of the pinch (above), so whether one of these MSA streams is used as a utility or just integrated normally as a process stream into the HENS base problem would not really make any difference in utility requirement.

However for situations in which the MSA streams do cross the pinch (using the same HENS problem from Shenoy, 1995) there would be a reduction in the utility need of the HENS problem when one of the MSA streams is integrated into the HENS base problem as a utility. This is illustrated on Table 4.2 below.

Table 4.2: Results for treating MSA streams as HENS utility streams for different MSA stream temperatures

Options (°C)	MENS	HENS				CHAMENS
		ΔT_{min}	Pinch Temp	AOC	ACC	
30	*162.3*	*24*	*113*	*96*	*168.4*	*426.7*
20	*170.8*	*24*	*113*	*99.3*	*166.1*	*436.2*
10	*167.2*	*24*	*113*	*109*	*158*	*434.2*

Though there are hardly any differences in the CHAMENS TAC costs between the mass exchange temperatures presented on Table 4.2 above, however these costs are about 16.5% lower than the least cost on Table 4.1. The AOC and ACC of the HENS are significantly lower on Table 4.2 compared with Table 4.1. Note that a predetermined value of 24°C is still being used for the ΔT_{min}. The heat to be rejected to cold utility is the same in each of the mass exchange temperatures, 665 kW, however the HENS AOC of the 10°C mass exchange temperature is the highest, this is because cold utility at a temperature as low as 10°C (CU_3 on Table A.11 in the Appendix A) is more expensive at those at higher temperatures. This is also the reason for which that of 20°C (CU_2 on Table A.11 in Appendix A) is higher than that of 30°C.

Note that the costs presented on Table 4.2 are only possible if the MSA stream to be used will itself be satisfied as far as its heat demand is concerned, so each of these options still has to be investigated, their respective GCCs will be used to examine the best positioning for the concerned MSA.

For two reasons the results presented on Table 4.2 are not the best, some optimisation of the ΔT_{min} still has to be carried out, this is because of the traditional reason of supertargeting and also because the best positioning of the MSA to be used as a utility in the HEN base case has to be established using the GCC. The best positioning for the MSA is such that its own heat demand has to be fulfilled because this also minimises the TAC of the MENS since its heat capacity flowrate is the optimum flow needed by the mass exchangers. Also a good positioning needs to be established for the said MSA using the HENS base case GCC such that much of the utility needs of the HENS base case is satisfied in the best possible and cheapest way.

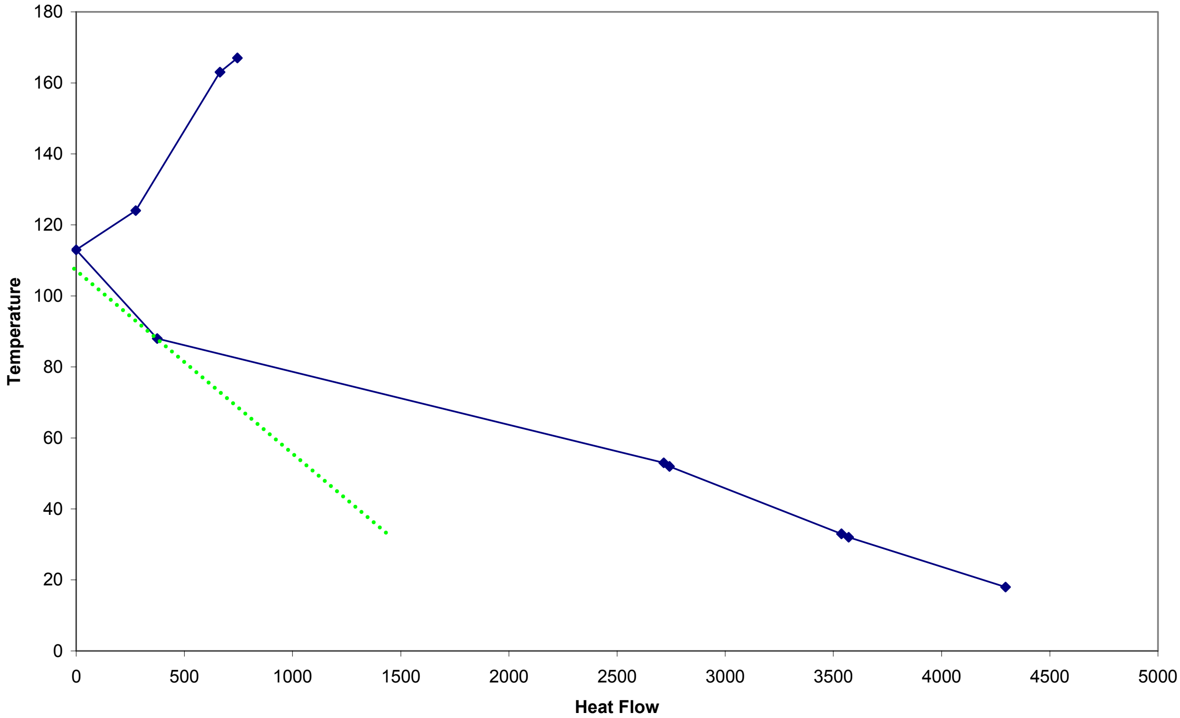

Figure 4.1: Positioning of an MSA on the Thermal Grand Composite Curve – 1st possibility.

The MSA positioning in Figure 4.1 above only satisfies the heat requirements of 5.102 kg/s of the MSA for it to absorb mass at 30°C and be stripped at 100°C. What this implies is that the remaining 7.248 kg/s has to be taken care of separately outside the HENS base case but this will not be optimal hence this positioning is not good enough. Also 2,795.9 kW of cold utility will still have to be purchased, this will produce a cumbersome layout.

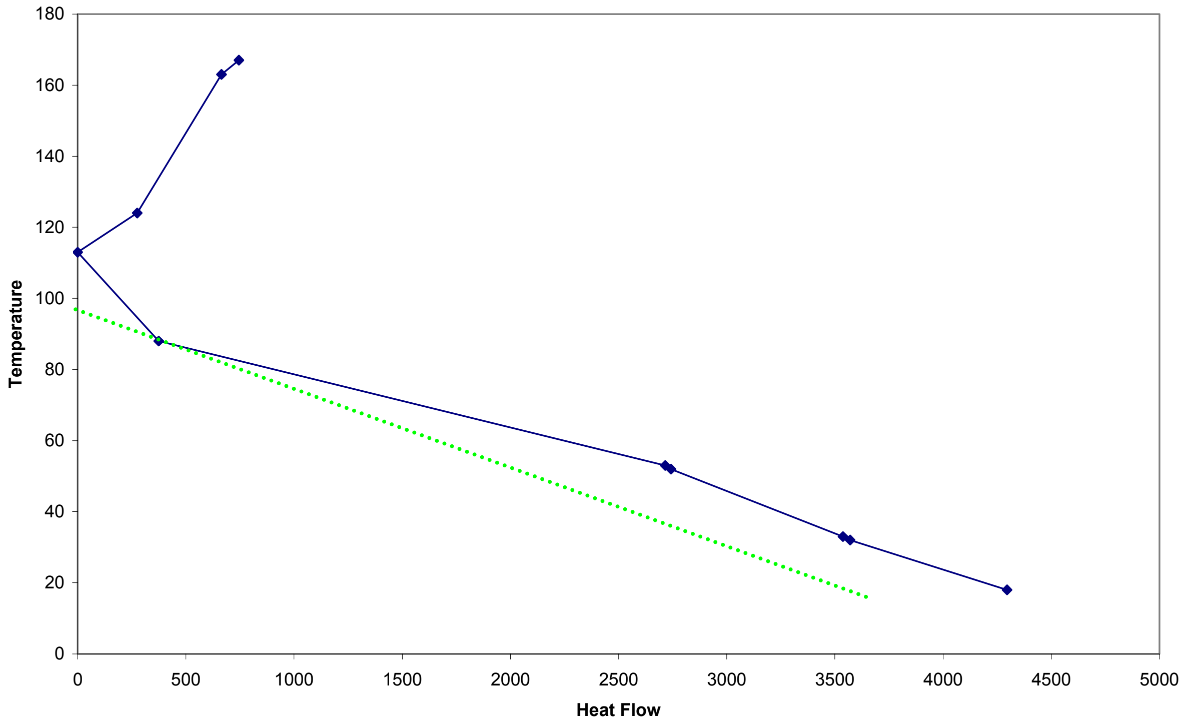

Figure 4.2: Positioning of an MSA on the Thermal Grand Composite Curve – 2nd possibility.

The MSA positioning in figure 4.2 above will make for the MSA to be used as an absorbent at 30°C but it will not be taken to the stripping temperature of 100°C but instead 96°C, hence reaching the target temperature of 100°C will have to be done outside of the HENS base case heat exchange network, this will also produce a cumbersome plant layout. Also 872.48 kW of cold utility would still have to be purchased so as to satisfy the cold utility demand of the HENS base case.

The two positioning schemes just examined shows that there are so many ways in which the MSA can be positioned so as to help in reducing the cold utility demand of the HENS base problem but this is dependent on the shape of the HENS GCC, hence the need to still optimise the $\Delta T_{\min}$ as this will change the pinch location which will allow for some other positioning possibilities for the MSA such that much (if not all) of its heat demand would be satisfied in the cheapest way possible.

Note that by integrating the twin MSAs into the HENS base problem in the traditional way of treating them process streams and carrying out a supertargeting results in a HENS TAC of

366,200 $/yr, adding the MENS cost to this gives a CHAMENS TAC of 528,513 $/yr. This is lower than the results presented on Table 4.1.

A thorough optimisation was carried out and coincidentally the optimal ΔT_{min} also produces a pinch location, 5°C, which allows the MSA to be used at a mass exchange temperature of 30°C and also be taken to the target temperature of 100°C for stripping. This is illustrated below.

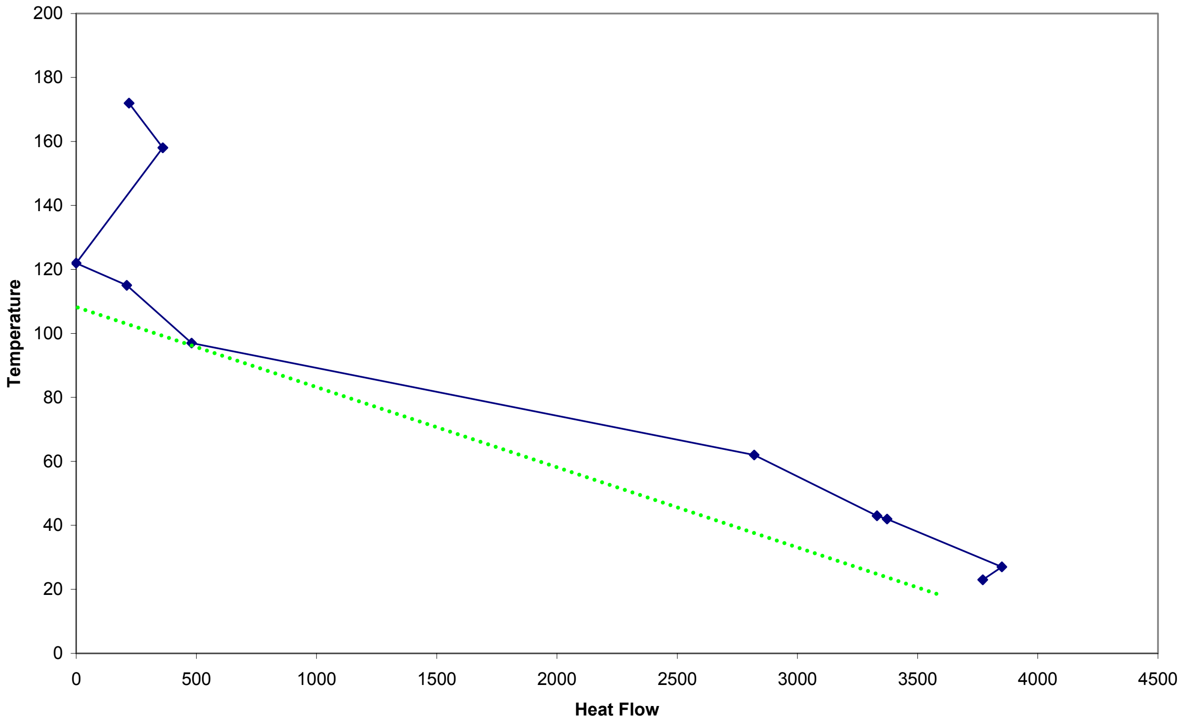

Figure 4.3: Positioning of an MSA on the Thermal Grand Composite Curve – optimal position.

The HENS TAC for the above positioning scheme is 227,456 $/yr, adding this to the MENS TAC results in a CHAMENS TAC of 389,756 $/yr.

4.4 Conclusions

Two approaches of combining the synthesis of heat and mass exchanger networks have been considered in Example problem 4.1. It can be deduced from the second technique of this example problem that combined heat and mass exchange network problems are highly interactive and that there exists opportunities for saving costs. This problem through the sequential synthesis approach has revealed the many topologies which exist in the combined network and also gives the designer a feel of how each of these topologies contribute to the CHAMENS total annual cost.

It has been demonstrated that the heat exchange grand composite curve could be used as a framework for optimising the combined system since the best positioning of the MSA streams as utility in the heat exchange operation could easily be identified on the grand composite curve.

Also, it is seen that combining the synthesis of heat and mass exchangers is beneficial not only to the mass exchanger network, but to the heat exchanger network too. This is because the use of the MSA as a utility in the heat exchanger network helps in reducing the utility need of the heat exchange operation, also the capital cost of the HEN is reduced because the MSA streams are operating at a reduced heat capacity flowrate.

5 SOFTWARE DEVELOPMENT

5.1 Introduction

We have written a software package that will analyse both heat and mass exchange networks independently. We have also added the capability to analyse water pinch networks.

The main software package was developed as a master's degree project by Khaya Ndwandwe (Ndwandwe, 2003), and the water pinch addition was done by Prashant Bansal (Bansal, 2004) as a research internship.

The User Manual for the original package is given in Appendix B, while the addition of the water pinch feature is discussed in Section 5.3 below. Khaya Ndwandwe's master's thesis is available on request. Section 5.3 is adapted from a report by Prashnat Bansal, the full version of which is also available on request.

5.2 Software for the Analysis of Heat and Mass Exchanger Networks

As it stands this computer package can be used for analysis of heat and mass exchange systems on their own, in order to establish which system dominates.

It is also useful for iterative calculations to establish the interaction between the heat and mass exchange systems. This is based on the presumption that comparing targets provides a valid determination of what could be achieved in the design of such systems.

This approach is justified on the basis of experience that has shown that it is always possible to achieve the utility targets (whether energy utilities or MSA utilities), and that capital costs targets for both energy and mass exchange systems can be approached to within less than 10%.

A fundamentally different approach is being developed for the situations in which there is interaction between the water-using (or mass transfer) and energy-using (or energy transfer) systems. This requires a more complex methodology in which conceptual Pinch Technology techniques are combined with mathematical programming optimisation techniques, such as Mixed-Integer Non-Linear Programming (MINLP).

5.3 Extension for Water Pinch Analysis

5.3.1 Overview

This section describes the development a user friendly program for the application of Pinch Technology approach for the problem of minimization of water consumption in process industries. The program has been incorporated as an extension to the software developed for heat and mass exchange network synthesis described in Section 5.2. The program being developed makes use of an Excel spreadsheet for data input and output of results. The program is written in Visual Basic for Applications (VBA) which is an integrated part of the Excel software.

The program is flexible, wherever possible, to allow the user to choose between different available options. This helps in analysing the problems in different aspects and choosing the optimum solution. The graphical user interface is described and the program structure of various targetings is also described with the help of flow charts

There are many packages available in the area of heat exchange network synthesis; however, this is a unique package consisting of all the three applications of Pinch Technology, Heat exchange networks, Mass exchange networks and Water Pinch Analysis.

5.3.2 Introduction to Water Pinch analysis

Water is used in most Chemical process industries for a wide range of applications. In process industries water is largely used as a solvent for removing contaminants from other process streams. There can be many processes which require water. The processes might have different requirements for water and would produce waste water streams with varying concentrations of contaminants. An integrated design can be developed in which water streams are transferred between processes to minimize overall water consumption. Reducing wastewater affects both effluent treatment and freshwater costs (Wang, Smith, 1994). The design of highly integrated processes can be achieved by recognising that such processes require networks for the distribution of resources such as heat and mass that are both consumed and produced within the process (Towler, 1996). A very useful tool for developing integrated process design is Pinch Technology. Pinch Technology has already been successfully applied to Heat and Mass exchange process. The present author is interested in using Pinch Technology for minimising overall water consumption in a chemical process plant. This approach for optimising overall water consumption is known as Water Pinch analysis.

Water Pinch analysis is based on an extension of pinch analysis techniques for heat exchange network design processes. It assumes each water-using operation as being described by the mass transfer of a certain contaminant from the process itself to the water stream. By specifying the maximum allowable inlet and outlet contaminant concentrations for each operation, a limiting profile can be constructed. (Figure 5.1)

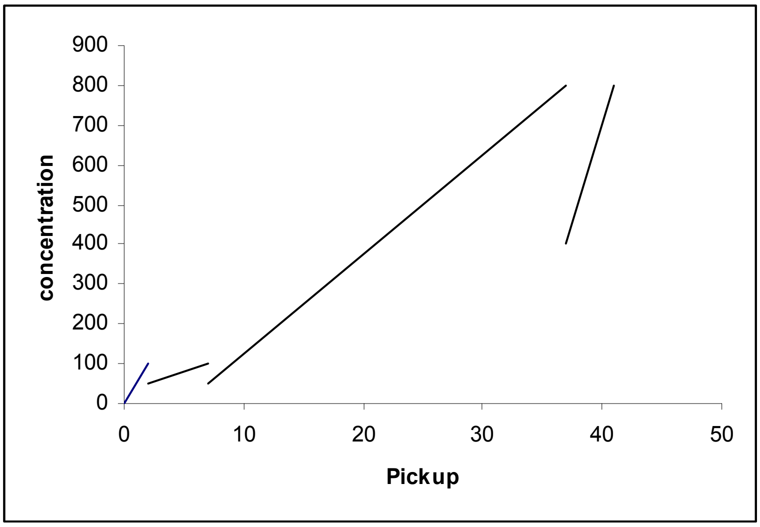

Figure 5.1: Different processes with concentration limits

These are combined to form a limiting composite curve (Figure 5.2), against which a water supply line can be matched. The inverse of the slope of this line gives the target for the minimum fresh water and wastewater. The point that limits the slope of the line has been termed the water pinch point (Figure 5.3).

This is basic targeting for minimising water requirement. Further reduction in water requirement can be achieved by using processes of Regeneration and Recycling, either independently or simultaneously. Wastewater can be regenerated by partial treatment to remove the contaminants, which would otherwise prevent its reuse, and then reused in other operations (Wang, Smith, 1994). Water can also be recycled. But this has its own restrictions like in some cases recycling between processes in not feasible due to build up of contaminants.

The methodology can be considered to be based on mass transfer model. Water Pinch analysis can be considered as a special type of mass exchange network synthesis (MENS) problem in that only water is used as an mass separating agent or MSA (Hallale, Fraser, 1998).

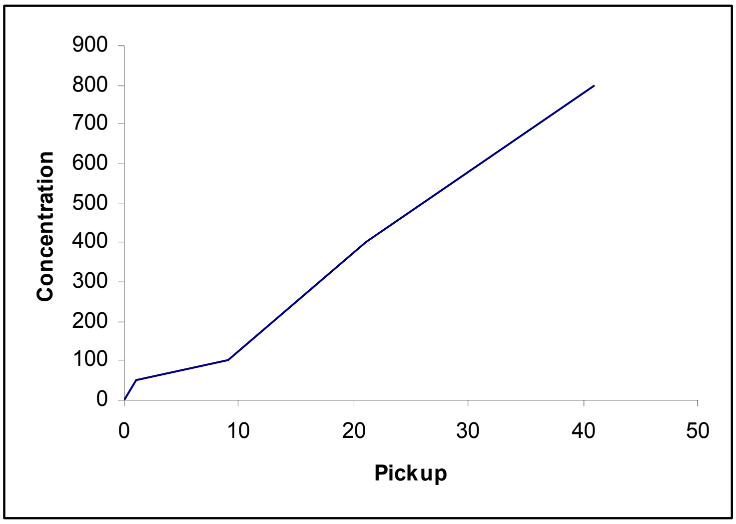

Figure 5.2: Composite curve for different processes

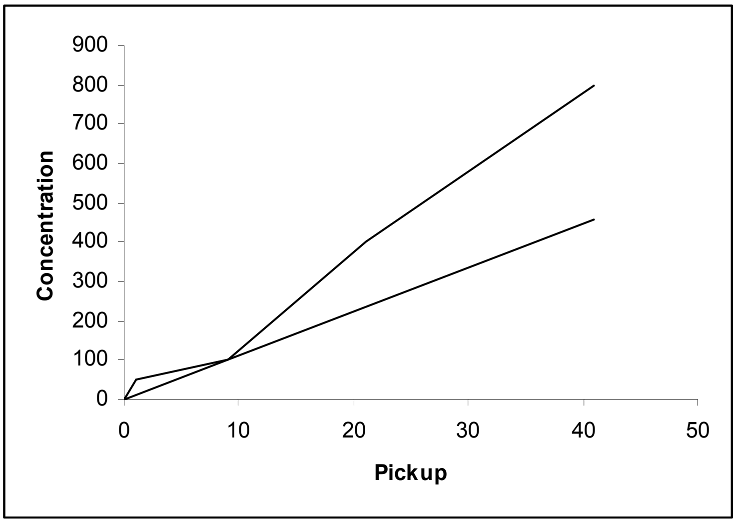

Figure 5.3: Minimum water target line

5.3.3 Approach

The program uses targeting for calculating minimum water flow rate using basic targeting as well as using regeneration and recycling of water. The program also takes care of water insufficiency problems above the pinch point concentration. Section 5.3.5 has been devoted to the problems encountered and approach used in minimising water flow rate above the pinch point concentration.

The targeting in the program are basic targeting, Regeneration of water below and, if required, above pinch point and finally Recycle and/or Regeneration of water below and, if required, above pinch point. There are all possible options available to the user for above pinch regeneration and recycle targeting while running the program. The approaches used for water insufficiency problem for part of processes above pinch have been described in detail with the help of charts.

5.3.4 The Program

This section presents the development of the program for Water Pinch analysis. The script used is Visual Basic for Applications. The Excel spreadsheets are used for input and output of the data to the program. The program is developed in a way to allow the user to be in full control of the analysis. Options have been provided wherever required to allow the analysis of different aspects of the problem. The development of program has been described as step by step process beginning from the structure of the program to the linkages in the major procedures of the program.

5.3.4.1 Graphical User Interface (GUI)

The program originally designed for Heat and Mass exchange networks has an inbuilt graphical user interface and a toolbar supporting all major links to the program functions. The links for water pinch section have been fused with the original menu and toolbar. This has been illustrated using the flow chart in Figure 5.4. To begin the end user will click the *start running the program* button at the beginning resulting in appearance of the main control form asking to choose between *Heat Exchange Network Synthesis, Mass Exchange Network Synthesis* and *Water Pinch Analysis*. When *Water Pinch Analysis* is clicked another form appears to choose to go back to *main control* or proceed to *minimum water flow rate*. Clicking *minimum water flow rate* leads to the input worksheet for Water Pinch Analysis.

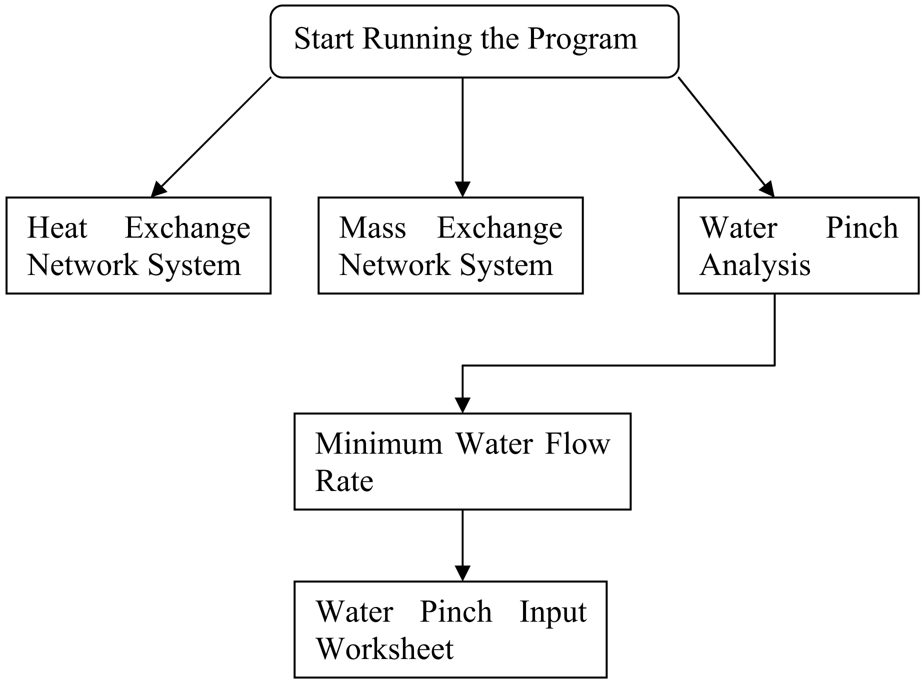

Figure 5.4: The user interface sequence to select between different functions of the program.

In addition to the above user interface, the toolbar menu for Water Pinch Analysis is also added in the existing toolbar. However, it must be noted that the water pinch analysis section of the program has been separately developed and merged with the existing package for HENS and MENS.

5.3.4.2 Water Pinch Analysis

The following types of targeting are analysed: Basic Targeting, Regeneration of water below & above pinch point concentration and Recycle and Regeneration of water also below and above pinch point concentration. The program structure for whole of the program has been concisely displayed using a flow chart (Figure 5.5).

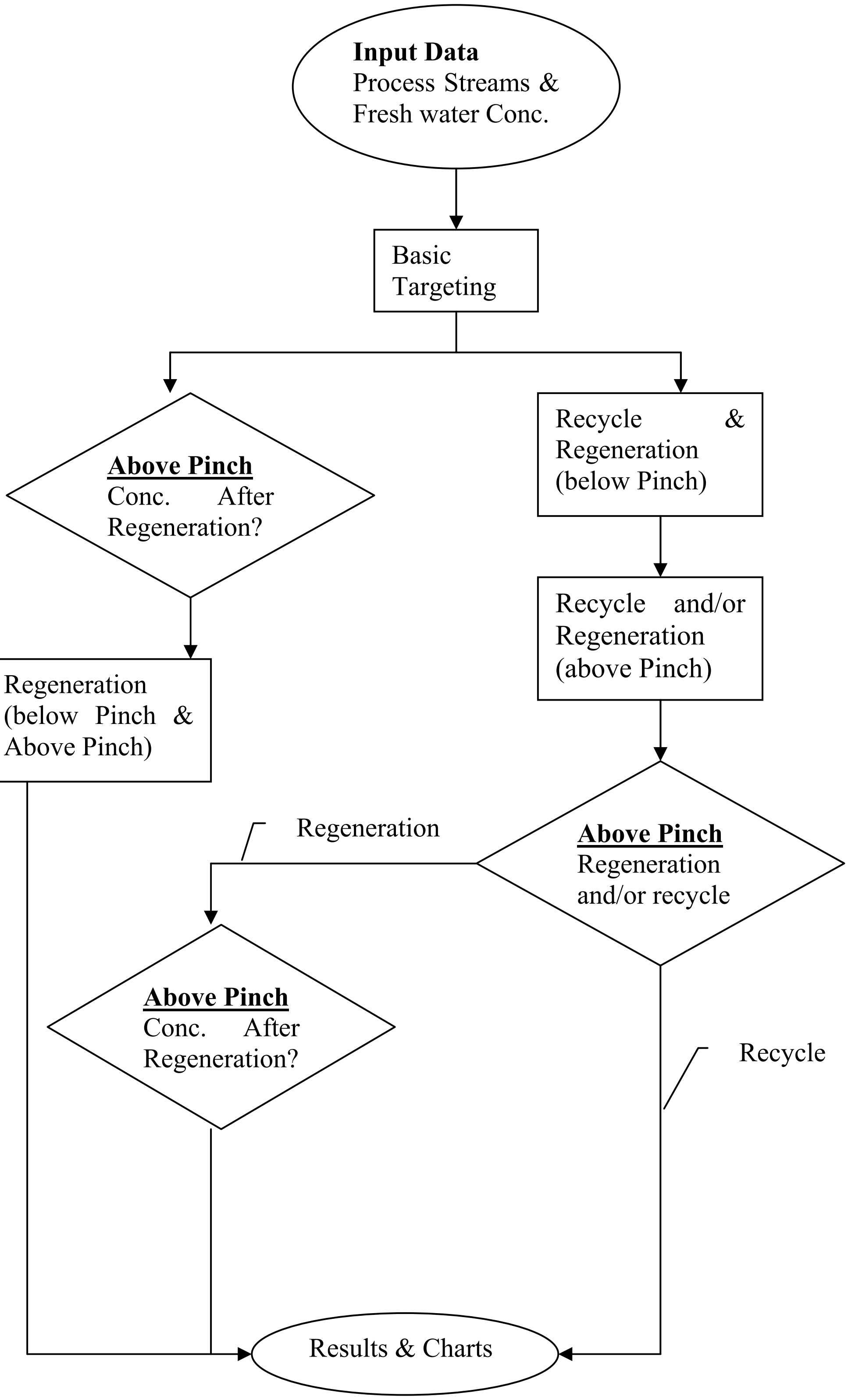

Figure 5.5: The Program structure in the form of a flow chart incorporating linkage of the major procedures to each other.

5.3.4.2.1 Program Structure for Basic Targeting

Each independent section of the program consists of a major procedure which in turn comprises several minor procedures in a definite order. Each minor procedure accomplishes a specific task.

The command button provided for minimum water flow rate calls the major procedure *waterpinch*, which in itself calls several minor procedures in a specified order.

The procedure for basic targeting uses the algorithm for flow rate targeting developed by Wang and Smith (1994). This procedure is similar to the Problem Table Algorithm used for Heat Exchanger Network Synthesis.

The user must input the process stream information in the form of mass load carried by each stream and maximum inlet and outlet concentration of the water for each process stream. Also, the user must furnish the fresh water concentration. Clicking the command button for minimum water flow rate leads to a separate output sheet for display of results. The command buttons for the chart have been provided on both input and output worksheets.

5.3.4.2.2 Program Structure for Regeneration of water

As stated in the previous section, this targeting also consists of a major procedure, *waterregen,* which in itself consists of several minor procedures. The concentration after regeneration for below pinch operation must be entered, otherwise the program will ask the user to enter a value.

In regeneration targeting, water is allowed to reach the pinch concentration, and then regenerated completely to the specified concentration. The flow rate thus obtained is the minimum flow rate required.

If regenerated water line intersects the composite curve above the pinch point, it suggests that the minimum flow rate obtained below the pinch is not sufficient for above pinch processes. Then, water requires further single or multiple regenerations above the pinch point. The approaches used in solving these problems have been described in detail in the next chapter of this report.

5.3.4.2.3 Program Structure for Recycle and/or Regeneration of water

Unlike the program for regeneration, in which regeneration below the pinch and above the pinch, if required, are analysed through a single command button, the programs for recycle and/or regeneration below the pinch and above the pinch, if required, can be analysed separately through different command buttons.

In recycle and regeneration targeting, water is allowed to go to the pinch concentration following the initial slope of the composite curve, which is the inverse of the minimum flow rate required. When the water reaches the pinch concentration, it is regenerated to the specified concentration. The line between the regeneration point and the pinch point gives the total flow after regeneration. The difference between this and the freshwater flow is the amount of water that needs to be recycled in addition to the minimum water required.

In some cases, recycle of water is not required and water can be regenerated to some higher concentration to maintain the same flow rate after regeneration. It must be noted that in this case the concentration after regeneration is not the same as specified by the user in the input worksheet.

If the minimum flow rate water line from the pinch point is not sufficient for the above pinch part of the composite curve, then recycle and/or regeneration of water are required above the pinch. The approaches used to solve this problem will be discussed in detail in the next chapter.

5.3.4.3 Charts & Input Data Management

The source data for all the charts gets saved in Excel, but to produce the charts, user must request them. The command buttons for all the charts are provided in both input and output worksheets. The charts are independent of each other. During the production of every chart, the source data for that particular charts gets saved in a different place in the worksheet, so any change in the original source data does not affect the already produced chart. However, there is a limit to the number of each type of chart the user can produce. User will be notified when the limit will be reached, and then the cache history of that particular chart needs to be cleared from the link provided in the *chart* menu of the toolbar.

The feature of managing the input data has been added to all the three parts of the package *HENS, MENS* and *Water Pinch Analysis*. A *Save Data* command button has been provided at the top left corner of every input worksheet of the package. This button links to a program, different for every input worksheet, which saves the input data of that specific input worksheet. A name must be provided for each data set. The stored data sets can be retrieved or deleted by the *Load Data* command button which is provided right below the *Save Data* button. The data sets are saved on a worksheet of the package itself, so they are carried with the package. The clicking of the *Load Data* command button results in appearance of a form which lists all the data sets stored for that particular input worksheet. Any of the listed data sets can be loaded or deleted using respective command buttons provided on the form. All the previous input, output or calculated data is removed, with permission from user, from the worksheets when a new data set from the stored sets is loaded. Before manually entering a new data set, the *Clear All* button on the top left corner must be clicked.

There is also a provision of attaching comments with each saved data set which the user can use for storing any characteristic results observed while analysing that data set for reference in future. The attached comments appear on the *Load Data* form when the respective data sets are selected from the list.

5.3.5 Problems above the Pinch Point

When the water is regenerated or recycled, its flow rate no longer remains same as that obtained by basic targeting. So, when the water line crosses the pinch point it may cross the composite curve at the pinch point or at some point above the pinch point. In any of the above situations, the minimum water flow rate which was sufficient for the part of the process below the pinch point no longer remains sufficient for the part of the process above the pinch. In that case, water needs to be again recycled or regenerated or both above the pinch point. This chapter describes the approaches applied for such cases. First the case of regeneration is considered in which the flow rate of water remains the same during all the regeneration processes and then recycle and/or regeneration is described where the flow rate may change.

5.3.5.1 Regeneration above the Pinch Point

If the water line crosses the composite curve at some point above the pinch point, then at that point water needs to be regenerated. If, after one regeneration, the water line again intersects the composite curve, then the flow rate is still not sufficient for the remaining part of the process. That means that the water needs to be regenerated again at the point of next intersection. In this way water is recursively regenerated till there are no more intersections with the composite curve or the water is sufficient for the remaining process. The concentration after regeneration can be the *Pinch concentration* or the *concentration of the previous regeneration point* or the *previous point of the composite curve*. Each of these cases has been illustrated with the help of charts in Figures 5.6 – 5.9. Figure 5.6 illustrates the regeneration curve when no regeneration is done above the pinch point.

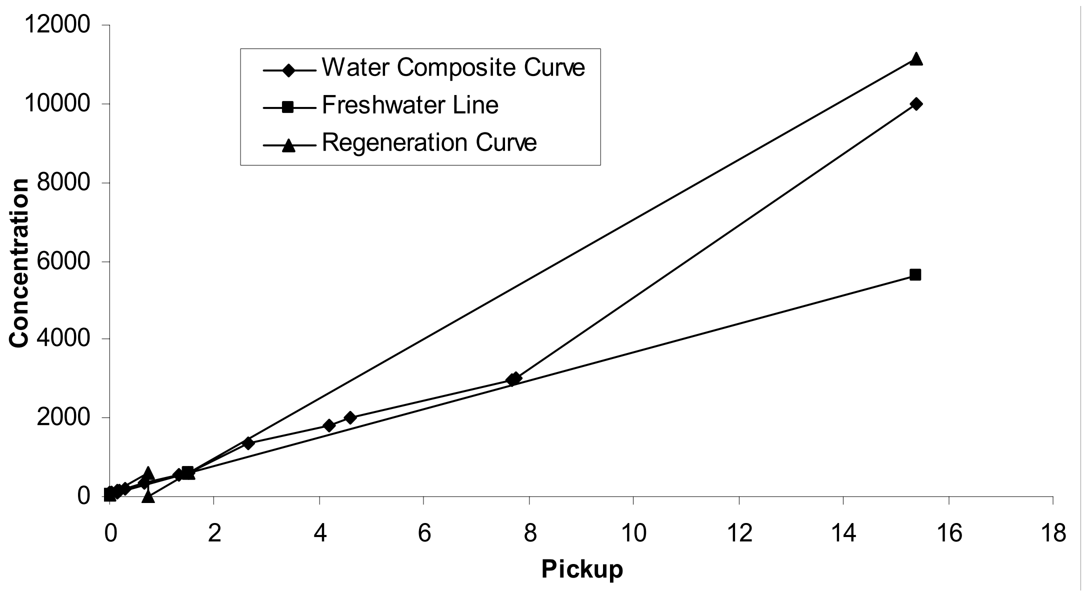

Figure 5.6: Regeneration Curve with no regeneration above pinch point

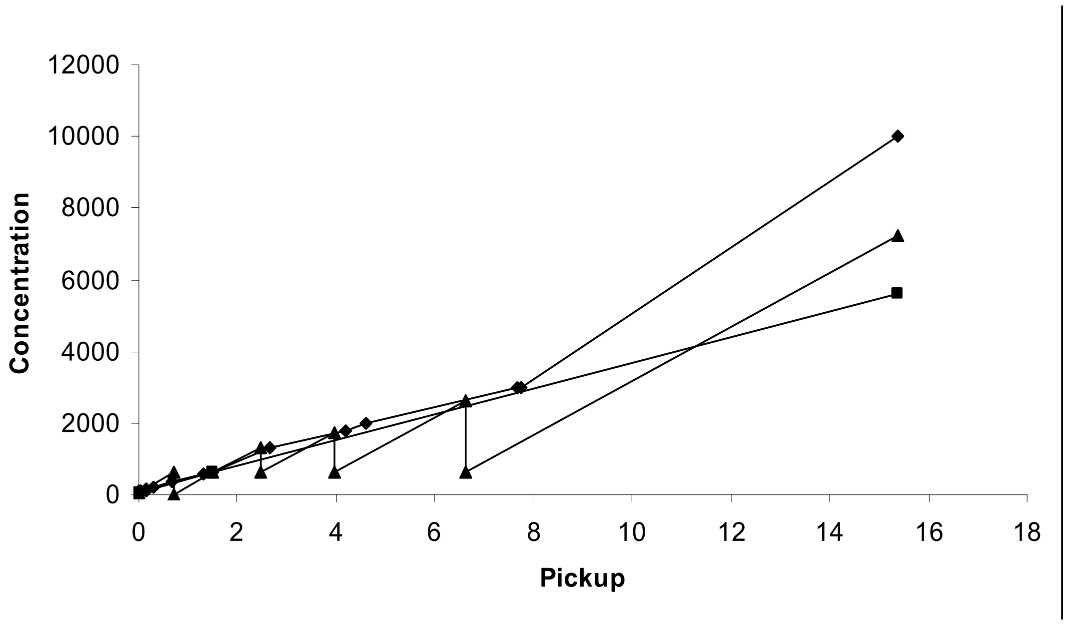

Figure 5.7: Regeneration above Pinch with Conc. after regeneration as Pinch Conc.

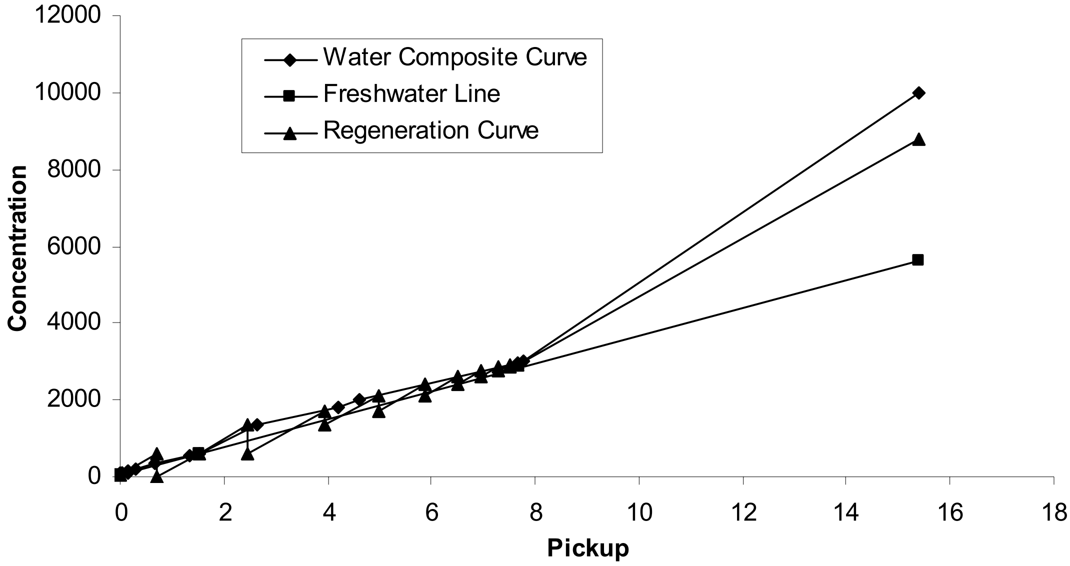

Figure 5.8: Regeneration above Pinch with Conc. after regeneration as Conc. of previous regeneration point

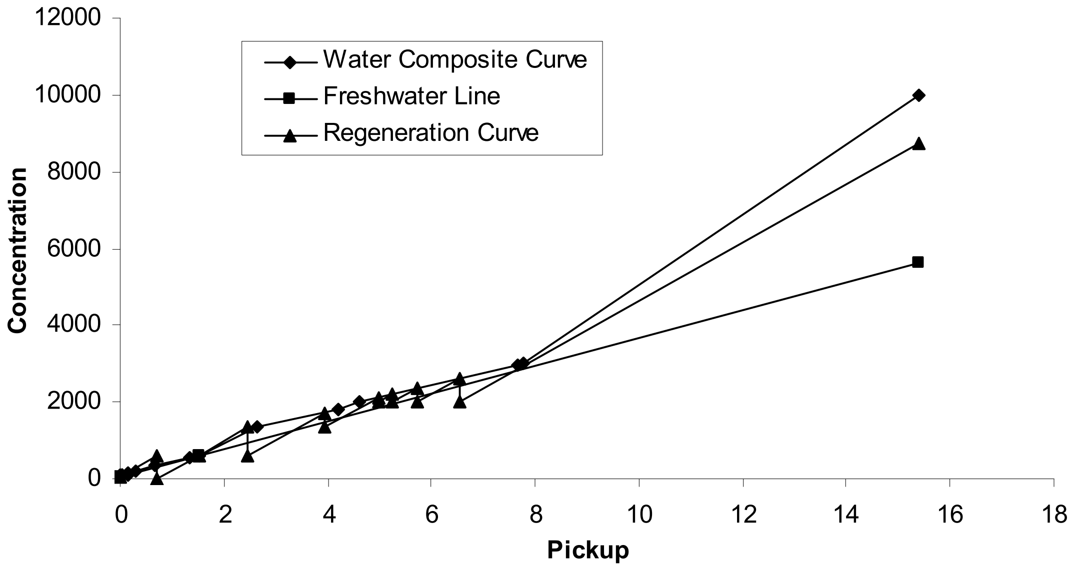

Figure 5.9: Regeneration above Pinch with Conc. after regeneration as Conc. of previous point of composite curve

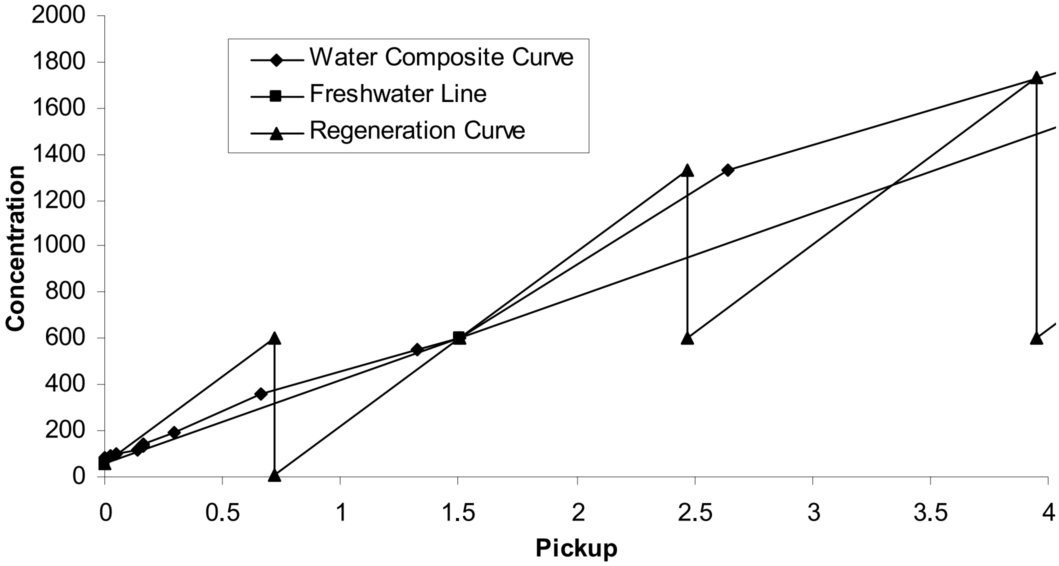

Figure 5.10: Regeneration of water above the pinch just after pinch (Magnified View)

The number of regenerations required and the amount of regeneration per regeneration vary with the different values chosen for concentration after regeneration. It can be seen that the least numbers of regenerations are required for conc. after regeneration as pinch concentration but at the same time the amount of regeneration per regeneration are largest in that case. These vary with different input data sets.

In the data set used for the preparation of the charts, the regeneration water line crosses the composite curve at the pinch point. In this case, water is allowed to reach the concentration of the next point on the composite curve after the pinch point before regenerating it to the pinch concentration (Figure 3.10)

5.3.5.2 Recycle and/or Regeneration above the Pinch Point

When the water is recycled below the pinch the flow rate of water no longer remains the same as the initial minimum flow rate. So, when the water line crosses the pinch point, it may intersect the composite curve at any point above the pinch point or it may cross the composite curve at the pinch point. In either case, the initial minimum flow rate of water is insufficient for part of the process above the pinch point. So, water needs to be again recycled and/or regenerated. The program offers flexibility to the user in terms of choosing among *Only Regenerations* or *Only Recycles* or both *Regeneration and Recycle* above the pinch point.

The *Only regeneration* case above the pinch is similar to as described in the previous section of regeneration above the pinch point. The other two case have been illustrated with the help of charts in Figures 5.9 – 5.10.

In the O*nly Recycle* case (Figure 5.11), water is recycled only once above pinch. This is done by taking the minimum slope line from the pinch point which just touches the composite curve at a point above the pinch point. In the case of both *Regeneration and Recycle* (Figure 5.12) water is regenerated once and recycled once, if required after regeneration. The concentration after regeneration can be chosen between the *pinch concentration* and *conc. of previous point on composite curve*. The option of concentration of previous regeneration point is not available for this case as there is only single regeneration. Please note that there is no freshwater line in the curves used for illustration for these cases for better clarity.

In the case where the water line crosses the composite curve at the pinch point, only recycling of water is allowed because in this case, if water is regenerated as before at the next point on the composite curve, that would be the case similar to the *Regeneration and Recycle* or *Only Regeneration* case discussed above in this section.

The option left is of *Only Recycle*. So, there is no regeneration in this case.

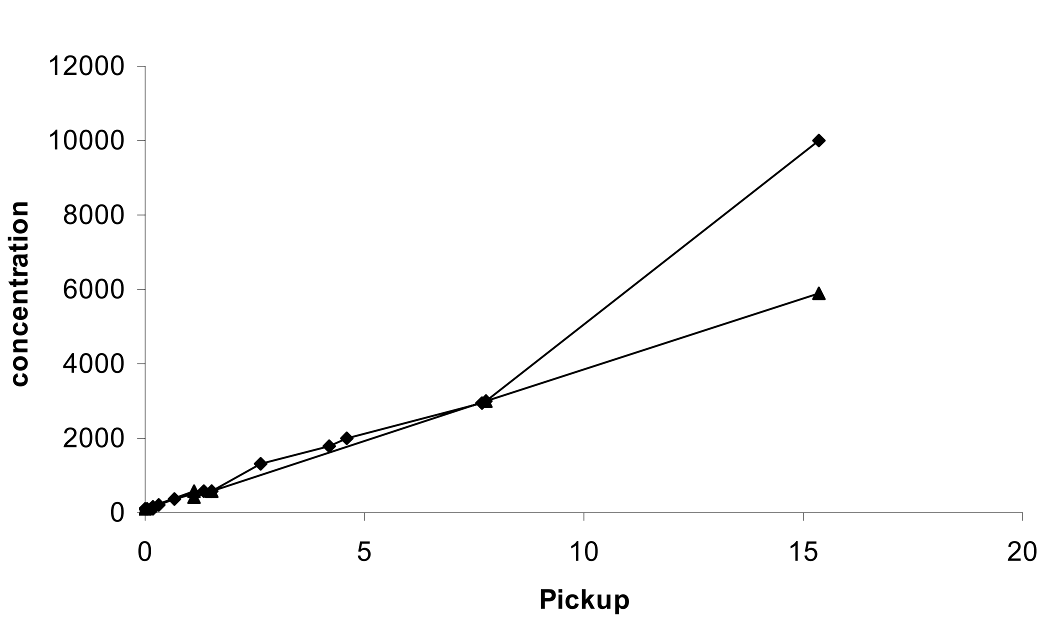

Figure 5.11: Only Recycle of water above the Pinch Point

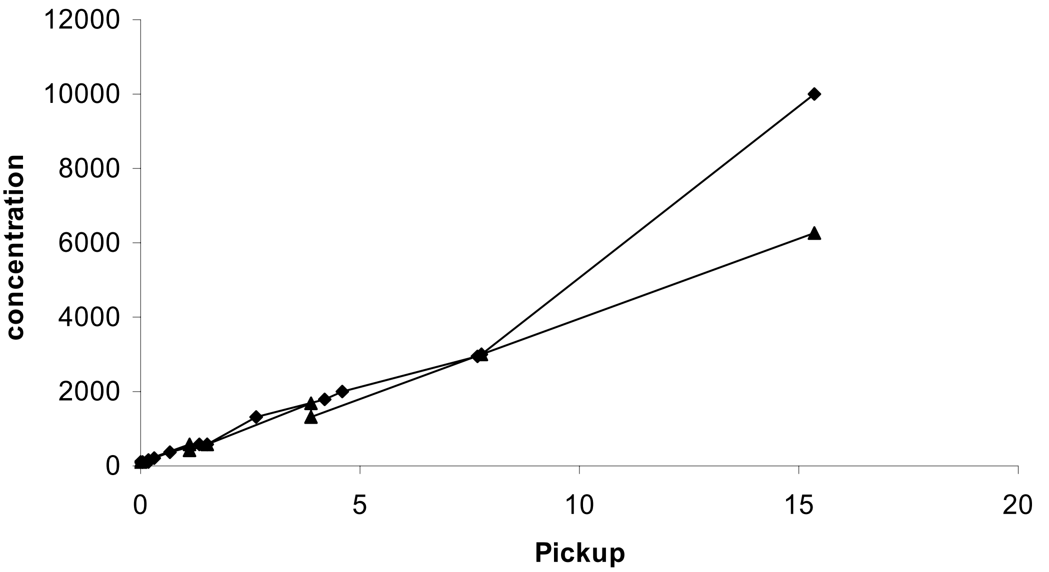

Figure 5.12: Regeneration and Recycle of water the above Pinch Point

5.3.6 Conclusions

The objective of the project was to develop a user friendly program for water pinch analysis. The focus is on targeting. The program offers flexibility, wherever possible, by providing the decision making for the proceeding direction to the user. The program is a valuable tool that can be used to analyse different aspects of the solution of the problem.

As said earlier, this package contains all the three applications of pinch technology HENS, MENS and Water Pinch Analysis, with the first two developed by Mr. Khaya Ndwandwe. The addition of the data management system within the program makes data sets easier to maintain.

The program also incorporates the techniques developed during the project for solving the problems of regeneration and/or recycle of water above the pinch point. These problems were encountered during the development of the program while analyzing some specific data sets. These techniques have been discussed in detail in the previous section. This emphasis of the program on the solution to the problem of insufficiency of water above the pinch point makes the program unique among available similar packages. The project is open, new additions can be made to program to improve it. Currently, the program focuses only on targeting; network design features can be added to the program in the future.

6 CONCLUSIONS

The contribution of the UCT team to this project has been to develop a methodology and tools for the analysis and design of systems in which the heat and mass exchanger networks are not independent, but interact with each other, with a view to being able to apply these techniques to systems in water conservation could be achieved through energy conservation. Considerable progress has been made towards the objective of having a methodology and tools to handle all conceivable situations in which both heat transfer and mass transfer occur, but there remain areas that still need to be resolved.

6.1 Design Approaches Developed

In this study two basically different types of systems have been identified. In the first type of system either the heat or mass exchange system may be used to enhance the performance of the other system. In this case the system which is optimised by the other one is termed the foundation problem.

The most common example of this type is a water-using (or mass exchange) operation that can be improved by use of heat exchange, with the heat exchange being supplied by hot and cold utilities. Here the water-using (or mass transfer) system is the foundation problem, and its performance would be enhanced by changing the temperatures of the water-using streams (or the mass separating agents). Something which would be less common would be a heat exchange system which is improved by means of utility water or utility mass separating agents.

In the second type of system has both a water-using (or mass transfer) system as well as hot and cold process streams (the heat exchange system), and there is interaction between them, so neither can be used as the foundation problem.

It should be noted that most of the example problems that have been tackled in this project have been problems in which water was the mass separating agent used for removal of contaminants (Examples 3.1, 3.3 and 4.1). Furthermore, the optimisation carried out in the examples was to minimise total annual cost rather than water usage. However, exactly the same approach can be used with modifications to the objective function to maximise water conservation, energy conservation or any desired combination of the two. In principle, the 'cost' function can be defined to account for factors other than simple financial costs, for example environmental costs, where these can be satisfactorily quantified.

6.1.1 Problems in which energy utilities are used to enhance water use or mass exchange

Based on the three different CHAMENS problems considered in section 3, a synthesis algorithm for achieving optimal designs can be described as follows:

6.1.1.1 MENS problems with one MSA

- Identify the most dominant variable and discretise (each being a topology), in this case, the mass exchange temperature is the most dominant of the variables and is not influenced by other variables. The search for the optimum is carried out within each of these temperature options (topologies) with the supply temperature for the only available MSA being the first topology while the lowest working temperature for the MSA is the last.
- Within each topology, the optimum ε is identified and for each optimum ε the $\Delta T_{\min}$ is optimized. The best $\Delta T_{\min}$ is noted so that it can then be compared with the best $\Delta T_{\min}$ from other ε. The least combination in terms of cost of ε - $\Delta T_{\min}$ is taken as the best for the concerned topology.
- The second step is repeated for all the temperature topologies and the least ε - $\Delta T_{\min}$ combination is taken as the optimum solution.

Note however that this is beneficial in situations in which the HENS cost is not dominant. However this approach is still good in that it helps to identify the dominant network in terms of costs between the HENS and MENS since a thorough search is carried out at all the variables that affect the costs of each of these networks so that the least combination of HENS and MENS can be easily compared with the MENS base problem (i.e. at the supply conditions with no option of introducing HENS).

6.1.1.2 MENS problems with non-overlapping MSAs

Each of the MSAs in this type of MENS problem is restricted to each side of the pinch, the process MSA being above while the external is below. The procedure highlighted above for MENS problems with one MSA is followed for each side of the pinch division here as well.

But for cases in which the process MSA at a low mass exchange temperature is not able to take away alone the entire mass load, the following steps should be followed.

- Identify temperature topologies for both process and external MSAs, i.e. above and below the pinch.
- Carry out a one-one mapping of the two temperature topologies at each mass exchange temperature and then follow the procedure stated for the MENS problem with just one MSA.

6.1.1.3 MENS problems with overlapping MSAs

The procedure for the MENS problems with non-overlapping MSAs is also followed here, the difference lies in the fact that the mapping of the temperature topologies would result in a matrix which will be somewhat difficult to handle manually since within each topology there still exists variables which need to be optimized.

6.1.2 Problems in which energy utilities are used to enhance water use or mass exchange

Two approaches of combining the synthesis of heat and mass exchanger networks have been considered in Example problem 4.1. It can be deduced from the second technique of this example problem that combined heat and mass exchange network problems are highly interactive and that there exists opportunities for saving costs. This problem through the sequential synthesis approach has revealed the many topologies which exist in the combined network and also gives the designer a feel of how each of these topologies contribute to the CHAMENS total annual cost.

It has been demonstrated that the heat exchange grand composite curve could be used as a framework for optimising the combined system since the best positioning of the MSA streams as utility in the heat exchange operation could easily be identified on the grand composite curve.

Also, it is seen that combining the synthesis of heat and mass exchangers is beneficial not only to the mass exchanger network, but to the heat exchanger network too. This is because the use of the MSA as a utility in the heat exchanger network helps in reducing the utility need of the heat exchange operation, also the capital cost of the HEN is reduced because the MSA streams are operating at a reduced heat capacity flowrate.

6.1.3 Water Pinch Analysis

The technique known as water pinch analysis has a somewhat wider scope than the use of water as a MSA, since water is used in processes for many diverse purposes other than mass separation, including its use as a heat transfer medium. The approach used in water pinch analysis to handle this diversity of application has been to require that all process requirements be expressed purely in terms of quantity and quality constraints for the water streams, so that the analysis does not have to consider the nature of the processes which give rise to the constraints. The preceding development of CHAMENS therefore does not fully address the water pinch problem, and further work is required to include all aspects of water use into the methodology. In section 5.3 a start has been made by including water pinch capability into the targeting software.

6.2 Software Development

A software package has been written for targeting both heat and mass exchange networks independently. It also has the added capability to target water pinch networks.

As it stands this computer package can be used for analysis of heat and mass exchange systems on their own, in order to establish which system dominates.

It is also useful for iterative calculations to establish the interaction between the heat and mass exchange systems. This is based on the presumption that comparing targets provides a valid determination of what could be achieved in the design of such systems.

This approach is justified on the basis of experience that has shown that it is always possible to achieve the utility targets (whether energy utilities or MSA utilities), and that capital costs targets for both energy and mass exchange systems can be approached to within less than 10%.

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APPENDIX A: DATA FOR EXAMPLE PROBLEMS

Table A.1: Stream data for Example 3.1(Halalle & Fraser, 1998).

Rich Streams	G (kmol/h)	y^s (kmol SO_2/kmol inert gas)	y^t (kmol SO_2/kmol inert gas)
R_1	50	0.01	0.004
R_2	60	0.01	0.005
R_3	40	0.02	0.005
R_4	30	0.02	0.015

MSA	L^c (kmol/h)	x^s	x^t
S_1	∞	0	-

MSA	L^c (kmol/h)	z^s	z^t
W_1	∞	0	0.02

Equilibrium relations

S_1 at 100°C:

$$y = 700x \quad \text{(from international critical tables, 2003)}$$

S_1 at 30°C:

$$y = 35.71x - 0.0026$$

S_1 at 20°C:

$$y = 25.464x - 0.0018$$

S_1 at 10°C:

$$y = 14.887x - 0.0012 \quad \text{(from Perry et al., 1984)}$$

Table A.2: MSA and utilities costs for Example 3.1

S_1 ($/ton)	HU ($/kW.yr)	CU_1 ($/kW.yr)	CU_2 ($/kW.yr)
1.28	100 (121 ^{o}C -120^{o}C)	10 (15 – 25^{o}C)	30 (5^{o}C – 10^{o}C)

Stripping steam cost: $0.128/kmol

Table A.3: Equipment data for Example 3.1 (Coulson et al., 1993)

Operating time:	8600h/yr
Column capital cost (installed):	\$ $12{,}800 H_t^{0.95} D^{0.6}$
Trays:	\$ $608e^{0.8D}$ per tray
	D is column diameter (m)
	H_t is column height (m)
Tray efficiency:	20%
Annualisation factor:	0.2
Inactive height:	3m
Heat exchange cost (installed):	$30{,}000 + 750A^{0.81}$
Annualisation factor:	0.2

Table A.4: Stream data for Example 3.2
(Srinivas & El-Halwagi, 1994).

Rich streams	G (kg/s)	y^s	y^t
R_1	104	8.83×10^{-4}	5.00×10^{-6}
R_2	442	7.00×10^{-4}	5.00×10^{-6}

MSAs	L^c (kg/s)	x^s	x^t
S_1	40	0.07557	0.115
S_2	∞	1.00×10^{-6}	1.00×10^{-5}
S_3	∞	0.001	0.01

Equilibrium relations

For white liquor, S_1:

$$m_1 = (5.86807 \times 10^{-8}) \times 10^{(0.01024T_1)}$$

For 15 wt% *N*-methyl-2-pyrrolidone, S_2:

$$m_2 = 1.1907T_2 - 332$$

For 15 wt% MDEA, S_3:

$$m_3 = (9.386 \times 10^{-10}) \times 10^{(0.0215T_3)}$$

Table A.5: Stream thermal data for Example 3.2

Stream	Supply temperature (K)	Target temperature (K)	Lower bound temperature (K)	Upper bound temperature (K)	Average Specific heat capacity (kJ/kgK)
R_1	298	298	288	313	1.00
R_2	298	298	288	313	1.00
S_1	368	368	368	368	2.50
S_2	313	313	298	313	2.40
S_3	310	310	280	330	2.40
HU	394	393	394	393	4.2
CU_1	288	298	288	298	4.2
CU_2	278	283			4.2

Table A.6: MSA and utilities costs for Example 3.2
(Srinivas & El-Halwagi, 1994).

S_2 (\$/kg)	S_3 (\$/kg)	HU (\$/kW.yr)	CU_1 (\$/kW.yr)	CU_2 (\$/kW.yr)
0.007	0.001	100 (121°C - 120°C)	10 (15°C - 25°C)	30 (5°C – 10°C)

Stripping steam cost: \$0.007/kg

Supply and target composition, 0 and 0.08

Table A.7: Equipment data for Example 3.2
(costs taken from Papalexandri et al., 1994 & Shenoy, 1995)

Tray column cost (installed):	4552 N_{stages} \$/yr
Heat exchange cost (installed):	30,000 + 750$A^{0.81}$
Annualisation factor:	0.2

Table A.8: Stream data for Example 3.3.

Rich streams	G (kg/s)	y^s (mass fraction)	y^t (mass fraction)
R_1	3.5	0.058	0.006
R_2	1.5	0.054	0.007

MSAs	L^c (kg/s)	x^s (mass fraction)	x^t (mass fraction)	b
S_1	25	0.0017	0.0071	0
S_2	40	0.0025	0.0085	0
S_3	∞	0	0.017	0

Equilibrium relation for the temperature range of 50°C to 70°C is $y = (0.1107T - 2.4159)x$

m at 100°C = 12.28

Table A.9 Stream thermal data for Example 3.3

Stream	Supply temperature (°C)	Target temperature (°C)	Lower bound temperature (°C)	Upper bound temperature (°C)	Average Specific heat capacity (kJ/kg°C)
R_1	25	25	7	47	1.00
R_2	25	25	7	47	1.00
S_1	55	55	10	70	4.2
S_2	70	70	10	70	4.2
S_3	30	30	10	30	4.2

Table A.10: Equipment data for Example 3.3
(Costs from Peters and Timmerhaus, 1991)

For continuous contact columns,

Shell cost (installed): $ $618M^{0.66}$ (M in kg)

Packing: 2.54 mm Raschig rings
*K*w : 0.02

For staged columns,
Cost per equilibrium stage: $ 22760 (Papalexandri et al., 1994)

Annualisation factor: 0.2
Operating time: 8150 hrs/yr

Heat exchange cost (installed): $30{,}000 + 750A^{0.81}$
Annualisation factor: 0.2

S_3 ($/kg)	HU ($/kW.yr)	CU_1 ($/kW.yr)	CU_2 ($/kW.yr)
0.005	100 (121°C - 120°C)	10 (15°C - 25°C)	30 (5°C – 10°C)

Table A.11: Hot and cold stream data for Example 4.1 (Shenoy, 2005)

Stream	Type	T^s(°C)	T^t(°C)	FCP(kW/°C)
1	Hot	175	45	10
2	Hot	125	65	40
3	Cold	20	155	20
4	Cold	40	112	15

HU ($/kW.yr)	CU_1 ($/kW.yr)	CU_2 ($/kW.yr)	CU_3 ($/kW.yr)
120 (180°C - 179°C)	10 (15°C - 25°C)	20 (10°C – 20°C)	30 (5°C - 10°C)

The mass exchange data for this problem is the same as for Example 3.1 and may be found in Tables A.1, A.2 and A.3.

APPENDIX B: USER MANUAL FOR HENS AND MEN SYSTEMS ANALYSIS SOFTWARE

The purpose of this document is to provide the user with a quick reference when running the program. It begins by presenting the Graphical User Interface (GUI) which allows the user to navigate between Heat Exchanger Network (HENS) and Mass Exchanger Network (MENS). This is then followed by a special design menu system in Excel, which is automatically loaded when the user opens the program. It will be noted from this document that the worksheets are not presented explicitly because the user does not need to know the functions of them as the program leads the user to the correct worksheet. However, if the user is interested in knowing the worksheet, this is presented in the study. This document ends by briefly reviewing the purposes of the submenus and presenting the data require for executing these submenus. It will also be noted from this document that there is a brief review of units that might cause confusion, however, it is worthwhile pointing out that the user can use any system of units as long as there is consistence.

1. Graphical User Interface (GUI)

The user must click "**Start Running the program**" command button at the beginning of targeting. It is worthwhile pointing out that upon opening the file the program takes the user directly to this command button. "**The Main Control Form**" will then appear prompting the user to select between **Heat Exchange Network Synthesis (HENS)** and **Mass Exchange Network Synthesis (MENS)**. When **HENS** is selected, the "**HENS Form**" will appear prompting the user to select among **Grassroots Targeting**, **Retrofit Targeting**, and **Multiple Utility Targeting**, and similarly for **MENS** (Figure 1).

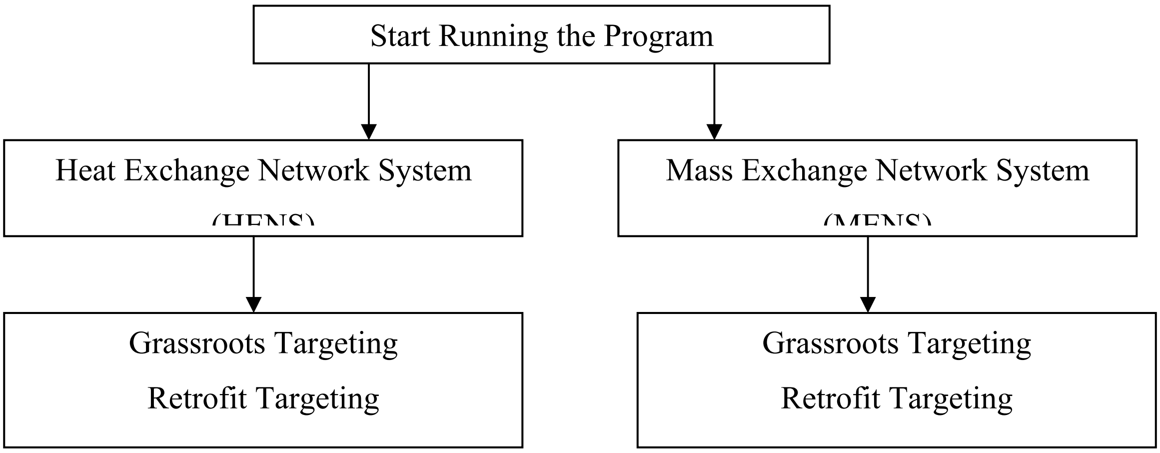

*Figure 1: The user interface, which allows the user to select between **HENS** and **MENS** and the type of targeting to be executed within **HENS** and **MENS**.*

It must be pointed out, however, that when the user selects Grassroots Targeting in MENS, the "**Problem Type Form**" will appear prompting the user to select between **Problem with only one MSA** and **Problem with Multiple MSAs**.

When the user selects one the above the program will lead the user the correct input worksheet. For example, when the user selects **HENS** followed by the **Grassroots Targeting** from the GUI, the program will activate the "**INPUTHENS**" worksheet. It is for this reason that the worksheets will not be presented explicitly.

2. **The menu**

In Excel, there is a specially designed menu which prompts the user to select the type of analysis to be executed by the program. This is partly demonstrated in Figure 2.

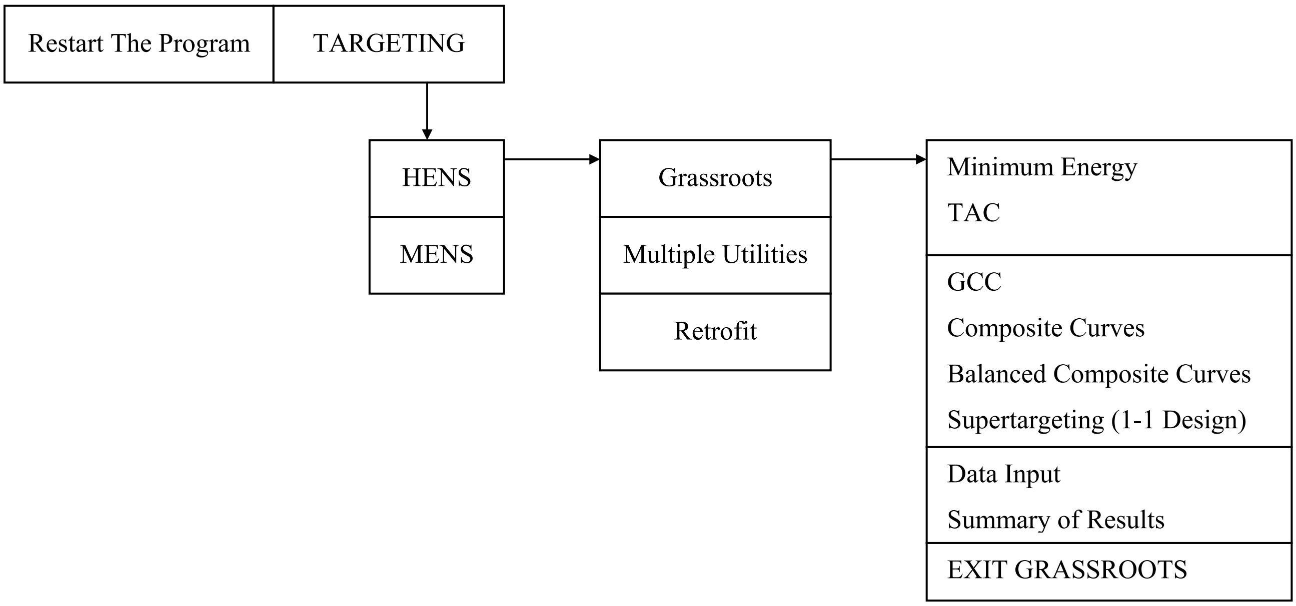

Figure 2: The menu system which allows the user to select the type of the analysis to be executed by the program.

The "**Restart The Program**" command button leads the user to the "**Start Running the Program**" command button (Figure 1). When the user selects the "**TARGETING**" command button, the "**HENS**" and "**MENS**" command buttons appear allowing the user to choose between them. When "**HENS**" command button is clicked, the "**Grassroots**", "**Multiple Utilities**", and "**Retrofit**" command buttons will then appear allowing the user to select the analysis to be executed by the program. Suppose the user selects the "**Grassroots**" button (Figure 2), the command buttons shown in Figure 2 will appear allowing the user to decide on the analysis to be executed by the program. The code attached to each of the command buttons is independent of the code for the other buttons (i.e. a user can run TAC without running Minimum Energy first). .

It is worthwhile to point out that the data for all curves are kept in the database of the program. Therefore, to view these curves, the user must request them using the submenus.

3. **Heat Exchanger Network Synthesis (HENS)**

3.1. Grassroots targeting

The menu system is divided into three command buttons (submenus) i.e. Minimum Energy, TAC, and Supertargeting. The objective and input data for these command buttons are summarized below.

Minimum Energy

This command button determines the minimum energy (i.e. minimum hot and cold utilities) using the *Problem Table Algorithm*, and constructs the Composite Curves (CC) and Grand Composite Curve (GCC).

The input data required is stream inlet temperature, stream outlet temperature, heat flow capacity flowrates, and the minimum approach temperature.

TAC

This command button determines all the targets (minimum energy, minimum area, minimum units, minimum shells, minimum operating cost, minimum capital cost, and Total Annual Cost).

The input data required is stream inlet temperatures, stream outlet temperatures, stream heat flow capacity flowrates, minimum approach temperature, inlet and outlet temperature of the utilities, stream heat transfer coefficients, the cost per unit load of each hot and cold utility, annualization factor, cost law coefficients for each stream, and the reference cost law coefficients. Data is input on the **INPUTHENS** worksheet.

Supertargeting

This command button determines the optimum minimum approach temperature and Total Annual Cost (TAC) for each of 1-1 design and 1-2 design.

In addition to all data mentioned above, the number of iterations and the temperature range (start and end temperatures) are required.

It is worthwhile pointing out that the program does check the validity of these specifications. For instance, the program determines the maximum and the minimum allowable minimum approach temperatures, and it will therefore overlook any specification outside this range. The number of iterations must be greater then ten and less than fifty. This is applicable to both HENS and MENS.

3.2. Multiple Utilities

The command button "**Utility Usage** " in the menu is for determination of the optimum utility usage for both cold and hot utilities.

The input data required is stream inlet temperatures, stream outlet temperatures, stream heat flow capacity flowrates, minimum approach temperature, and the priority indices of the individual cold and hot utilities. Data is input on the **MULTIPLEHENS** worksheet.

3.3. Retrofit

The command button "**Retrofitting**" in the menu is for determination of the optimum network which saves the greatest amount of energy subject to a specific payback period or investment limit.

The input data required is stream and utility inlet and outlet temperatures, stream heat flow capacity flowrates, the area of the existing network, the utility usage of the existing network, the cost per unit load of hot and cold utilities, the reference cost law coefficients, average area per match and/or average area per shell (calculated from the existing network) , and payback period or investment limit. Data is input on the **RETROFITHENS** worksheet.

4. Mass Exchanger Network Synthesis (MENS)

4.1. MENS with only one external MSA

Two categories of MENS are considered: Stagewise Exchangers and Continuous-contact Exchangers. The program only considers Grassroots Targeting. The menu system is divided into three command buttons i.e. Minimum MSA, TAC, and Supertargeting.

Minimum MSA

This command button determines the minimum MSA and the pinch compositions using the limiting composite curve of Wang and Smith (1994) and construct the y-x composite curve.

For Stagewise and Continuous-contact exchangers, the inlet and outlet composition for rich streams, inlet composition and the equilibrium data of the external lean stream, stream densities, and the minimum composition difference in the lean phase must be inputted as a data. Data is input on the **INPUTMENS** worksheet.

It is worthwhile pointing out that the program does not have unit conversion features, thus it is the responsibility of the user to ensure that the units are consistent. To clarify this, I'll demonstrate this using the case study for grassroots targeting of stagewise mass exchange networks (see Section 5.2.1). Here, *G* is given in kmol/hr. Therefore the water flowrate will be also in kmol/hr. Now, suppose G was given in g/min, then the water target will be in g/min. It is very important that the units be consistent, and also that the operating cost units are consistent with them.

TAC

This command button determines all targets at once i.e. MSA, number of stages (stagewise), height (continuous), number of units, operating cost, capital cost, and Total Annual Cost (TAC).

In addition to the data mentioned in Minimum MSA, the tray efficiency (stagewise), mass transfer coefficient (continuous), the cost of external MSA, and the annualization factor are required. As before, data is input on the **INPUTMENS** worksheet.

Now, the water target will be in kmol/hr (see Minimum MSA), however, cost of water is given \$/ton and the plant operates for 8600 hr/yr. The task for the user is to input the annual operating cost which will be in accordance with the water target. This is how to work out the annual operating cost input:

- I must know the final units which I want, in this case I want the units in \$/yr
- The cost of water is given in \$/ton, therefore, I must convert this to \$/kmol using the molar mass of water.
- Now, I must use operating time (8600 hr/yr) to introduce the time factor.
- The annual operating cost input must be in (\$/yr)/(kmol/hr) which is the combination of water cost and operating time.
- Therefore, I must input 201.24 (\$/yr)/(kmol/hr) so that when I multiply this by the water target in kmol/hr, I will get the operating cost in \$/yr

The other trick in problems with only one external MSA is in the determination of the diameter of the exchangers. The flowrate, *G*, must be in kg/s which is in accordance with the densities in kg/m^3. Therefore, *G*, which is in kmol/hr, must be converted to kg/s using the molar mass of air (taken to be the mixture of oxygen and nitrogen ignoring other gases).

In continuous-contact exchanger, the user must ascertain that the units of the mass transfer coefficient are in accordance with the units of *G*. This information is used to calculate the HTU which is given by equation 1.
Now, *S* is in m^2 and *G* is in kmol/hr, therefore, the user must convert the mass transfer coefficient ($K_y a$) to (kmol/hr)/m^3.

Supertargeting

This command button determines the TAC over a range of minimum composition differences and the optimum minimum composition difference in the lean phase.

In addition to all data mentioned above, the number of iterations and the minimum composition difference range (start and end minimum composition difference) are required. As for HENS, the number of iterations must be greater then ten and less than fifty.

4.2. MENS with multiple MSAs

Two categories of MENS are considered: Stagewise Exchangers and Continuous-contact Exchangers. The analyses which are presented in this section are: Grassroots Targeting, Multiple Mass Separating Agent (MSA) Targeting, and Retrofit Targeting.

4.2.1. Grassroots Targeting

The menu system is divided into three command buttons (submenus) i.e. Minimum MSA, TAC, and Supertargeting. The objective and input data for these command buttons are summarized below.

Minimum MSA

This command button is for determination the excess capacity of the process MSAs to remove mass and the mass that needs to be removed by external MSAs, using the Tabular Method. It also determines the flowrate for each MSA.

Stream data, the minimum composition difference in the rich phase, and the factor for each external MSA are required as the input data. Data is input on the **INPUTMENSM** worksheet.

TAC

This submenu determines all targets (minimum MSA, flowrate for each MSA, minimum number of stages (stagewise), minimum mass (continuous), operating cost, capital cost, and TAC)

In addition to the data mentioned in minimum MSA, lumped coefficient (continuous), the capital cost per equilibrium stage (stagewise), the cost of MSAs, and the cost law coefficients (continuous) are now required. As before, data is input on the **INPUTMENSM** worksheet.

Supertargeting

This command button determines the TAC over a range of minimum composition differences and the optimum minimum composition difference in the rich phase.

In addition to all data mentioned above, the number of iteration and the minimum composition difference range (start and end minimum composition difference) are required. As for HENS, the number of iterations must be greater then ten and less than fifty.

4.2.2. Multiple MSA Targeting

The command button "**MSAs Usage** " in the menu is for determination of the optimum MSAs usage for both process and external.

Stream data, minimum composition difference in the rich phase, and the factor for each external MSA must be provided to the program as input.

4.2.3. Retrofit Targeting of MENS

The command button "**Retrofitting**" in the menu is for determination of the optimum network which saves the greatest amount of MSAs subject to a specific payback period (there is no investment limit specification in MENS).

The input data required is stream data, the factor for each external MSA, the cost for each MSA, the number of stages of the existing network (stagewise), the MSA usage of the existing network (total process MSA usage and total external MSA usage), the capital cost per equilibrium stage (stagewise) the mass of exchangers (continuous), the cost law coefficients (continuous), and the payback period. Data is input on the **RETROFITMENS** worksheet.

PART 2

Water Conservation Through Energy Conservation

Case Study: African Explosives, Modderfontein

Student:	**Ms Nongezile Nyathi**
Research Leader:	**Professor Thokozani Majozi**
Institution:	**University of Pretoria** **Department of Chemical Engineering** **Pretoria**
Research Period:	**July 2004 to May 2006**

PART 2

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1 INTRODUCTION

Most industries use significant amounts of cooling water to remove excess energy from processes. Cooling towers are most commonly used to remove the excess energy. This is always accompanied by evaporation of water which results in water loss from the cycle and concentration of salts contained in the cooling tower. The concentrated cooling water leaves the cooling tower as cooling water blowdown, thus contaminating the water system. Loss of water via evaporation and cooling water blowdown has the effect of increasing the amount of water required as makeup, thus increasing the freshwater consumption. The industries that have a problem with high cooling water consumption and wastewater generation include, power generation sector, the chemical and petroleum sector, the metallurgical sector as well as the pulp and paper sector. The major contaminants in the nitrates production facilities are nitrates, which leave the system as effluent in the form of blowdown. There is thus a need to design cooling water systems with low effluent production and high cooling tower performance.

Most methodologies tend to assess the cooling tower performance by analyzing the cooling tower as a separate entity from the rest of the cooling water system components. They concentrate on improving the performance by investigating the design characteristics of the cooling tower whilst disregarding interactions between the cooling tower and the rest of the cooling water network components. Bernier (1994) looked at the different parameters of the cooling tower which affect its performance. The cooling water parameters which mostly affect the performance of a cooling tower are wet bulb temperature and the flowrates of the air and water. It was observed that reducing the flowrate of the cooling water increases the cooling tower performance. However, reducing the cooling water flowrate results in an increase in the return temperature to the cooling tower. Thus, the reduction of the cooling water flowrate is limited by the maximum permissible return temperature. High temperatures can lead to problems in the cooling tower, e.g. fouling, thus a reduction in the heat transfer rate of the cooling tower. On the other hand, Milosavljevic and Heikkilä (2001) developed a mathematical model for a counter flow wet cooling tower based on one-dimensional heat and mass equations using the measured heat transfer coefficient. Khan et al. (2003) and Fisenko (2004) also developed models for investigating the performance characteristics of counter flow cooling towers. However, these models do not look at techniques for reducing effluent or the interactions between the cooling tower and the rest of the cooling water network.

The problem of effluent reduction or wastewater minimization has been investigated by several authors in the past years. Most of the work has been focusing on situations where water is used in reducing the amount of contaminants in the process streams. Wang and Smith (1994) addressed the minimization of wastewater in process industries. They introduced the limiting water profile approach, where the maximum permissible inlet and outlet concentrations are used to construct the limiting cooling water composite curve. The methodology first sets the target for minimum wastewater and then the network is designed which ensures that the targets are met. Furthermore, Wang and Smith (1995) extended their work and developed a technique for targeting minimum wastewater for fixed flowrates. In their work they also addressed the issue of targeting for multiple sources of freshwater. Kim et al. (2001) introduced a methodology for the design of cooling systems for effluent temperature reduction. This focuses on the reduction of the effluent temperature rather than the amount of effluent produced. These conceptually based methods provide physical insights and design features for water systems.

Kim and Smith (2001) developed a cooling water system design methodology, which takes into consideration all the components of the cooling water systems, i.e. the cooling tower as well as the unit operations using cooling water. It is an adaptation of the graphical technique introduced by Wang and Smith (1994) for wastewater minimization based on pinch principles. The technique allows the designer to set targets for minimum cooling water requirement through the exploitation of reuse and possibly recycle opportunities. The minimization of cooling water requirements implies higher return temperature. This combination of operational parameters, that is, low flowrates and high return temperature has been shown to improve cooling tower performance (Bernier 1994; Kim and Smith 2001). The drawback of this technique is that it does not incorporate the pressure drop which is associated with the reduction in cooling water flowrates. This problem was addressed by Kim and Smith (2003) in their automated cooling water systems design based on mathematical programming. Furthermore, Kim and Smith (2004) developed a methodology aimed at reducing the cooling water makeup. This is achieved by introducing water recovery between wastewater-generating processes and cooling systems while the cooling tower can reliably manage the increased heat load. Their technique incorporates pressure drop in the problem formulation and the selection of the best design is dependent on the values of the pressure drop. The lower the pressure drop the more acceptable the design. Whilst these techniques can be applied to systems with a single cooling water source, they cannot be readily applied to systems with multiple cooling water sources.

This report presents a graphical technique for cooling water networks that enables targets to be set for systems with multiple cooling water sources. The targeting procedure is first developed assuming fixed inlet and outlet cooling water conditions for each cooling water using operation. The maximum acceptable inlet and outlet temperatures of the cooling water are used. These are set by the minimum temperature difference, ΔT_{min}, for each water using operation. For heat exchange units operating at temperatures above the boiling point of water, setting maximum inlet and outlet water temperatures is not straightforward, as simple use of ΔT_{min} between cooling water and process stream might suggest partial or full evaporation of cooling water in the exchange unit. For example, in a unit with process stream at 410^0C, using a ΔT_{min} of 20^0C would suggest cooling water outlet temperature of 390^0C, which is not practical. In these situations, engineering insight and process understanding become imperative. The design which meets the target is then developed. The application of the method is illustrated using an example as well as a case study from an existing industrial facility.

2 OBJECTIVES OF STUDY

The objectives of the study as originally stated in 2001 are as follows.

(i) Conserve the use of water by the process industry through thermal energy conservation.

(ii) Reduction of salination through the reduced cooling need by the process industry.

(iii) Develop a rigorous and rational technique to optimize cooling circuits for simultaneous water and energy conservation.

After assessing the case study which was chosen for the project, the objectives of the project were extended. The additional aim of the project was to develop a graphical methodology to target and design cooling water networks, using basic principles of Pinch Analysis, for systems with multiple cooling water sources. The extension of the research project objectives was motivated by the observation that the case study system had two cooling water sources and could not be fully analysed using the techniques currently available, which only address systems with single cooling water sources. In short, the problem addressed in this report can be stated as follows:

Given,

(i) a set of cooling towers with different supply temperatures,

(ii) maximum capacity for each of the cooling towers,

(iii) a set of cooling water using operations with limiting temperature requirements and

(iv) the duty requirements for each of the cooling water using operations,

determine the minimum amount of cooling water required by the overall cooling water network as well as the optimal amount required from each of the cooling towers, without compromising the performance of each cooling tower.

Additionally, the implications of the technique developed on it’s interaction with the cooling tower as well as the cooling tower performance and effluent production were investigated.

3 COOLING WATER NETWORK DESIGN

The cooling water network (CWN) design is performed in two parts, namely targeting and design. These parts are discussed in detail below.

3.1 Targeting

Targeting involves the setting of cooling water supply targets from the cooling tower into the associated cooling water using network. The cooling water composite curve is constructed as suggested by Kim and Smith (2001) for single cooling water sources by combining all individual profiles into a single curve within temperature intervals. However, there are two scenarios that can arise in the presence of multiple cooling water sources. If the cooling water sources have very high design capacities and significantly high maximum return temperatures, all the cooling water used will be supplied by the cooling water source with the lowest supply temperature (primary source). Thus the water supply line will be similar to that for systems with a single cooling water source. This observation is demonstrated in Figure 3.1.

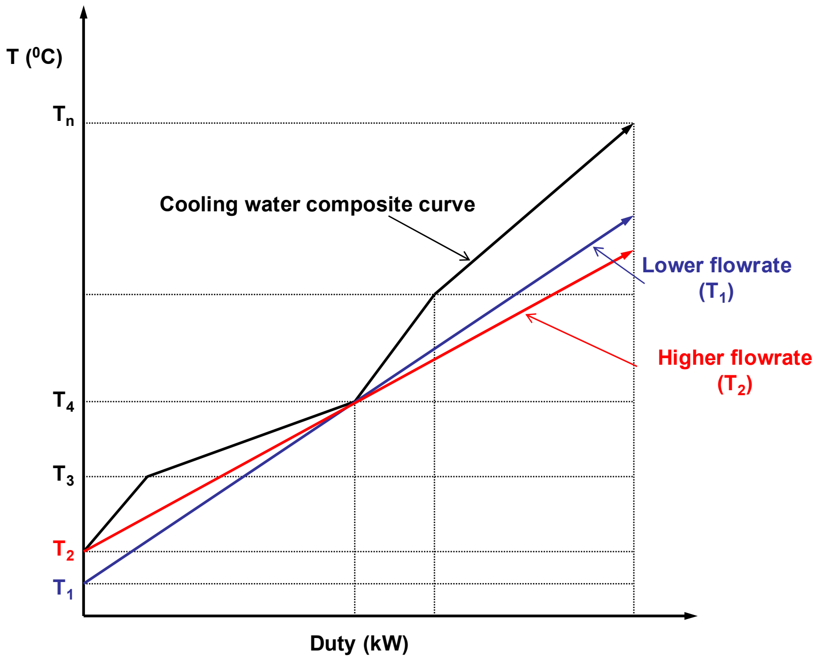


Figure 3.1 Cooling water targets for cooling water sources with unlimited capacity

Figure 3.1 shows that the flowrate for the cooling water source with a lower supply temperature (T_1) is lower than that with a higher supply temperature. Thus less water will be required if it is supplied solely from the primary source. However, the lower flowrate is concomitant with higher return temperature for the same heat duty (Figure 3.1). It is, therefore, evident that in a situation where the flowrates are unlimited and return temperatures not critical, the source with minimum supply temperature will always be the sole supplier. This renders the other supplies redundant. The targeting is thus performed as outlined by Kim and Smith (2001) for single cooling water sources, where the flowrate is minimized by ensuring that the water supply line forms a pinch with the limiting cooling water composite curve. Any cooling water supply line beyond that which forms a pinch with the limiting composite curve does not satisfy the cooling requirements of the system.

However, in cases where the minimum water requirement for the cooling water system is higher than the design capacity of the primary source, the cooling water from the cooling water sources with higher supply temperatures has to be used to supplement the primary cooling water supply. In this particular case, targeting is no longer straightforward. The steps followed in targeting for the cooling water supply are outlined below.

Step 1 Primary cooling water source

Maximize the amount of cooling water used from the primary source by adjusting the gradient of the cooling water supply line until its value corresponds to the maximum flowrate. This step is illustrated in Figure 3.2. At this point, supplementary water from higher temperature sources is required in order to meet the target for the entire cooling water system.

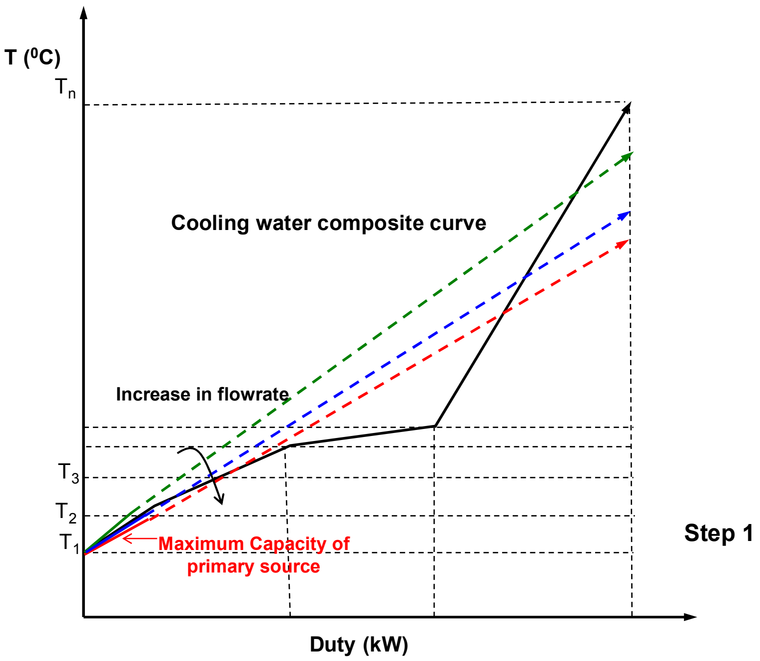


Figure 3.2 Setting the target for primary cooling water source

Step 2 Intermediate cooling water sources

All the subsequent cooling water supply lines represent the overall flowrate of the previous cooling water sources and the one being targeted at that stage. The cooling water supply line for the intermediate cooling water sources is set by either the maximum capacity of the cooling water source or the pinch point. If the maximum capacity is reached before a pinch is formed with the limiting cooling water composite curve, then the cooling water source with the next closest supply temperature is used to supplement the cooling requirement. However, if the pinch is formed before the maximum capacity is reached, the rest of the cooling water sources need not be used because the cooling water requirement will be satisfied. Thus the rest of the cooling water sources become redundant. This step is illustrated in Figure 3.3.

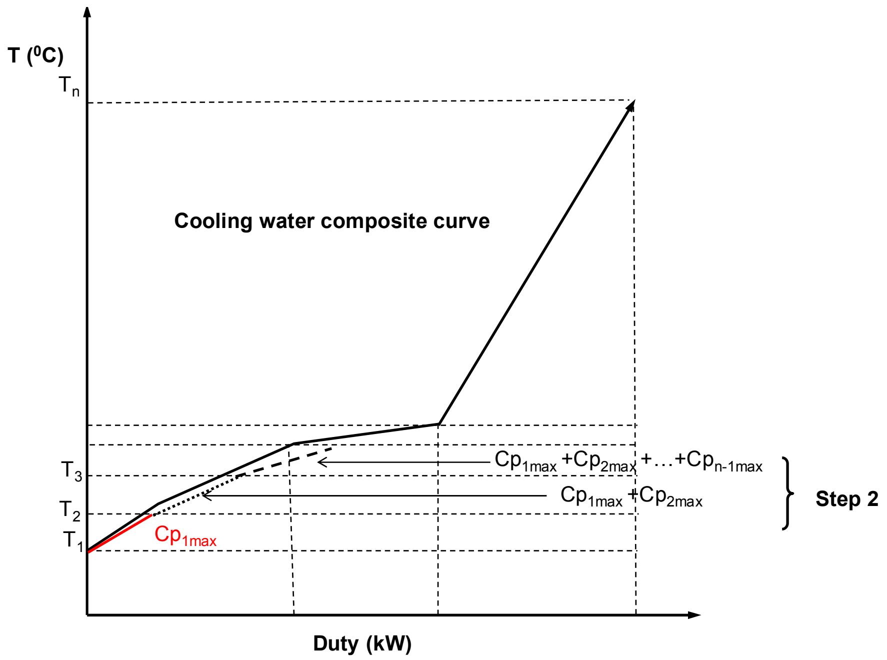


Figure 3.3 Setting the targets for intermediate cooling water sources

As shown in Figure 3.3, the gradient of the cooling water supply line decreases with the addition of an extra cooling water source as it represents the sum of all the cooling water flowrates from all the water sources that have been used.

Step 3 Cooling water source with the highest supply temperature

If a pinch is not formed while targeting for any of the intermediate cooling water sources, the cooling water source with the highest supply temperature has to be used. The overall amount of cooling water used by the whole system is set by minimizing the amount of cooling water from the last cooling water source. This is done by ensuring that the final supply line forms a pinch with the cooling water composite curve. The flowrate obtained from this line represents the overall cooling water requirement for the system. This is shown in Figure 3.4.

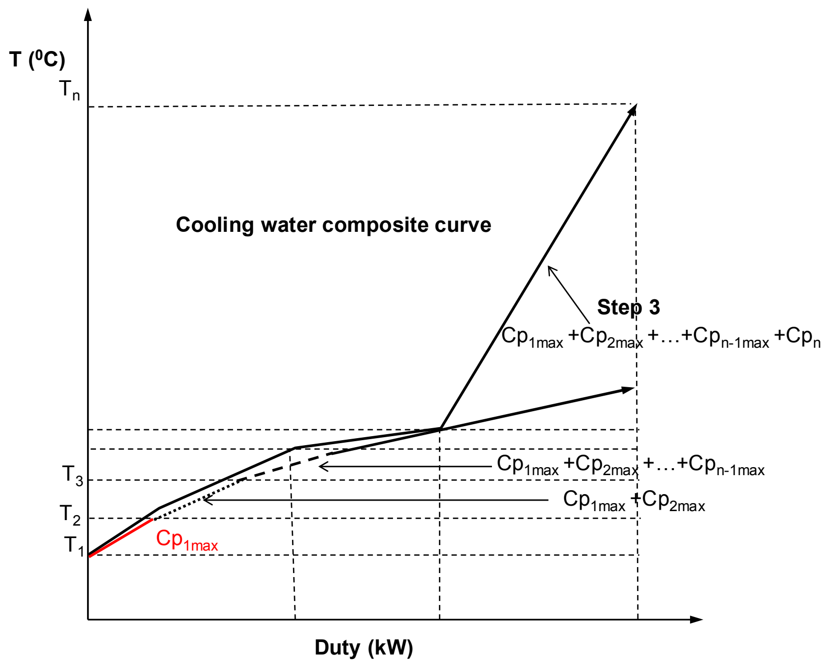


Figure 3.4 Targeting steps for systems with multiple cooling water sources

3.2 Design Procedure

The design step follows the targeting step and it meets the target set. The design procedure for systems with unlimited cooling water capacities is similar to the water mains method for single cooling water sources (Kim and Smith, 2001). The water mains on a grid diagram represent the cooling water source, the pinch point as well as the highest exit temperature of the water using operations. Other intermediate water mains are possible depending on the maximum supply and target temperatures of the cooling water. However, the design procedure for systems with limited cooling water supply from the primary cooling water source is an extension of the procedure suggested by Kim and Smith (2001). Each cooling water source is represented by a water mains and the grid diagram also has water mains representing the pinch point and the highest exit temperature. The procedure has five steps.

The first step is to generate the grid diagram consisting of the cooling water mains representing all the cooling water sources, the pinch temperature, the intermediate temperatures and the highest exit temperature. Then, the cooling water using operations are plotted in accordance with their maximum supply and target temperatures on the grid diagram. This is shown in Figure 3.5.

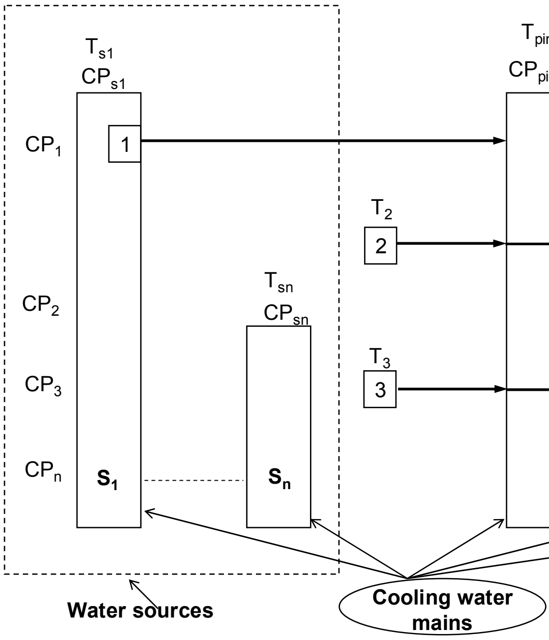


Figure 3.5 Step 1 of the design procedure

The second step is to connect the cooling water operations to the water mains. The cooling water from the source mains is used in ascending order, starting with the water supplied by the primary source. This is shown in Figure 3.6.

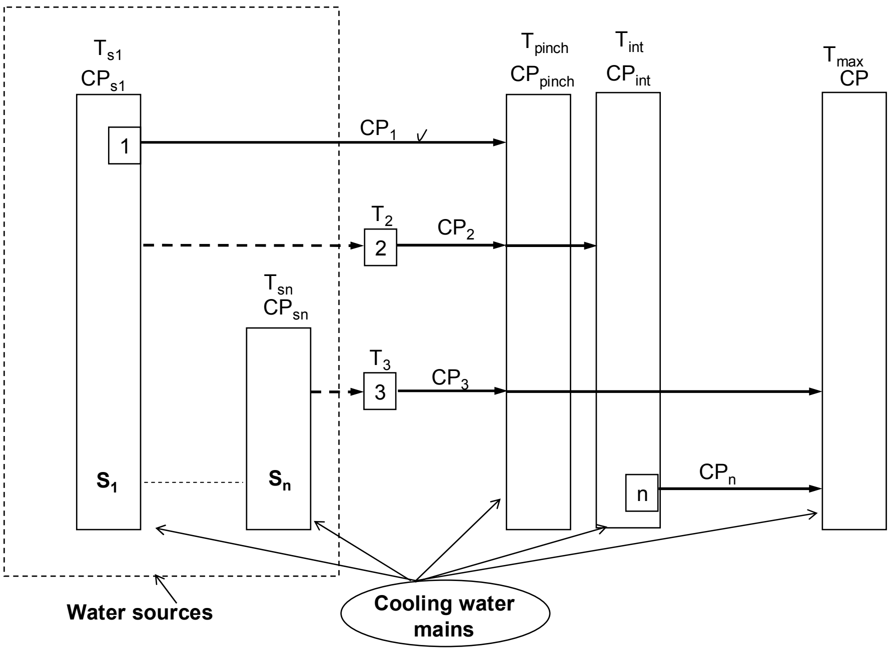


Figure 3.6 Step 2 of the design procedure

The ticked stream in Figure 3.6 indicates that the cooling requirement for the cooling water using operation has been satisfied.

The third step is to merge operations that cross the intermediate cooling water and pinch mains. This is shown in Figure 3.7.

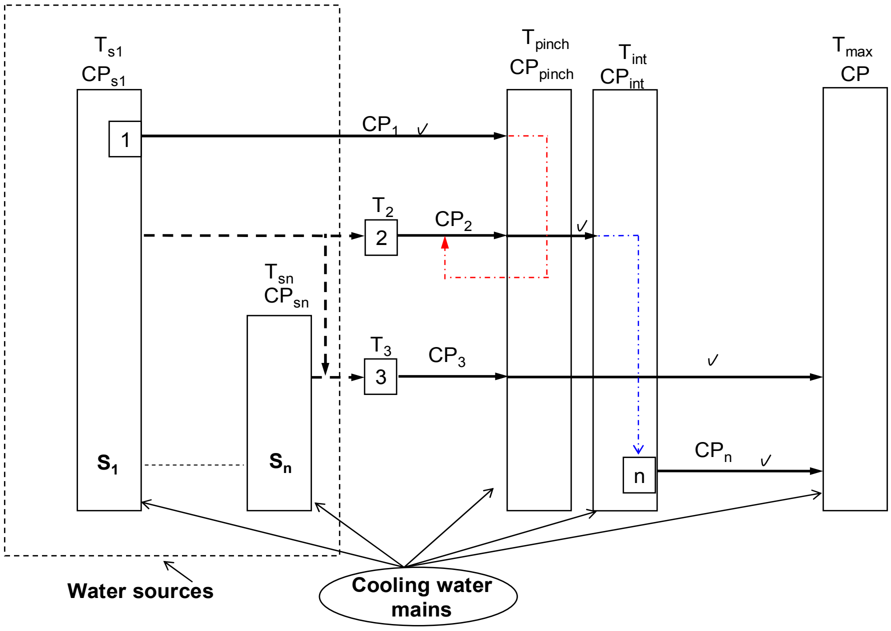


Figure 3.7 Step 3 of the design procedure

The fourth step is to remove the intermediate and pinch mains as shown in Figure 3.8.

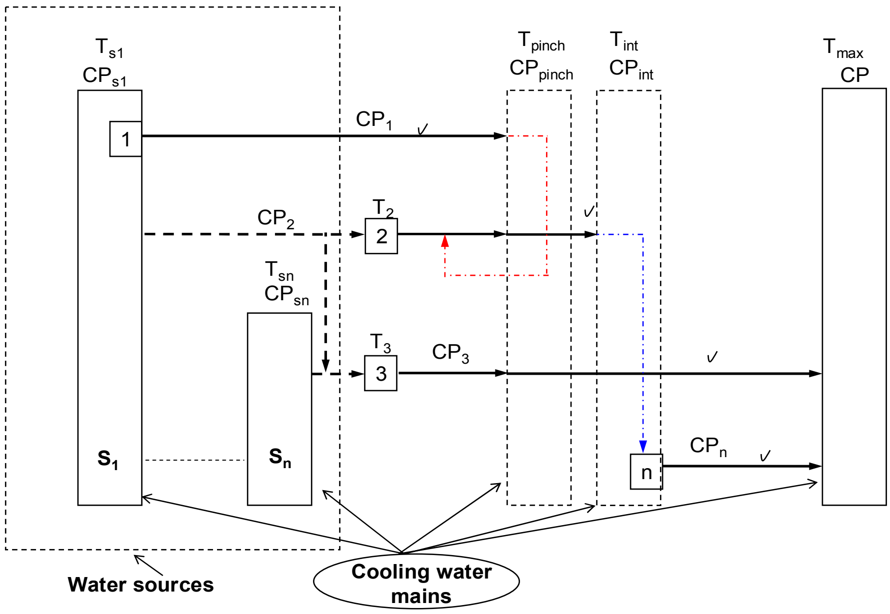
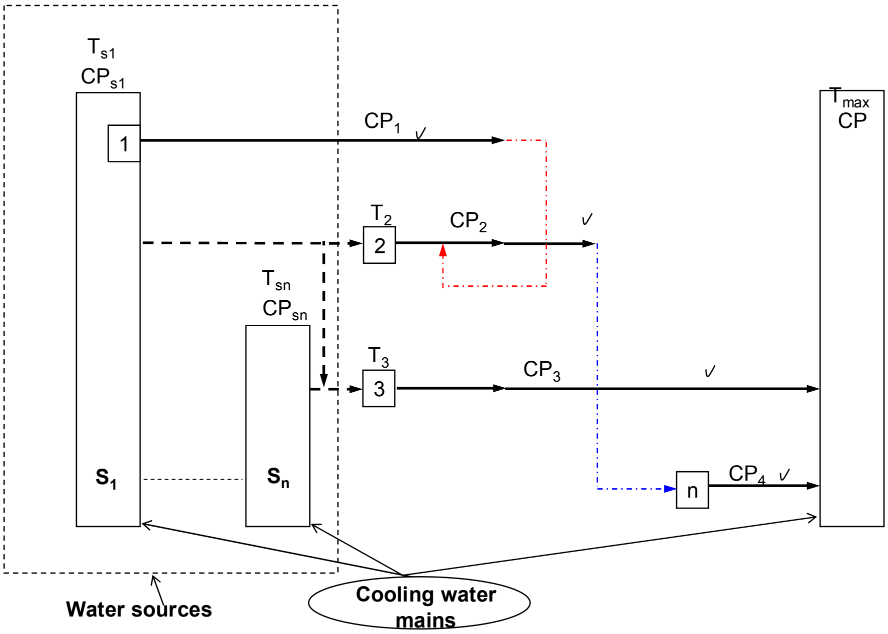
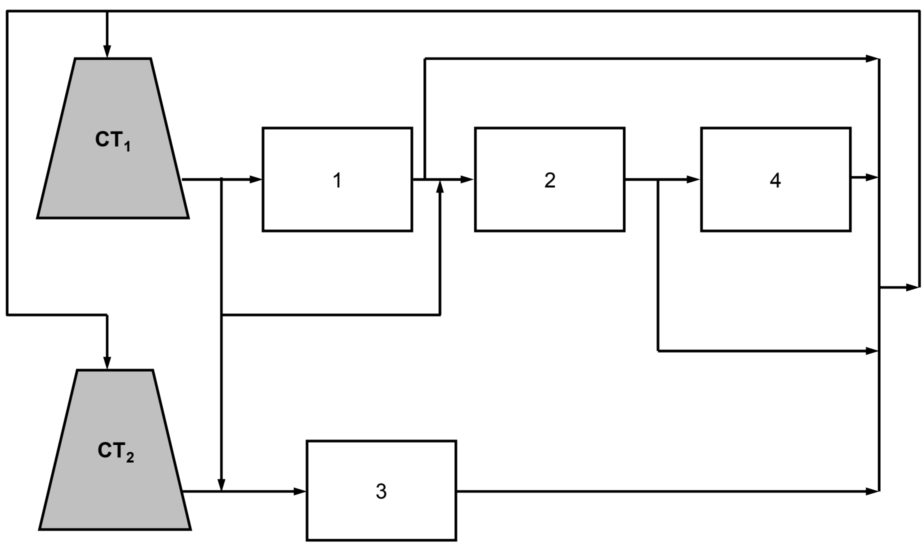


Figure 3.8 Step 4 of the design procedure

The fifth step is to connect the operations directly, which yields the final design as shown in Figures 3.9(a) and 3.9(b).



(a)



(b)

Figure 3.9 Step 5 of the design procedure

4 ILLUSTRATIVE EXAMPLE

In this example, the cooling water network comprises of four cooling water using operations. These cooling water using operations are supplied by two cooling towers A and B with supply temperatures of 20°C and 25°C, respectively. The maximum design capacities for cooling tower A and B are 69 ton/hr (80 kW/°C) and 43 ton/hr (50 kW/°C), respectively. Table 4.1 below shows the limiting cooling water data used. Cooling tower A supplies heat exchangers 1 and 2 and cooling tower B supplies heat exchangers 3 and 4.

Table 4.1 Limiting cooling water data

Heat Exchanger	$T_{hot,in}$ (^{0}C)	$T_{hot,out}$ (^{0}C)	CP (kW/^{0}C)	Q (kW)
1	25	40	30	450
2	35	40	160	800
3	25	75	34	1 700
4	50	75	12	300

Cooling water inlet temperature from cooling tower A = 20°C

Cooling water inlet temperature from cooling tower B = 25°C

Initially, the system was analysed as two independent subsystems (case 1). Then the overall system was analysed using the new technique for targeting for multiple cooling water sources (case 2). The targeting and design procedures are detailed in sections 4.1 and 4.2 below.

4.1 Targeting

The targeting procedure for case 1 is similar to that discussed by Kim and Smith (2001). That is, the limiting cooling water composite curves are constructed for the subsystems and the cooling water supply line is matched against them. The supply lines have the highest possible gradients to ensure that the flowrate is minimized. This is set when the water supply line forms a pinch with the limiting cooling water composite. The pinch point represents the region where the driving forces go to a minimum, but not necessarily zero (Wang and Smith 1994). The targets for cooling tower A and cooling tower B are shown in Figure 4.1.

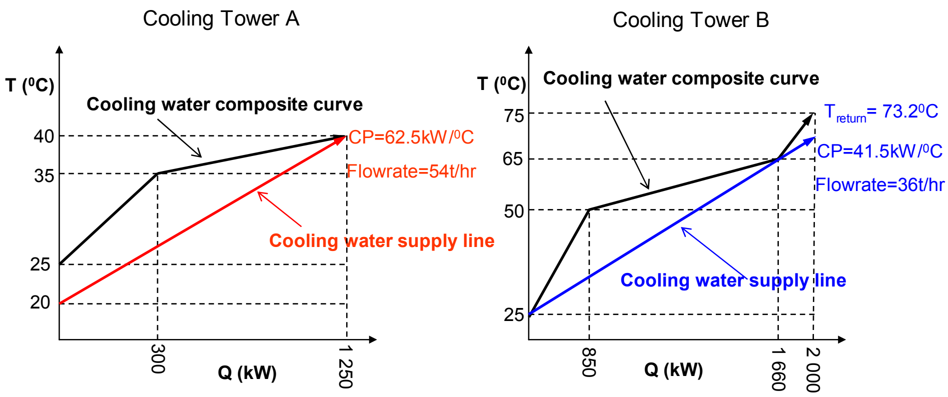


Figure 4.1 Cooling water targets for system analysed using case 1

Figure 4.1 shows that when the system is analysed as separate subsystems, the cooling water requirements for cooling tower A and cooling tower B are 54 ton/hr (62.5 kW/°C) and 36 ton/hr (41.5 kW/°C). Both of these are less than the maximum design capacities for the cooling towers. The return temperatures of cooling tower A and cooling tower B are 40°C and 73.2°C, respectively. The return temperature of cooling tower B is very high and could be unacceptable due to some constraints such as fouling and corrosion. Thus there could be a need to reduce the return temperature to cooling tower B.

The targeting procedure used for case 2 has been introduced in section 3.1 above and will be discussed in detail in this section. The amount of cooling water supplied by the cooling tower with the lowest supply temperature (primary source) is maximized to ensure that the overall requirement is minimized. The maximum value is set by the maximum capacity of the cooling tower. The cooling water used from the subsequent sources is also maximized as long as the pinch point is not reached. Otherwise the amount used from the subsequent cooling water sources is set by the pinch. However, if the pinch point is not formed when using the intermediate cooling water sources, the target for the source with the highest supply temperature is set by ensuring that the final cooling water supply line forms a pinch with the limiting cooling water composite curve. The final cooling water supply line represents the overall cooling water requirement. Targeting this way ensures that the overall cooling water requirement is optimized. In the example used in this report, there are only two cooling water sources (primary and secondary), thus the amount of cooling water from the primary source will be maximized and that from the secondary source will be minimized. The target set is shown in Figure 4.2.

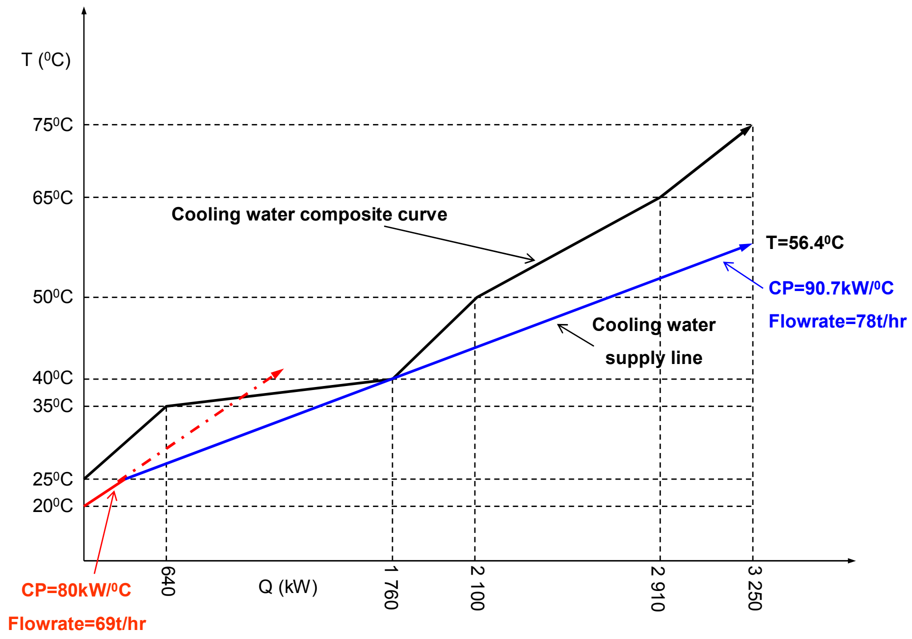


Figure 4.2 Targets for case 2

Figure 4.2 shows that targeting holistically significantly reduces the overall cooling water requirement (from 90 ton/hr to 78 ton/hr). The overall cooling water requirement (78 ton/hr) is more than the maximum design capacity of cooling tower A (69 ton/hr) thus, cooling tower B has to be used to supplement it. Furthermore, the return temperature to cooling tower B is also significantly reduced (from 73.2°C to 56.4°C). The overall performance of the cooling towers is improved, i.e. less water is required for the removal of the same amount of heat.

4.2 Design Procedure

When designing for case 1, the subsystems are designed as independent systems using the water mains method as described in section 3.2 above. Lines representing the cooling water using operations are placed on a grid diagram, indicating the maximum inlet and maximum outlet temperatures as well as the cooling duty required in terms of the heat capacity flowrate, CP. The next step is to connect the cooling water operations which are below the pinch (those that are not connected to the water mains) to the water mains. This is followed by connecting the cooling water operations that cross the pinch mains to fulfill the cooling requirement.

Then, the intermediate and pinch mains are removed. Finally the cooling water operations are connected directly. The final cooling water network design for case 1, which meets the target set in Figure 4.1, is shown in Figure 4.3.

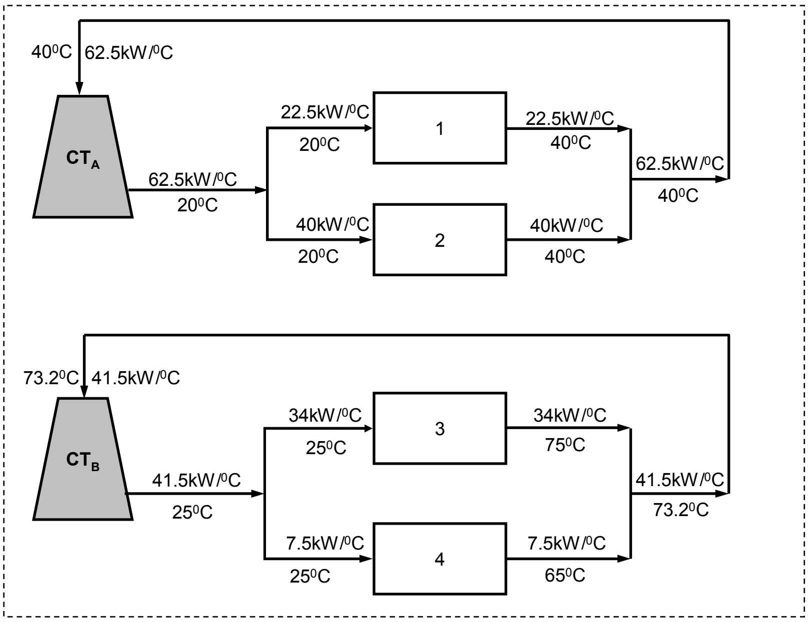


Figure 4.3 Final cooling water network design using case 1

For case 2, the system is analysed in a holistic manner. The network is first supplied by the primary source and then the secondary source is used to fulfill the overall cooling water requirement. The steps for designing the network are shown in Figures 4.4 to 4.8.

Step 1 Generate the grid diagram with the water mains representing all the cooling water sources, the pinch point, the intermediate temperature(s) and the highest exit temperature. Plot all the cooling water using operations as shown in Figure 4.4.

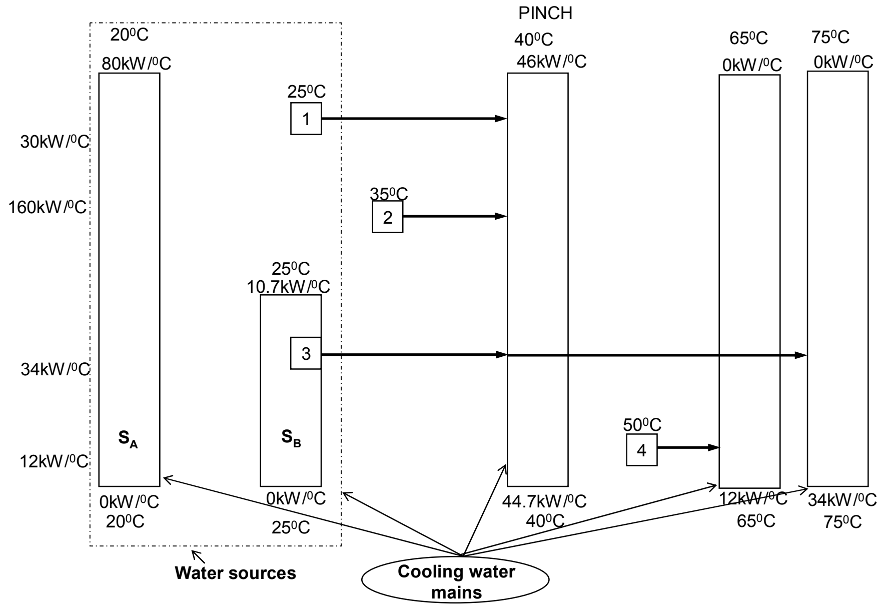


Figure 4.4 Design procedure step 1

Step 2 Connect the operations to the water mains as shown in Figure 4.5.

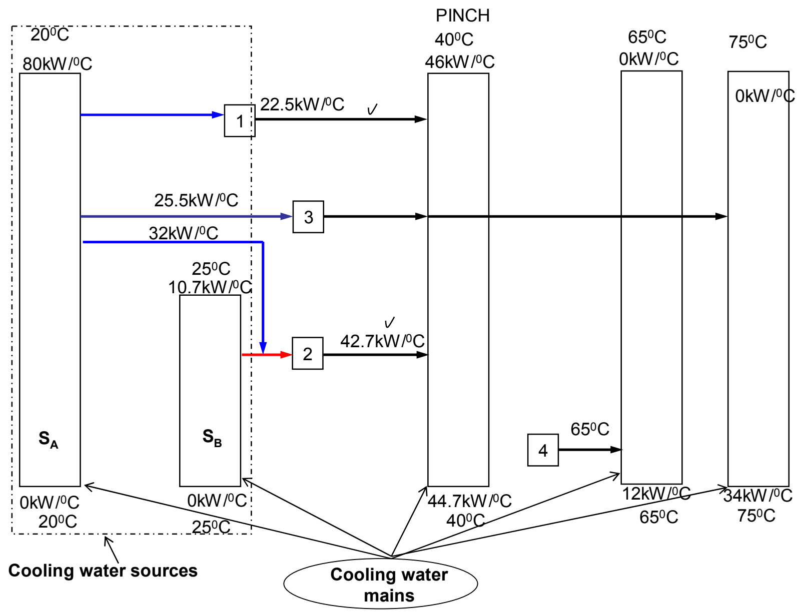


Figure 4.5 Step 2 for the design procedure

Step 3: Merge all operations that cross the pinch as shown in Figure 4.6.

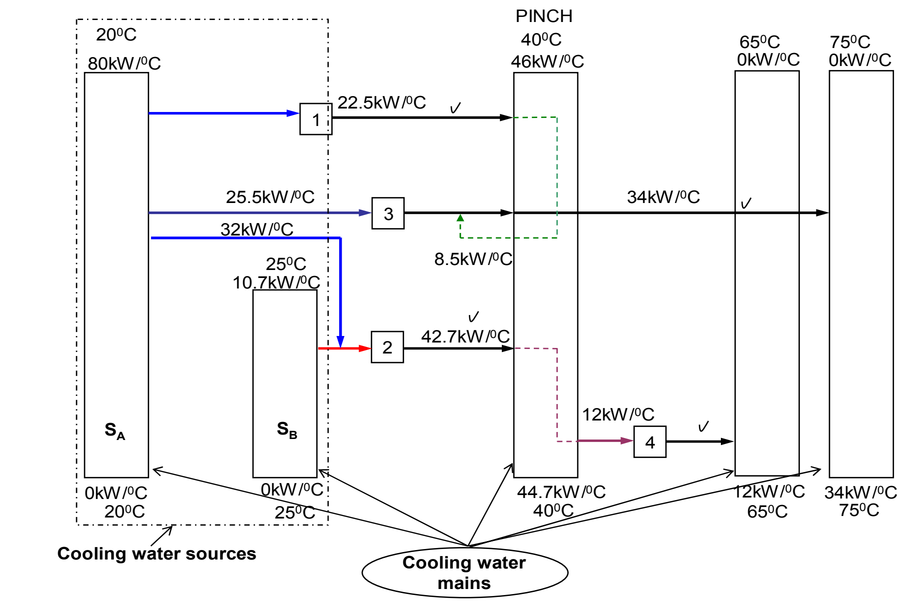


Figure 4.6 Step 3 for the design procedure

Step 4 Remove the intermediate pinch as shown in Figure 4.7.

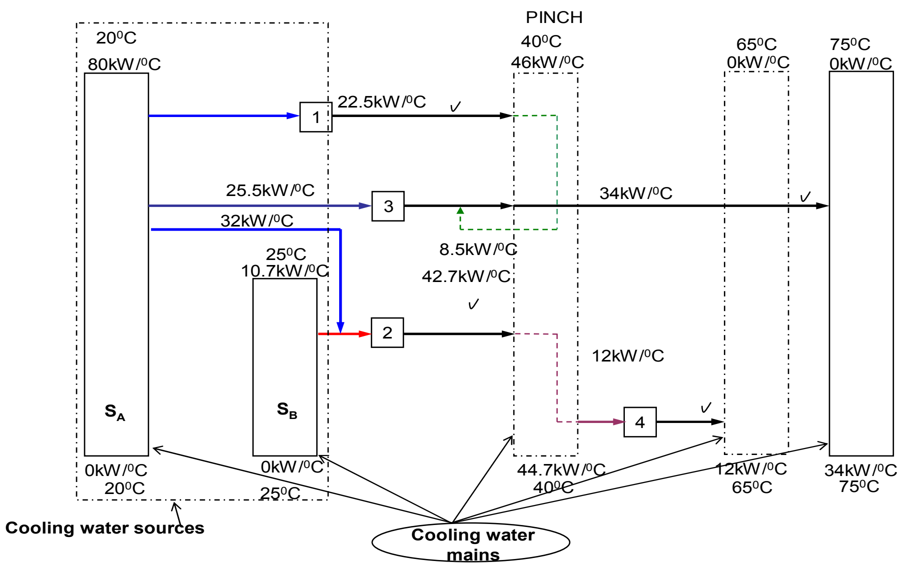


Figure 4.7 Step 4 of the design procedure

Step 5 Connect the cooling water operations directly as shown in Figure 4.8.

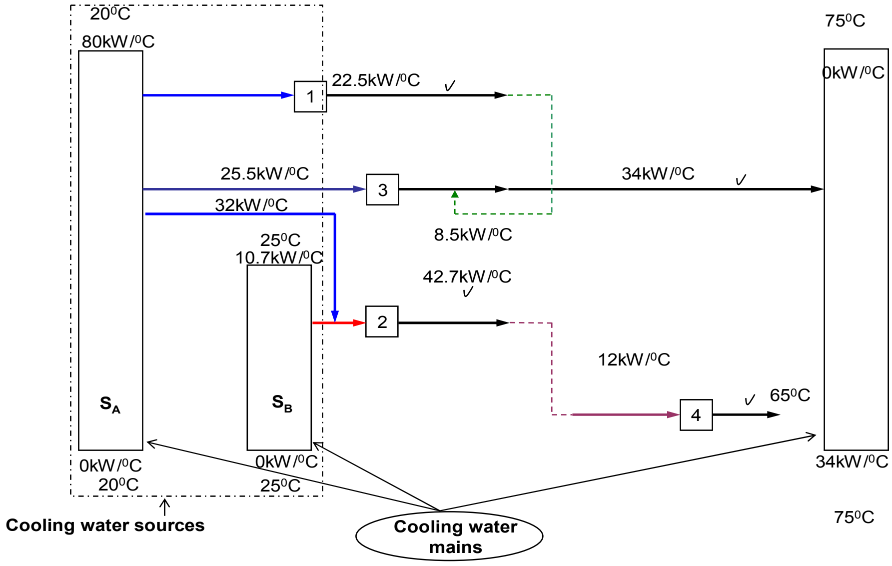


Figure 4.8 Step 5 of the design procedure

The final design obtained for case 2 which meets the target set in Figure 4.2 is shown in Figure 4.9. This shows the actual layout of the cooling water network, with the cooling towers and cooling water using operations in place. Cooling water operation 2 is supplied by both cooling tower A and cooling tower B. This forms the main interaction between cooling tower A and cooling tower B. The rest of the cooling water operations are supplied by one cooling tower or by other operations, i.e. water from other operations is reused.

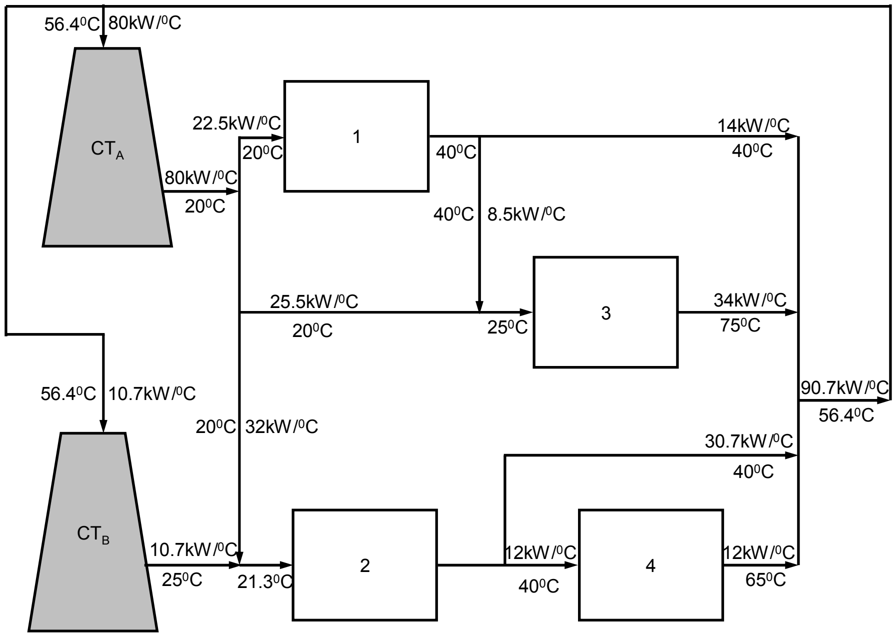


Figure 4.9 Final design for the illustrative example using case 2

4.3 Results and Discussion

Table 4.2 summarizes the results obtained for cases 1 and 2, which includes the overall cooling water requirements and the overall performance of the cooling towers. The overall performance of cooling tower A and cooling tower B for cases 1 and 2 was analysed using an artificial performance factor (φ) represented by Equation 4.1.

$$\varphi_k = \frac{\Delta T_k}{Flowrate_k}, k \in K = \{k \mid k = Cooling\ Tower\} \tag{4.1}$$

In Equation 4.1, ΔT_k is the temperature difference between the return temperature and the supply temperature of cooling tower *k*. The flowrate is the amount of cooling water required to cool the cooling water using operations. Since the intention of this investigation is to reduce flowrate, thereby increasing return temperature, an increase in the factor φ is associated with improved cooling tower performance.

Table 4.2 Comparison of case 1 and case 2 results

	Flowrate (ton/hr)	**Performance Factor (φ) (^{0}C.s/kg)**
Case 1		
Cooling Tower A	54	1.3
Cooling Tower B	36	4.9
Overall	**90**	
Case 2		
Cooling Tower A	69	1.9
Cooling Tower B	9	12.3
	78	

The increase in the performance factors for both cooling towers as shown in Table 4.2, suggests an overall increase in the cooling tower performance for both cooling tower A and cooling tower B (Bernier, 1994). Furthermore, the overall cooling water requirements presented in Table 4.2, show that analyzing the system in a holistic manner reduces the overall amount of cooling water required, thus improving the performance of the cooling towers. Although the amount of cooling water required from cooling tower A is increased, the overall performance of the cooling tower is improved. When assessing the results for cooling tower B, it can seen that the flowrate required decreases significantly and the return temperature also decreases because there is mixing between the water supplied by cooling tower A and cooling tower B when heat is removed from the cooling water using operations.

5 APPLICATION TO AN AFRICAN EXPLOSIVES LIMITED (AEL) PROCESS

The process used is for the production of nitrates. At steady state, the process generates enough steam to fulfill the heating requirement and excess steam is exported to other sections of the facility. Figure 5.1 below shows the preliminary targeting results of the process using heat exchanger network design.

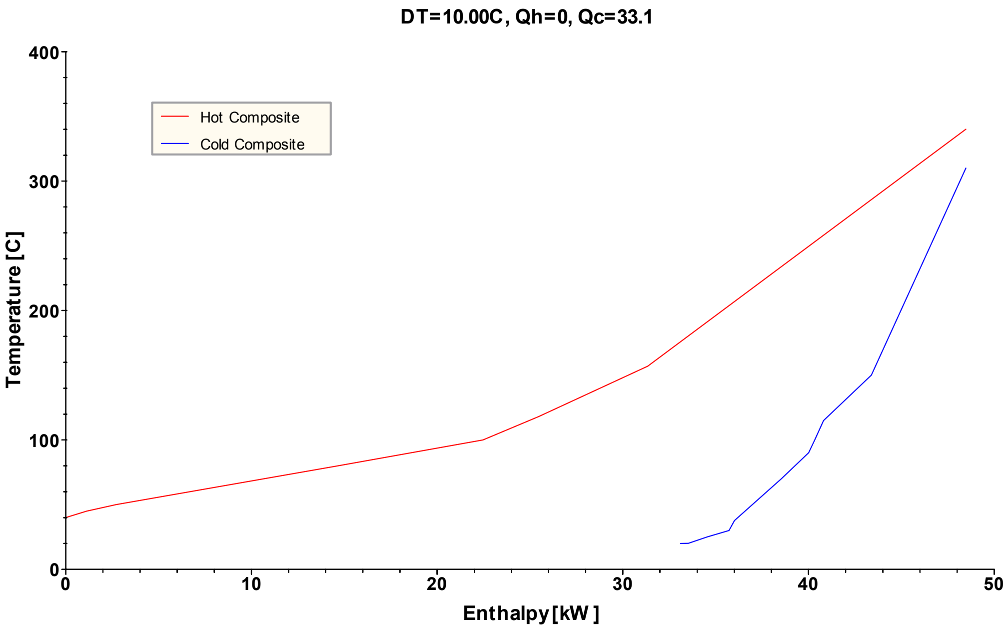


Figure 5.1 Utility targets for the heat exchanger network

Figure 5.1 confirms that there is no external hot utility required and also shows that the external cold utility required is 33.1 MW. Hence the focus of the study was on the optimization of the amount of cooling water used in the system. The cooling water network is supplied by one counter-current induced draft cooling tower. The cooling water network is predominantly heat exchangers with a parallel-series configuration as shown in Figure 5.2. The process stream data of the case study is shown in Table 5.1 and the current cooling water data is given in Table 5.2.

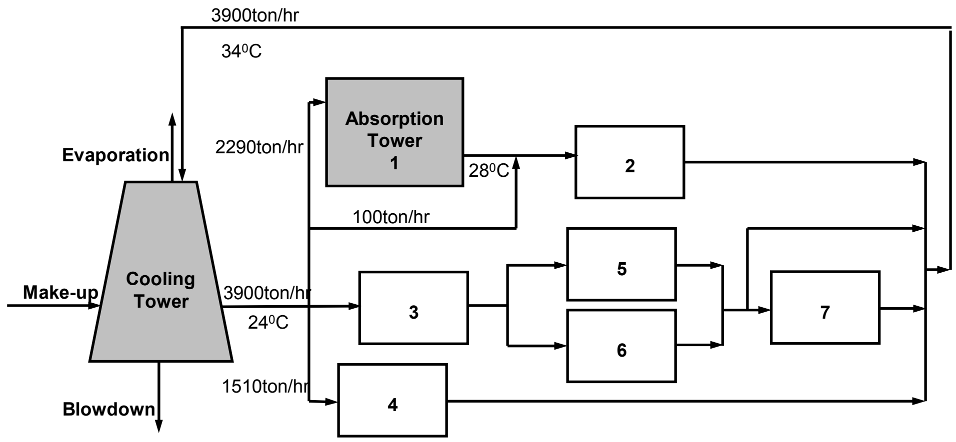


Figure 5.2 Cooling water network for a nitrates production facility

Table 5.1 Process stream data for the case study

Heat Exchanger	T_{supply} (^{0}C)	T_{target} (^{0}C)	Duty (kW)
1	52	25	10 700
2	115	45	16 700
3	100	40	13 500
4	48	39	300
5	118	50	1 100
6	114	50	4 400
7	20	30	-2 000

Table 5.2 Current cooling water data for the case study

Heat Exchanger	T_{supply} (^{0}C)	T_{target} (^{0}C)	Duty (kW)
1	24	28	10 700
2	28	34	16 700
3	24	32	13 500
4	24	29	300
5	32	34	1 100
6	32	36	4 400
7	35	34	-2 000

Currently the process requires 3900 ton/hr of cooling water with about 59% (2290 ton/hr) used by the absorption tower. 41% (1610 ton/hr) of the cooling water supplied by the cooling tower is used by the rest of the heat exchangers before it is returned to the cooling tower at a higher temperature. Currently the return temperature to the cooling tower is 34°C and the supply temperature is 24°C. Some of the cooling water is lost in the cooling tower through evaporation, windage and blowdown. Blowdown is necessary for the prevention of salts and nitrates accumulation in the system. Water lost is replaced by a freshwater makeup stream.

Since most of the inlet temperatures of the process streams have temperatures above 100°C it is evident that the limiting cooling water data cannot be set by directly using the minimum temperature difference on each end of the operation. Subtracting the minimum temperature difference from the process temperatures on each end of the heat exchangers to obtain the limiting cooling water temperature is not straightforward in this case as it will result in the return temperature close to or above 100°C. Hence, engineering insight and knowledge of the process is required to obtain the limiting cooling water data. The limiting cooling water data was thus obtained by adding 10°C to the current cooling water exit temperatures of the heat exchangers as shown in Table 5.3.

Table 5.3 Limiting cooling water data for the case study

Heat Exchanger	**T_{supply} (^{0}C)**	**T_{target} (^{0}C)**	**Duty (kW)**
1	24	28	10 700
2	28	44	16 700
3	24	42	13 500
4	24	29	300
5	32	44	1 100
6	32	46	4 400
7	35	44	-2 000

The exit temperature of heat exchanger 4 was not changed due to limited information on the unit operation. Also, for practical reasons, the exit temperature of the absorption tower (water using operation 1) was not changed.

In the assessment of the network, it is evident that the cooling water network has two cooling water sources, i.e. the cooling tower (primary source) and the absorption tower (secondary source), as shown in Figure 5.3. This system is unique in that, the cooling water required by the secondary source is supplied by the primary source. The absorption tower is treated as a secondary cooling water source rather than one of the cooling water using operations due to the fact that its cooling water supply is always fixed. As a process requirement, the amount of cooling water required by the absorption tower is fixed and cannot be manipulated. Therefore, in this case, the objective is to maximize the amount of cooling water that is reused from the secondary source, whilst minimizing the amount of water from the primary source. This is the direct opposite of the case presented in section 3.1 and illustrated in the previous example. The analysis is, therefore, reversed as detailed in the following sections.

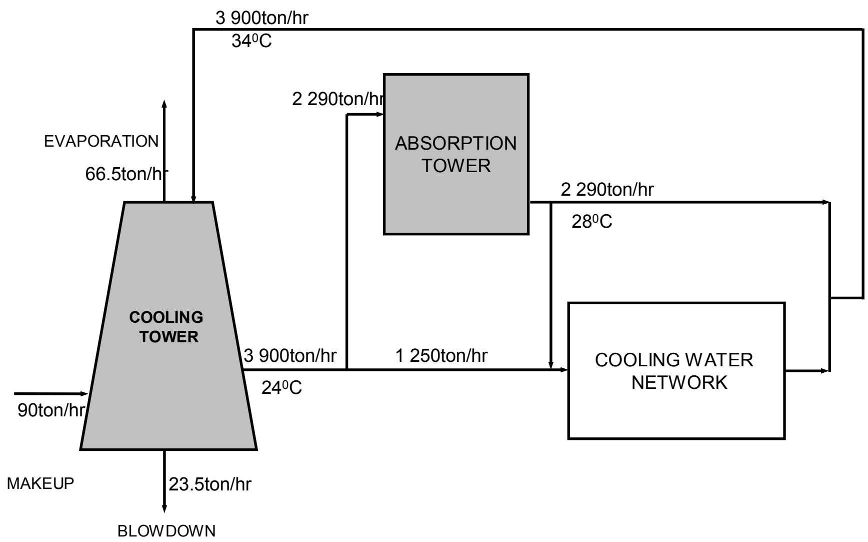


Figure 5.3 Two sources of cooling water to the cooling water network

5.1 Targeting

The case study analysed is a *special system* in that, in order to obtain an optimal solution, the amount of cooling water from the secondary cooling water source should be maximized instead of maximizing the cooling water from the primary source as required in ordinary systems presented earlier in this report. In this case, the secondary cooling water source has a fixed cooling water requirement and this is supplied by the primary cooling water source, as shown in Figures 5.2 and 5.3. In order to minimize the overall amount of cooling water required from the cooling tower the amount of cooling water supplied directly from the cooling tower to the other cooling water using operations should be minimized, since the stream to the absorption tower is fixed. This can only be achieved by maximizing the amount of cooling water reused from the secondary cooling water source, i.e. the absorption tower. The procedure for constructing the cooling water supply line for this case is described below. Water using operation 7 is not included in the construction of the limiting cooling water curve, because in that unit, cooling water is used as a hot stream. This is characterized by higher inlet cooling water temperature than the exit temperature. The limiting cooling water composite curve is only constructed considering the operations where the cooling water is used as a cold stream which is heated from a lower to a higher temperature.

The amount of cooling water used from the primary source is minimized by allowing its supply line to form a pinch with the composite curve at a temperature equal to or below that of the subsequent cooling water source. Figure 5.4 illustrates targeting when two cooling water sources supply a system of cooling water using operations.

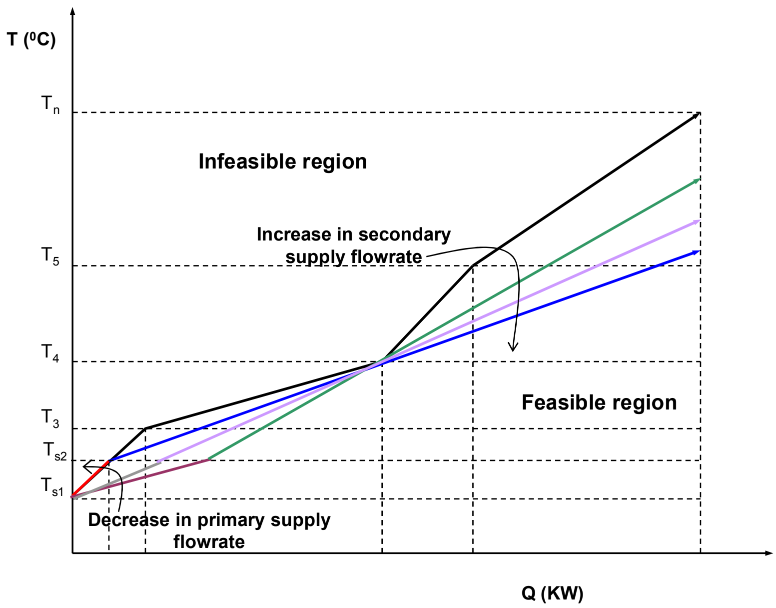


Figure 5.4 Targeting procedure for *special systems*

From Figure 5.4, it can be seen that as the amount of cooling water from primary source is decreased, the amount required from secondary source is increased as shown by the arrows. The limit is set when the cooling water supply line for the primary cooling source forms a pinch with the limiting cooling water composite curve. In the illustration in Figure 5.4, this occurs when the cooling water supply line is exactly on top of the limiting cooling water composite curve. Further decrease in primary cooling water supply would result in infeasibility as the composite curve forms the boundary between the feasible and infeasible regions. Targeting in this manner ensures that as much cooling water as possible is used from the secondary cooling water source.

The cooling water target set for the case study is shown in Figure 5.5.

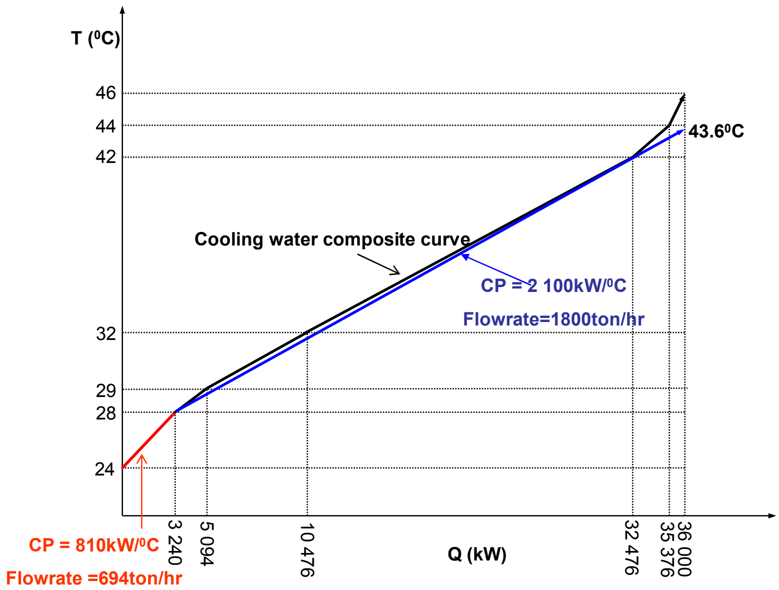


Figure 5.5 Target for case study

Figure 5.5 shows that the supply line for the primary cooling water source is directly on top of the cooling water composite curve. The overall target shown in Figure 5.5 for part of the network is 1800 ton/hr. This includes the cooling water obtained directly from the primary source (694 ton/hr) and part of the cooling water which is used in the secondary source (1106 ton/hr). The cooling water from the secondary source which is not reused anywhere else in the network (1184 ton/hr) is recombined with water from the rest of the cooling water network before being returned to the cooling tower (primary source). Thus, the temperature shown at the end of the cooling water supply line in this case does not reflect the return temperature to the cooling tower. The return temperature is obtained by calculating the temperature of the mixture of cooling water from the secondary source which is not reused anywhere else in the system and the cooling water from the rest of the network. In this case, the final temperature is 37°C.

5.2 Design Procedure

The design procedure adopted is similar to that of ordinary cooling water systems with multiple cooling water sources. On the grid diagram each cooling water source is represented by water mains. The pinch point and the exit temperature are also represented by water mains. The cooling water using operations are supplied by the primary cooling water source before the cooling water from the secondary source can be used. The design of the final network is performed in five steps as outlined in section 3.2 of this report. The final cooling water network design obtained for the case study is shown in Figure 5.6. Table 5.4 shows the current cooling water requirements as well as the reduced cooling water requirements obtained using the methodology developed.

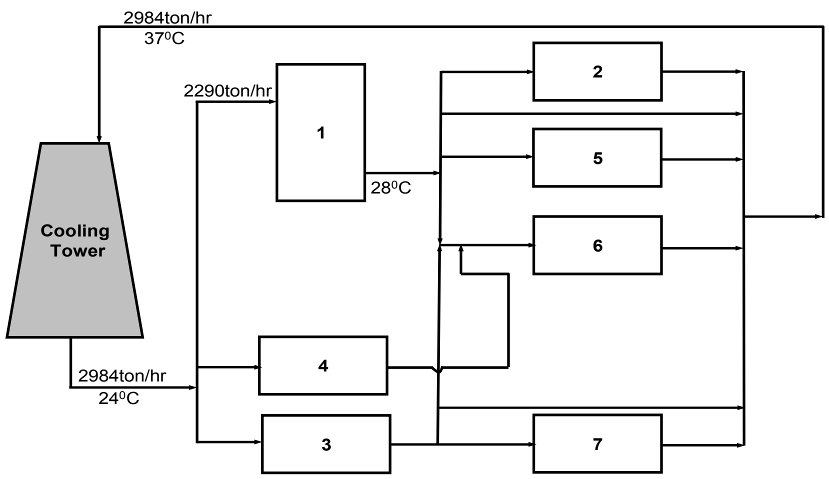


Figure 5.6 Improved cooling water network design for case study

Table 5.4 Cooling water requirements for the new improved cooling water network

Heat Exchanger	T_{supply} (^0C)	T_{target} (^0C)	Flowrate (ton/hr)	New Flowrate (ton/hr)
1	24	28	2 290	2 290
2	28	44	2 390	895
3	24	42	1 450	643
4	24	29	60	51
5	32	44	450	59
6	32	46	900	269
7	35	34	1 700	214

6 DISCUSSION

Analysing the nitrates production facility using the new methodology results in significant reduction in the amount of cooling water required by the individual cooling water using operations as well as the overall cooling water requirement. The cooling water requirement is reduced by 23%. The return temperature is slightly increased from 34°C to 37°C. The impact of this increase in the return temperature to the performance of the cooling tower and the exit cooling water at the bottom of the cooling tower were investigated using a cooling tower model discussed in the following section.

When looking at Figures 5.2 and 5.6 there are no major changes in the overall layout of the process. There are a few additional pipes that will need to be added. Considering the benefit of the reduced utility requirements, it could be worthwhile to make the necessary changes. However, the effects of the pressure drop will have to be investigated before any decision is made. This does not form part of the presentation made in this report.

7 COOLING TOWER MODEL AND EFFLUENT REDUCTION CONSIDERATIONS

The cooling tower model developed by Kim and Smith (2001) was used to analyse the thermal performance of a case study cooling tower. The model was developed for a mechanical draft countercurrent cooling tower, with air entering at the bottom and leaving at the top and cooling water entering at the top and leaving at the bottom of the cooling tower. The main assumption of the model was that the flowrate of the cooling water remains constant from the top to the bottom of the tower.

Moreover, the model also included Equations (7.1), (7.2) and (7.3) for calculating evaporation (*E*), blowdown (*B*) and makeup (*M*), respectively (Perry, 1997).

$$E = 0.00085(1.8)F_2(T_2 - T_1) \tag{7.1}$$

$$B = \frac{E}{CC - 1} \tag{7.2}$$

$$M = E + B \tag{7.3}$$

Where, E is the evaporation, B is the blowdown rate, M is the makeup stream CC is the cycles of concentration, F_2 is the cooling water flowrate, T_2 and T_1 are the inlet and exit cooling water temperatures, respectively.

Blowdown is the effluent produced by the cooling tower. It is removed from the cooling tower to reduce the concentration of the insoluble salts and nitrates which accumulate when cooling water is evaporated. When the salts are allowed to concentrate, they can deposit on the tubes of the heat exchangers thus causing fouling which affects the heat transfer rate. Likewise, when the nitrates are allowed to accumulate, they can cause acidification of water and subsequent corrosion of the pipeline. The results obtained using the model are discussed below.

Table 7.1 below shows the current flowrates for evaporation, blowdown and freshwater makeup as well as the results obtained using the above equations. The results are based on a cooling tower running at 6 cycles of concentration, which is the current setting of the cooling tower under investigation.

Table 7.1 Cooling tower evaporation, blowdown and makeup

	Current T_{L1}**=24^{0}C,** T_{L2}**=34^{0}C**	**New** T_{L1}**=23.4^{0}C,** T_{L2}**=37^{0}C**
E (ton/hr)	60	62.6
B (ton/hr)	23.5	12.5
M (ton/hr)	83.5	75.2

The results in Table 7.1 indicate that when the inlet cooling water temperature at the top of the cooling tower is 37°C, the exit cooling water temperature at the bottom of the cooling tower is 23.4°C. When using these conditions (T_{L1}=23.4^{0}C and T_{L2} = 37^{0}C), the blowdown rate is reduced by 47% and the evaporation rate is increased slightly (4%). This implies that the makeup stream is reduced by 10%. Thus the overall cooling water effluent produced and cooling water consumption are both reduced by using the lower flowrate.

8 CONCLUSIONS AND RECOMMENDATIONS

The conclusions that can be drawn from the research study conducted are discussed below.

1. Analyzing a system with multiple cooling water sources discretely results in higher cooling water requirements. A graphical technique for setting targets in systems comprising multiple cooling towers has been developed. Its performance has been demonstrated using an illustrative example system with two cooling water sources and four cooling water using operations whereby it reduced the cooling water requirement by 13%. Although this method has been demonstrated on systems with two cooling water sources, it can be readily applied to more complex systems with more than two cooling water sources. The adaptation of the methodology to a special system has also been demonstrated through a case study, where the cooling water requirement was reduced by 23%.

2. To obtain the optimum solution when using multiple cooling towers with different supply temperatures, all the cooling water from the primary source should be used first before using water from any other cooling water source. The target for the cooling tower with the highest supply temperature is set by the pinch.

3. When the new methodology was applied to an existing nitric acid production facility, results showed that there exists a potential to reduce the overall cooling water requirement from 3900 ton/hr to 2984 ton/hr, i.e. 23% reduction. This reduction is concomitant with a slight increase in the return temperature from 34°C to 37°C.

4. The cooling tower model developed by Kim and Smith (2001) was used to demonstrate that the high return temperature of 37°C obtained with the new cooling water network would not adversely affect the supply temperature to the cooling water network. The results from the model indicated that when the return temperature was 37°C, the inlet cooling water temperature to the cooling water network was 23.4°C. This is lower than the current value of 24°C, which shows that more heat is removed by the cooling tower, thus the performance of the cooling tower is improved.

5. The model was also used to investigate the impact of the new cooling water flowrate on the effluent production and the requirement of cooling water makeup. The results obtained showed that there exists a potential to reduce the blowdown rate by 47% and the freshwater makeup by 10%.

6. Reducing the blowdown rate by 47% has a potential to reduce the blowdown treatment cost by almost R480 000 per year.

7. The amount of salination was reduced although the heat duty remains the same because the amount of salts discharged to the water system is reduced as the amount of blowdown leaving the cooling tower is reduced.

Based on the conclusions given above, the following recommendations can be made:

1. Heat exchanger network design (HEN) should be done prior to designing the cooling water network, to investigate the possibility of reducing the overall amount of external utilities that are required by the process thus saving energy and reducing operating costs.

2. The cycles of concentration of the cooling tower have a significant impact on the amount of effluent produced, thus the optimal value should be investigated as another way of reducing the amount of effluent produced.

3. The graphical technique presented in this report is such that the return temperature is not fixed, i.e. there is no limit to the value of the return temperature. In reality, one finds that the maximum return temperature is set by either fouling considerations, corrosion or design considerations of the cooling tower packing. In these instances, the final water supply line is set by the maximum acceptable return temperature. It is possible that this line would not form a pinch with the limiting cooling water composite curve, thus it will not be possible to obtain the minimum cooling water requirement directly. The water mains method presented is based on the concept of the pinch point and can not be readily applied to cases where there is no pinch. In this case, the pinch migration method suggested by Kim and Smith (2001) can be adopted. In this method, the limiting cooling water composite curve is allowed to move along the temperature axis until a new pinch is

formed. The details of how to find the new pinch point and how to modify the composite curve are given in Kim and Smith (2001). The pinch migration and temperature shift method enables design with any target temperature (Kim and Smith, 2001). The cooling water flowrate obtained this way may be minimum but not necessarily optimal.

4. The graphical technique as presented in this report assumes that premixing and post mixing are acceptable. Premixing refers to a situation where, cooling water from different cooling water sources is mixed before it is used in any water using operation. Post mixing refers to a situation where cooling water which has been used in the cooling water using operations is mixed before it is returned to the cooling water sources. There may exist situations where premixing is not acceptable due to geographical constraints or maximum supply temperature acceptable. Moreover, there may be situations where post mixing is not allowed due to the maximum return temperatures acceptable for the various cooling water sources or due to the process layout. For these reasons, there is a need to investigate a way of incorporating these constraints to the graphical technique. However, it is possible to set these constraints when mathematical formulation is used.

9 GLOSSARY

B	blowdown
CC	cycles of concentration
CP	heat capacity flowrate
E	evaporation rate
F_2	circulating water flow at cooling tower inlet
M	makeup water
Q	Heat duty
T	temperature
T_1	inlet water temperature for the cooling tower
T_2	outlet water temperature for the cooling tower
ΔT_{min}	minimum temperature difference

Greek letters

φ_κ	artificial performance factor

Subscripts

CW	cooling water
in	inlet conditions
int	intermediate
max	maximum
min	minimum
pinch	pinch point
return	return temperature
s	source

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PART 3

Technology Transfer and Capacity Building Reports

CAPACITY BUILDING REPORT

Four students were employed in this project, of whom three are black Africans, one is Indian and one is female. Professor Thokozani Majozi, the University of Pretoria lead researcher is also black African. Details are provided in Table CB1 below.

Table CB1. Students involved in WRC Project K5/1368

Institution	Student	Degree	Year	Race	Gender
University of Cape Town	Mr K. Ndwandwe	M.Sc. (Eng)	2003	B	M
	Mr A. Isiafaide	Ph.D.	In progress	B	M
Indian Institute of Technology, Bombay	Mr P. Basnal	B.Tech (Eng)	2004	I	M
University of Pretoria	Ms N.S Nyathi	M.Eng.	In progress	B	F

TECHNOLOGY TRANSFER REPORT

This project generated the following outputs in terms of technology transfer.

1 UNIVERSITY OF CAPE TOWN OUTPUTS

Computer software (1)

Targeting package for the analysis of heat and mass exchange systems, including special section on water pinch. This package runs on Excel.

Journal Publications (4)

"Determination of Mass Separating Agent Flows Using the Mass Exchange Grand Composite Curve," Duncan Fraser, Michael Howe, Andre Hugo and Uday Shenoy, 83(A12), 1381-1390, Chem Eng Research and Design, 2005.

"The influence of particle size on energy consumption and water recovery in comminution and dewatering systems", Mwale, A.H., Musonge, P., and Fraser, D.M., Minerals Engineering, 18, 915-926, 2005.

"A New Method For Sizing Mass Exchange Units Without The Singularity Of The Kremser Equation", Fraser, D.M., and Shenoy, U.V, Computers and Chem Eng, 28(11), 2331-2335, 2004.

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Theses (1)

"A Spreadsheet-Based Tool For The Synthesis Of Heat And Mass Exchange Networks", Ndwandwe, K.P., M.Sc.(Eng), 2003.

International conference publications (6)

"New Hybrid Method for Mass Exchange Network Optimisation," Emhamed, A. M.; Lelkes, Z.; Rev, E.; Farkas, T.; Fonyo, Z.; Fraser, D.M., European Symposium On Computer Aided Process Engineering – 15, Ed: Puigjaner, L. & Espuña, A., Elsevier, 2005, ISBN: 0-444-51987-4, p. 877-882.

"Selection of Mass Separating Agents in Mass Exchange Network Synthesis", Fraser, D.M., Howe, M., Hugo, A., and Shenoy, U.V., Proceedings of ECOS 2005 Conference, Trandheim, Norway, June 2005.

"Process Synthesis: Design For Improved Effectiveness", Fraser, D. M., Proceedings Regional Symposium on Chemical Engineering, Manila, 7-1 to 7-8, 2003.

"Hybrid Synthesis Method for Mass Exchange Networks", Msiza, A.K., and Fraser, D.M., European Symposium on Computer Aided Process Engineering - 13, Eds. A. Kraslawski and I. Turunen, Elsevier, Amsterdam, 227-232, 2003.

"A New Method for Sizing Mass Exchanger Units without the Singularity of the Kremser Equation", Shenoy, U., and Fraser, D.M., European Symposium on Computer Aided Process Engineering - 13, Eds. A. Kraslawski and I. Turunen, Elsevier, Amsterdam, Supplement, 9-14, 2003.

"Comparison of different mathematical programming techniques for mass exchange network synthesis", Szitkai, Z., Msiza, A.K., Fraser, D.M., Rev, E., Lelkes, Z., Fonyo, Z., Proceedings ESCAPE-12 Conference, Holland, 361-366, 2002.

Local conference publications (3)

"A New Method for Sizing Mass Exchange Units", U.V. Shenoy and D.M. Fraser, SAIChE Congress 2003, Sun City, 3-5 September 2003.

"Hybrid Synthesis Method for Mass Exchange Networks", A.K. Msiza and D.M. Fraser, SAIChE Congress 2003, Sun City, 3-5 September 2003.

"A Spreadsheet-Based Tool for Synthesis of Heat and Mass Exchange Networks", K.P. Ndwandwe and D.M. Fraser, SAIChE Congress 2003, Sun City, 3-5 September 2003.

2 UNIVERSITY OF PRETORIA OUTPUTS

Routine feedback sessions with AEL were given during the course of the project. The following summarizes the presentations and publications related to this research project.

Majozi T. and N. Nyathi, Process Design and Process Integration, *PRES'05 8th Conference on Process Integration, Modeling and Optimization for Energy Saving and Pollution Reduction, Giardini di Naxos, Sicily, 15-18 May 2005*: (Poster Presentation)

Majozi, T and N. Nyathi, "On cooling water and effluent reduction in systems with multiple cooling water sources – a pinch design philosophy", *Chemical Technology Innovations Awards,* November 2005 – *3rd Place*

Two journal articles have since been submitted to international journals.