INTERVAL BASED MINLP SUPERSTRUCTURE SYNTHESIS OF HEAT AND MASS EXCHANGE NETWORKS

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ABSTRACT

This study presents a new technique for synthesizing heat and mass exchange networks. The method involves generating superstructures using the temperature/composition interval concept from the physical insight approach. The superstructures are partitioned into temperature/composition intervals using the supply and target temperatures/compositions of either the hot/rich or cold/lean set of streams. The opposite kind of streams are made to participate (float) in all the intervals defined. Their ability to exchange heat/mass in these intervals is however subject to thermodynamic feasibility. The resulting superstructure is optimised as a mixed integer non linear programming (MINLP) model. The superstructure is hot/rich streams based if hot/rich streams are used to define the intervals otherwise it is cold/lean stream based.

In the superstructure, every stream has the potential of splitting into however many streams of the opposite kind there are in each interval in order to exchange heat/mass with such streams. The split branches are automatically mixed at equal temperatures/compositions. The total heat/mass exchanged by a stream in an interval defines the temperature/composition of the next interval boundary location.

This method does not involve partitioning the network into above and below the pinch regions. Moreover since the temperatures/compositions of streams at interval boundaries which they do not define but cross are treated as variables to be optimised, there is no strict adherence to the philosophy of vertical heat/mass transfer. This implies that streams with significantly different heat transfer coefficients can be effectively handled and the costs which contribute to the total costs can be simultaneously optimised.

Apart from the benefit of automatically mixing split streams at equal temperatures/compositions, another benefit of partitioning superstructures in this manner is that techniques for initialisation and setting of bounds are simplified since key variables such as temperatures/compositions which determine driving forces are used to set up problem specific superstructures.

The interval based MINLP superstructure (IBMS) for heat and mass exchange networks developed in this study has been applied to relatively small problems adapted from the literature. Such problems involve single and multiple utilities, single and multiple lean (process and external) streams, stagewise and continuous contact columns, regeneration, non-linear equilibrium relations, multiperiod heat exchange operations and combined heat and mass exchange networks. The solutions obtained are comparable with those in the literature in terms of cost and simplicity of networks, far much less computational effort and much easier initialisation and setting of bounds. The IBMS even gives better total costs or simpler networks in some cases.

This study is the first to use the same superstructure framework for heat and mass exchanger networks synthesis. It has also shown that the new IBMS technique is effective for finding near optimum solutions for a wide range of heat and mass exchange network problems.

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NOMENCLATURE

Abbreviations

AC	area cost coefficient
ACC	annualised capital costs
AE	area exponent
AOC	annual operating cost
CE	cold end
CHAMENS	combined heat and mass exchanger network synthesis
COG	coke oven gas
CS	cold start
CU	cold utility
CUC	per unit cost of cold utility
CUP	cheapest utility principle
CW	cooling water
DFP	driving force plot
DOP	duration of period
EMCD	exchanger minimum composition difference
EMAT	exchanger minimum approach temperature
EOR	end of operation
FCp	heat capacity flowrate
FLM	fairly linear model
GCC	grand composite curve
HE	hot end
HENS	heat exchanger network synthesis
HMPS	high medium pressure steam
HPS	high pressure steam
HRAT	heat recovery approach temperature
HS	hot start
HTU	height of theoretical units
HU	hot utility

HUC	cost per unit of hot utility
IBMS	interval based MINLP superstructure
LMTD	logarithmic mean temperature difference
LP	linear programming
LPG	liquefied petroleum gas
LPS	low pressure steam
MENS	mass exchange network synthesis
MILP	mixed integer linear program
MINLP	mixed integer non linear program
MinNU	minimum number of units
MinNST	minimum number of stages
MOC	minimum operating cost
MOR	middle of operation
MPS	medium pressure steam
MSA	mass separating agent
NB	total number of composition intervals (or stages)
NK	total number of temperature intervals (or stages)
NLP	non linear program
NOB	total number of composition locations (boundaries)
NOK	total number of temperature locations (boundaries)
NOP	number of period
NTU	number of theoretical units
OLD	optimum load distribution
RPA	remaining problem analysis
TAC	total annual cost
TCC	total capital cost
SOR	start of operation
SWS	stagewise superstructure
U	overall heat transfer coefficient
VGO	vacuum gas oil

Symbols

$\Delta T_{\min}$	minimum temperature difference
ΔT_{lm}	logarithmic mean temperature difference
Δy	rich stream composition difference
Δy_{min}	minimum composition difference in the rich phase
Δy_{lm}	logarithmic mean composition difference
$	conditional operator

General notations

CM	set of components
DS	mass exchanger column cross sectional area
$Qc_{\min}$	minimum cold utility
$Q_{H\min}$	minimum hot utility
h	stream film heat transfer coefficient
HU^{UP}	hot utility upper bound
Kya	overall mass transfer coefficient based on rich stream
m	equilibrium constant
N_C	number of cold stream
N_H	number of hot stream
N_R	number of rich stream
N_{real}	number of real stages
N_S	number of lean stream
N_{SP}	number of process lean stream
N_{SE}	number of external lean stream
T_c	temperature of cold stream
T_h	temperature of hot stream
w_i	mass load of stream
x	composition of lean stream
y	composition of rich stream

HENS notations in Chapter 3

Sets

H	hot process and utility streams
C	cold process and utility streams
K	temperature intervals in superstructure

Indices

i	hot process or utility stream
j	cold process or utility stream
k	index for temperature interval location (k = 1,….. NOK)

Parameters

AC	area cost coefficient
AE	area cost index
CF	fixed charge for exchangers
CUC	cost per unit of cold utility
HUC	cost per unit of hot utility
h_c	stream heat transfer coefficient
T_k	temperature of location or interval boundary k
T_i^s	supply temperature of hot stream i
T_i^t	target temperature of hot stream i
T_j^s	supply temperature of cold stream j
T_j^t	target temperature of cold stream j
$U_{i,j}$	overall heat transfer coefficient
Ω_h	upper bound for heat exchanged in match i,j
Γ_h	upper bound for driving force in match i,j

Binary variables

z_{ijk}	variable indicating the existence of match i,j in interval k in the optimal network

Positive variables

dt_{ijk}	driving force for match i,j in interval k
F_i	flow rate of hot stream i
F_j	flow rate of cold stream j
q_{ijk}	heat exchanged between stream i and stream j in temperature interval k
$t_{i,k}$	temperature of hot stream i at hot end of interval k
$t_{j,k}$	temperature of cold stream j at hot end of interval k

MENS notations in Chapter 4

Sets

R	rich process streams
S	lean streams (process and external mass separating agents)
V	regenerating streams
B	composition intervals in the superstructure

Indices

r	rich process stream
l	lean stream (process or external mass separating agents)
v	regenerating stream
b	index for composition interval location (b = 1,……,NOB)

Parameters

AC_l	annual operating cost per unit of lean stream l
AC_v	annual operating cost per unit of regenerating stream v
ACT_{rl}	annual cost per stage for staged columns involving rich stream, r and lean stream, l

ACT_{lv}	annual cost per stage for staged columns involving lean stream, l and regenerating stream, v
ACH_{rl}	annual cost per height for continuous contact columns involving rich stream, r and lean stream, l
ACH_{lv}	annual cost per height for continuous contact columns involving lean stream l and regenerating stream, v
CB_{rl}	fixed charge or exchanger installation cost for columns involving rich stream, r and lean stream, l
CB_{lv}	fixed charge or exchanger installation cost for columns involving lean stream l and regenerating stream, v
D^{rl}	area cost exponent for columns involving rich stream, r and lean stream, l
D^{lv}	area cost exponent for columns involving lean stream l and regenerating stream, v
m	slope of equilibrium line governing the transfer of component from rich stream r to lean stream l
m_v	slope of equilibrium line governing the transfer of component from regenerable lean stream l to regenerating stream v
K_w	lumped mass transfer coefficient
b_{int}	intercept of the equilibrium line
WF	weighting function
$X^S_{l,b}$	supply composition of lean (process or external) stream l which starts from composition interval b
$X^t_{l,b}$	target composition of lean (process or external) stream l which ends in interval b
$Y^S_{r,b}$	supply composition of rich process stream r which starts in interval b
$Y^t_{r,b}$	target composition of rich process stream r which ends in interval b
$Y^{*S}_{l,b}$	equilibrium supply composition of lean (process or external) stream l which starts in interval b

$Y_{l,b}^{*t}$	equilibrium target composition of lean (process or external) stream *l* which ends in interval *b*
Y_v^{*S}	equilibrium supply composition of regenerating stream *v*
Y_v^{*t}	equilibrium target composition of regenerating stream *v*
Z_v^s	supply composition of regenerating stream *v*
Z_v^t	target composition of regenerating stream *v*
Ω_m	upper bound for mass exchanged in match *r,l* in interval *b*
Ω_r	upper bound for mass exchanged in match *l,v*
Γ_m	upper bound for driving force in match *r,l* in interval *b*
Γ_r	upper bound for driving force in match *l,v*
ε_{min}	minimum composition difference

Binary variables

dw_{rlb}	binary variable denoting the existence of match *r,l* in interval *b* of the optimal network
w_{lvb}	binary variable denoting the existence of match *l,v* in the optimal network

Positive variables

dy_{rlb}	driving force between stream *r* and stream *l* in interval *b*
dx_{lvb}	driving force between lean stream *l* and regenerating stream *v*
G_r	flowrate of rich stream *r*
L_l	flowrate of lean stream *l*
M_{rlb}	mass exchanged between rich stream *r* and lean stream *l* in interval *b*
N_{rlb}	number of stages in staged column *rlb*
N_{lvb}	number of stages in staged column *lq*
QR_v	flowrate of regenerating stream *v*
$x_{l,b}$	composition of lean (process or external) stream *l* in composition location *b*
$y_{r,b}$	composition of rich process stream *r* in composition location *b*
$y^*_{l,b}$	equilibrium composition of lean (process or external) stream *l* in composition location *b*

w_{rlb} relaxed binary variable representing the existence of match, *r,l*, in interval *b*, in the optimal network

Notations in Chapter 5

Sets

P Operation periods

Indices

p index for operation period (p = 1,….. *NOP*)

Parameters

DOP duration of each period *p*

NOP number of periods

$T^s_{i,p}$ supply temperature of hot stream *i* for period *p*

$T^t_{i,p}$ target temperature of hot stream *i* for period *p*

$T^s_{j,p}$ supply temperature of cold stream *j* for period *p*

$T^t_{j,p}$ target temperature of cold stream *j* for period *p*

Ω_p upper bound for heat exchanged in match *i,j* in period *p*

$\Gamma_{i,j,p}$ upper bound for driving force in match *i,j* in period *p*

Positive variables

$A_{i,j,k}$ maximum area of match *i,j* in temperature interval *k*

$dt_{i,j,k,p}$ driving force for match *i,j* in temperature interval *k* and period *p*

$F_{i,p}$ flow rate of hot stream *i* in period *p*

$F_{j,p}$ flow rate of cold stream *j* in period *p*

$q_{ijk,p}$ heat exchanged between hot stream *i* and cold stream *j* in temperature interval *k* and period *p*

$t_{i,k,p}$ temperature of hot stream *i* at hot end of interval *k* in period *p*

$t_{j,k,p}$ temperature of cold stream *j* at hot end of interval *k* in period *p*

CHAPTER 1

INTRODUCTION

1.1 Background

The problem of process design is a multidimensional one; the design approaches that have been used in recent times involve integrating the systems that make up such processes. Heat integration (otherwise known as heat exchanger network synthesis, HENS) has been the most studied of the different processes involved in chemical systems. This was due to the rising cost of energy over the last four decades. Concerns are also being raised by environmental regulatory agencies on the effect of process industries emissions into the environment and this has necessitated developing integration methods for mass exchange (known as mass exchange network synthesis, MENS) as well. Process objectives which are usually optimised include; cost effectiveness, yield enhancement, and energy efficiency (El-Halwagi, 1997).

The conversion of raw materials to chemical products goes through many steps which include; 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 process 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, mixtures of by-products and unreacted feed are produced and such mixtures need to be separated. In essence, the reactor design defines the separation system requirements; these two stages (reactor and separation systems) in turn define the configuration of the heating and cooling systems. How much of process heat recovery is achieved determines the external heating and cooling utilities of the network. This hierarchy according to Smith (2005) could be represented symbolically by the layers of the “onion diagram” illustrated in Figure 1.1 below.

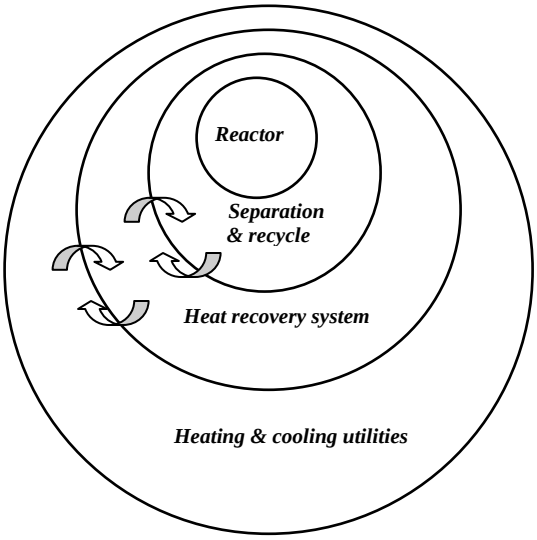


Figure 1.1: The Onion model showing the hierarchy of process design and the interaction between the separation and heat recovery layers (after Smith ,2005).

1.2 Synthesis of subsystems

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 make up the chemical process, such equipment includes: heat exchangers, reactors, mass exchangers, etc. The starting point of such designs has been from the reactor as illustrated by Figure 1.1. The interconnection of equipments and processes with one another has been accomplished by trial-and-error and heuristic design methods. Networks resulting from such design approaches cannot be guaranteed to be optimal in terms of costs and other design criteria because of the multidimensional nature of the various competing variables in a chemical system. Over time, the identification of subsystems (as shown in Figure 1.1) has enabled designers to tackle the process design problem in a holistic manner with techniques which involve physical and thermodynamic insights and mathematical programming.

The heat exchange layers (third and fourth layers of Figure 1.1) have received the most attention (Gundersen & Naess, 1988; Linnhoff, 1993). The second layer which is the mass exchange layer has also been studied (El-Halwagi, 1997; Hallale & Fraser, 1998, 2000a, & 2000b). Heat induced separation systems (such as distillation columns), heat and power

systems are being integrated into the heat exchange operations of a site (Shenoy, 1995) while reactor network synthesis is equally receiving attention (Smith, 2005). In all, design of chemical processes aims at total site integration.

There are 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, these call for a conceptual understanding of the interaction among these process variables so as to be able to establish design and synthesis techniques that will tackle the problem effectively in achieving the desired goals.

As mentioned earlier, synthesis approaches recently developed for the subsystems of chemical processes have been either insight or mathematically based. In the insight based approach the designer uses physical and thermodynamic concepts to set up and optimise the problem structure. With this approach, the designer can only consider one variable/structure at a time; hence it becomes difficult to handle problems of a multidimensional nature. However the designer can evaluate the performance of different possible networks of the problem ahead of any design. The design is subsequently initiated using the variables selected in the first step. The mathematical programming approach on the other hand involves setting up a framework which is believed to embed all possible alternative structures using mathematical constraints. The framework is subsequently optimised subject to the constraints in order to obtain the best structure.

1.3 Pinch Technology

Pinch Technology is a synthesis technique whose concept is based on physical and thermodynamic insights for the design of overall energy/mass separating agent (MSA) requirements of a process. The 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 point for a heat exchange network corresponds to the point of closest temperature approach between composites of the hot and cold sets of streams in the problem. Setting up a composite of streams on a temperature enthalpy diagram enables the heat load demand of

the streams to be treated in a global manner so that the enthalpy regions in which both composites participate can be regarded as the region of maximum energy recovery. The enthalpy regions of both composites which fall outside this section of process energy recovery will be satisfied by utilities. This procedure is known as utility targeting. The heat transfer area needed to meet such energy targets can also be determined from the temperature enthalpy plots. These two targets can easily be traded off against one another in order to get the optimal total cost target. The design is subsequently initiated using the values of the variables obtained in the targeting step (Townsend and Linnhoff, 1984).

El-Halwagi and Manousiouthakis (1989) developed a mass exchange analogue of the pinch synthesis method for heat exchange networks. Their method involved targeting for the minimum mass separating agent (MSA) needed to accomplish a separation task. However, they did not include targets for the mass exchange area. Hallale and Fraser (2000a & b) developed the $y - y^*$ tools for targeting the mass exchange area for both stagewise and continuous contact columns. El-Halwagi and Manousoiuthakis (1989) and Hallale and Fraser (2000a & b) also presented design methods with which to meet these targets.

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 mathematical models which are subsequently optimised. The steps involved include; the use of linear programming (LP) to target the pinch point and the corresponding minimum utility/MSA requirements. The minimum number of units that meets the targeted utility/MSA in the LP step is determined using mixed integer linear programming (MILP), (Papoulias & Grossmann, 1983). The final step involves initiating designs in a sequential manner to meet the targets in the first and second steps. The simultaneous approach on the other hand entails formulating as mathematical models the heat/mass exchange network using constraint and objective function equations which aim to minimize in a single step all the competing costs (Floudas and Ciric, 1989; Papalexandri *et. al.,* (1994). The problems are usually set up as non linear or mixed integer non linear programming (NLP/MINLP) models.

1.5 Motivation

The insight based approach has the advantage that each step is driven by the designer in a manner as to meet desired performance criteria; hence there are no variable initialisation problems. However these steps need to be repeated over a range of each of the decision variables thereby making the synthesis process tedious and time consuming. Also, it becomes increasingly difficult to establish a proper trade-off for multidimensional process design problems e.g. HENS problems involving multiple utilities and multiperiod operations or MENS problems involving regeneration, multiperiod operations, combined heat and mass exchange networks, etc.

The simultaneous mathematical programming approaches on the other hand can be set up to simultaneously trade-off the variables involved in the synthesis problem. However, setting up the models requires considerable expertise on the part of the designer. Also, proper variable initialisations and bound settings may pose a challenge due to the nature of the equation constraints which govern such engineering problems. The mathematical model solvers are left to determine the optimum operating conditions. These solvers have the tendency to route their search for the optimum network in the wrong direction due to the presence of non-linear and non-convexities in heat and mass exchange model equations. This is unlike the pinch technology method whose solution framework is determined by the designer. For the mathematical models which are simplified by excluding the non linear heat and mass balance equations a suboptmisation step may have to be done repeatedly for model solutions which involve the splitting of streams so as to determine the optimal split flows and mixing point temperatures.

In a bid to address the aforementioned problems which are encountered in the pinch technology and mathematical methods, models which harness the strengths of these two approaches are being developed. The reducible NLP superstructure of Comeaux (2000) for MENS is an example. This method uses a similar framework to the pinch composition interval approach. In the pinch intervals, the unknown interval compositions are determined by the supply or target compositions of the streams of the opposite kind participating in the same mass load intervals. In the NLP reducible superstructure, the unknown interval

compositions are model variables to be determined in the optimisation subject to the minimum composition difference which may also be set as a variable. The synthesis approach of Msiza (2001) which is also a hybrid of pinch technology and mathematical methods involves initialising the hyperstructure of Papalexandri *et. al*. (1994) using pinch solutions.

Yee and Grossmann (1990) used a simplified stagewise superstructure (SWS) where the supply and target temperatures of the hot and cold streams in the problem are used to define only the first and last stage temperatures while the intermediate temperatures are modelled as variables. Chen and Hung (2005a) and Szitkai, *et. al*. (2006) developed a mass exchange analogue of the SWS for HENS of Yee and Grossman (1990).

The methods of Papalexandri, *et. al*. (1994), Comeaux (2000) and Chen and Hung (2005a) include heat/mass balances and flow mixing equations. These equations have the tendency to increase the non linearity in the overall model thereby making it difficult for an optimum solution to be obtained in a reasonable time except proper initialisations are included in the model. Based on this reason, Yee & Grossmann (1990) and Szitkai, *et al*. (2006) did not include the non linear heat/mass balances and flow mixing equations in their models. The authors made assumptions that split streams would be mixed at equal temperatures/compositions. However for solution networks which involve splits, a suboptimisation step is needed in order to determine the individual flowrates of the split streams and exchanger exit temperatures. In addition, the models need special initialisations in order to get good solutions in reasonable times.

1.6 Objectives and methodology

This study will develop new synthesis techniques for heat and mass exchanger networks using an interval based MINLP superstructure (IBMS) approach. Heat/mass exchange superstructures are partitioned into intervals by defining the intervals using the supply and target temperatures/compositions of either the hot/rich or cold/lean set of streams while the streams of the opposite kinds are assumed to participate in all the intervals subject to thermodynamic feasibility. There are benefits in defining superstructure intervals in this

manner. Firstly, split streams will automatically be mixed at equal temperatures/compositions thereby helping to eliminate the need for non linear balances and mixing equations. Secondly, no special initialisation techniques are needed in order to optimise the superstructure since the superstructure is partitioned based on key variables which determine driving forces for areas and stages/heights in exchangers. Thirdly, the potential network structures in the superstructure are still screened in a simultaneous manner thereby allowing for the inclusion of multiple variables for optimisation.

The thesis will focus on problems involving single and multiple utilities for heat exchange and mass exchange. The IBMS method will also be extended to multiperiod operations (for heat exchange), regeneration operations and non linear equilibrium relations for mass exchange and combined heat and mass exchange network problems.

Chapter 2

The relevant literature for this study is reviewed in this chapter. 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 SWS of Yee & Grossmann (1990) for HENS and that of Szitkai, *et. al*. (2006) for MENS will be dwelt upon extensively in this chapter because these techniques form the basis for the IBMS synthesis methods developed in this study. Multiple periods of heat exchange operations as well as combined heat and mass exchange network synthesis are also reviewed.

Chapter 3

This chapter presents the model equations of the heat exchange IBMS method and its applications to HENS problems involving single and multiple utilities.

Chapter 4

The IBMS synthesis method model equations for MENs are presented in this chapter. The applications to MENS problems involving continuous contact and stagewise columns are demonstrated. A MENS problem requiring regeneration is also solved in this chapter using the IBMS model.

Chapter 5

The IBMS model for HENS is extended to heat exchange problems involving multiperiod operations. The necessary model equations and an application are presented in this chapter. The IBMS model for MENS is also extended to mass exchange problems having multiple process and external lean streams, non-linear equilibrium relations and combined heat and mass exchange networks.

Chapter 6

The conclusions drawn from this study will be presented in this chapter. Recommendations for future work will then be evaluated. The significance of this thesis to the field of process synthesis will be discussed as well.

CHAPTER 2

LITERATURE REVIEW

2.1 Introduction

This chapter is a review of the literature on the synthesis of heat and mass exchange networks where pinch technology and simultaneous mathematical programming methods have been applied. The sequential mathematical programming techniques are also briefly described. The techniques which have been applied to the synthesis of multiperiod operations for heat exchange and combined heat and mass exchange networks (CHAMENs) are also discussed. The chapter concludes by discussing the shortcomings of the existing methods for the synthesis of heat exchanger networks (HENs), mass exchanger networks (MENs) and CHAMENs.

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). The synthesis methods which have been applied to heat exchange networks include thermodynamic insight based (Pinch Technology) and mathematical programming.

The HENS problem 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.*

The key questions to be answered are; what heating/cooling utilities should be used and their heat load, what stream pairings and heat loads should be selected in order to get an optimal total annual cost (TAC) configuration?

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 1970`s prompted the extensive study in the area of HENS 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 in heat

exchange networks. Emphasis was later shifted from merely designing for energy optimal networks to cost optimal networks wherein trade-off between the operating and investment costs are established through targeting techniques before actual design is carried out. This optimisation method is known as supertargeting (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). This plot is a representation of the overall energy available in the hot streams (known as the hot composite curve) and the overall energy demand of the cold streams (known as the cold composite curve) on temperature versus cumulative enthalpy graphs. As illustrated by Figure 2.1 below, the point of closest temperature approach (ΔT_{min}) between the two composite curves (plotted on the same axes) is known as the pinch.

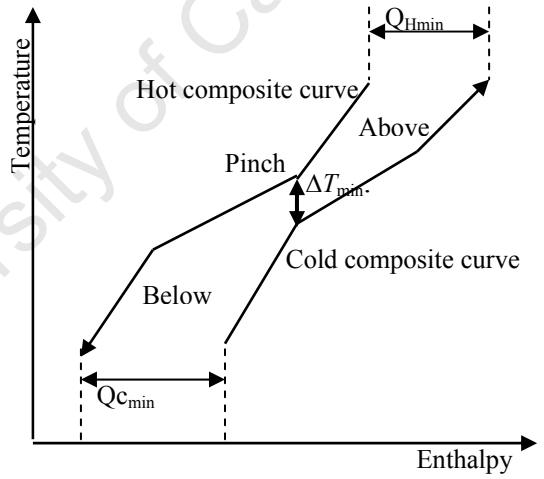


Figure 2.1: Construction of hot and cold composite curves on the same axes locate the pinch and give the minimum energy targets.

The region of overlap of the two curves corresponds to process to process heat recovery section. The overshoot of the hot composite relative to the cold composite is the minimum cold utility ($Q_{c,min}$) required to satisfy the heat load of the hot composite while the overshoot of the cold composite over the hot composite is the minimum hot utility ($Q_{h,min}$) required to satisfy the heat demand of the cold composite. $Q_{c,min}$ and $Q_{h,min}$ are the utility targets. These targets are known ahead of any detailed design. The points of

inflection on each of these curves correspond 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 they are called temperature or enthalpy intervals. The pinch divides the network into two thermodynamically independent regions, namely, above and below the pinch. The algebraic approach uses a tool known as problem table analysis which can also identify the pinch and minimum utilities targets (Linnhoff, *et al*. 1982).

2.2.1.2 Capital Cost Targets

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. However just the number of heat exchange units and total heat exchange area will be reviewed in this chapter.

Number of Units Target

The minimum number of units can be targeted ahead of detailed design in pinch technology; this is done separately for above and below the pinch. The minimum number of units is one less than the total number of streams (including utilities) on each side of the pinch as represented by Equation 2.1 (Linnhoff, *et al*. 1982);

$$N_{\text{units, pinch}} = (N_{St}\text{-}1)_{\text{Above pinch}} + (N_{St}\text{-}1)_{\text{Below pinch}} \quad (2.1)$$

where N_{units} is the number of units and N_{St}, the number of streams (including utilities). Partitioning at the pinch leads to an increase in the number of units because streams crossing the pinch will have to be counted twice.

Area targets

The minimum area requirement for a heat exchange network can also be determined ahead of design either graphically on the composite curves or algebraically; this process is known as area targeting. Area targeting is accomplished graphically by balancing the hot and cold composite curves using utilities. The resulting composite curve is known as the balanced composite curve which is illustrated by Figure 2.2 below.

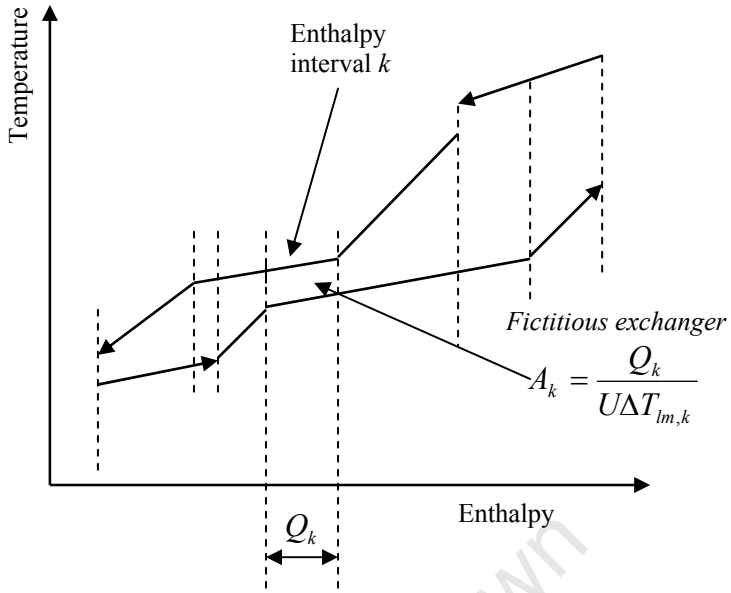


Figure 2.2: Division of the balanced composite curve into enthalpy intervals (Smith, 2005)

Vertical lines are drawn at each point of inflection to touch the opposite curve so as to identify segments on the graph; these segments are called enthalpy intervals. Each segment can be regarded as being equivalent to a fictitious countercurrent heat exchanger where the heat load corresponds to the enthalpy difference on the x-axis of the segment concerned. The vertical distance between the curves is the driving force of the fictitious heat exchanger. An ideal area can be calculated for each fictitious exchanger using the following equation (Townsend and Linnhoff, 1984):

$$A_k = \frac{Q_k}{U\Delta T_{lm,k}} \tag{2.2}$$

where: Q_k is the enthalpy change in interval k

U is the overall heat transfer coefficient

ΔT_{lmk} is the log mean temperature difference of enthalpy interval k

Note that $\Delta T_{\min}$ calculation leads to numerical problems, so a range of approximations have been proposed as discussed in Section 2.4.

For streams having equal heat transfer coefficients and assuming a vertical heat transfer pattern from the hot composite to the cold composite, the minimum total network area

can be obtained by using Equation 2.2. The equation is applied to each of the enthalpy intervals and summed over every one of them to obtain (Townsend and Linnhoff, 1984):

$$A_{\min,Network} = \frac{1}{U} \sum_{k}^{Intervals,K} \frac{Q_k}{\Delta T_{lm,k}} \tag{2.3}$$

where: K is the total number of enthalpy intervals.

For situations in which stream heat transfer coefficients differ by only an order of magnitude, Equation 2.3 will predict the total minimum area within 10 percent of the actual minimum (Smith, 2005).

Equation 2.3 assumes vertical heat transfer as well as a constant overall heat transfer coefficient which is not always the case in realistic situations. This is 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 heat transfer coefficient resistances are additive:

$$\frac{1}{U} = \frac{1}{h_i} + \frac{1}{h_j} \tag{2.4}$$

where: h_i is the hot stream film heat transfer coefficient

h_j is the cold stream film heat transfer coefficient

Applying Equation 2.4 to 2.3, the total minimum area requirement becomes:

$$A_{\min,Network} = \sum_{k}^{Intervals} \frac{1}{\Delta T_{lm,k}} \left[\sum_{i}^{Hot\ streams} \frac{q_i}{h_i} + \sum_{j}^{Cold\ streams} \frac{q_j}{h_j} \right]_k \tag{2.5}$$

where q is the enthalpy change of each stream. Equation 2.5 is called the *Bath formula* of Townsend & Linnhoff (1984).

Looking at Figure 2.3, vertical heat transfer requires that hot stream, A, which exists in interval 1 be matched with cold stream, C, which belongs to the same interval as A. This is because such a match (heat exchanger) will use temperature driving force exactly the way it is used in the interval (thus appearing vertical on the composite curve). This also applies to all intervals on the balanced composite curve where each stream in an interval

has to be matched with streams of the opposite kind in that interval. However, if there are more hot streams than cold streams or vice versa then stream splitting in proportional ratios would be required so as to meet the condition of vertical heat transfer. Following these rules religiously will result in a kind of design known as the spaghetti design (Linnhoff & Ahmad, 1990). It should be noted that the pinch design methods to be presented in Section 2.2.1.4 can be used to generate designs with as few streams as possible without having to generate spaghetti designs.

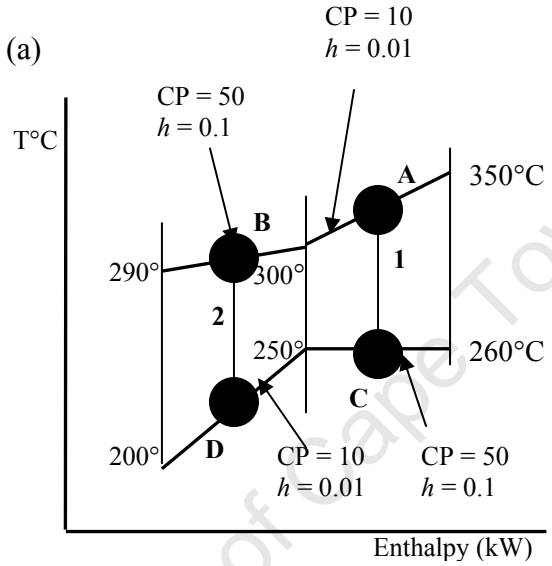


Figure 2.3: Vertical heat transfer (Smith, 2005)

In order to meet the area target in design for heat exchange problems whose stream heat transfer coefficients are significantly different, the vertical heat transfer assumption has to be relaxed and deviation from verticality employed. This is illustrated by Figure 2.4.

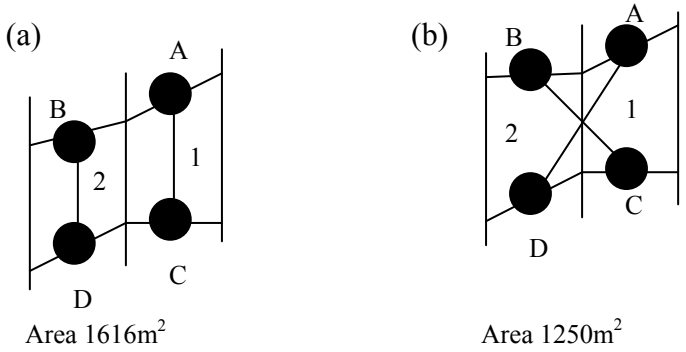


Figure 2.4: Non-vertical (criss-crossing) heat transfer matching (Smith, 2005)

In Figure 2.4, hot stream A has a low film coefficient and part of it exists in interval 1, cold stream C has a high film coefficient and part of it also exists in interval 1. Hot stream B has a high heat transfer coefficient and part of it exists in interval 2 while cold stream D has a low heat transfer coefficient and part of it exists in interval 2 as well. Matching stream A with stream C and B with D gives a total area requirement of 1616m^2 as illustrated in Figure 2.4a. But matching stream A with stream D and B with C as shown in Figure 2.4b gives a minimum area requirement of 1250m^2 which is less than that in Figure 2.4a. The A-D match (both streams 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 (Smith, 2005).

Strictly following the vertical heat transfer concept in stream matching for networks having multiple streams crossing the same intervals results in networks with many splits, hence a large number of matches. Networks of such nature as mentioned earlier are called spaghetti networks, they are not very practical because each exchanger will need an installation cost, thus resulting in a high capital cost and complex layout. However the vertical heat transfer concept can serve as a theoretical basis for designing to meet targets as used in the driving force plot (DFP) analysis by Linnhoff and Vredeveld (1984). The DFP involves evaluating each potential match on the balanced composite curves by comparing the driving forces of the matches with what it would have used on the balanced composite curve. While the DFP helps to give good designs the remaining problem analysis (RPA) by Ahmad (1985) and Tjoe (1986) can be used together with the DFP to improve the designs away from the pinch. The RPA evaluates the potential of matches meeting the target area on the bases of their area and not just temperature as it is with the DFP.

Equations 2.3 and 2.5 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 next.

Capital Cost Estimation

Procedures for converting the different targets discussed earlier into capital costs 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 network capital cost prediction, it is assumed that a single heat exchanger can be costed by the following relation:

$$\text{Cost (installed)} = a + bA^c \tag{2.6}$$

where A is the area of the heat exchanger, a, b and c are cost law constants which depend on material of construction, pressure rating and type of exchanger. The minimum network capital cost is given by (Smith, 2005);

$$\text{Network Capital Cost} = N\left[a + b\left(\frac{A_{\min}}{N}\right)^c\right] \tag{2.7}$$

where N is the minimum number of units.

Equation 2.7 is applied separately to above and below the pinch so as to ensure consistency between the capital cost and energy targets. The above and below the pinch capital costs are then added and annualised to get the annualised capital cost (ACC).

Hall, *et al*. (1990) applied cost weighting factors to each stream in order to establish capital cost targets for exchangers with non-uniform specifications. These cost factors are based on the exchanger design requirements. Jegede and Polley (1992) went further in their capital cost targeting for exchangers of non-uniform specifications by developing targeting techniques for estimating the distribution of both area and number of units between the different exchanger specifications. Their approach takes into account the area and units contribution of the exchanger requirements. The techniques of these two set of authors was worked by modifying heat transfer coefficient (h) values, so any technique that allows stream dependent h can use it.

2.2.1.3 Supertargeting

The targets for the minimum energy cost and the corresponding capital cost discussed in the previous sections are accomplished at a particular $\Delta T_{\min}$. If the targets are carried out at a higher value of $\Delta T_{\min}$, the energy costs increase while the capital cost decreases. On the other hand if a lower value of $\Delta T_{\min}$ is used for the targets, the energy costs decrease while the capital cost increases. This indicates that the costs can be traded-off against one another so as to obtain a $\Delta T_{\min}$ where the total annual cost (sum of annual operating and annualised capital costs) is a minimum. The minimum total annual cost (TAC) is known

as the TAC target and the technique of determining this TAC is known as supertarting. Initiating a design with the supertarget ΔT_{min} usually gives networks which require little or no evolution in order to meet the TAC target (Linnhoff and Ahmad, 1989).

2.2.1.4 Network Design

In order to meet the energy targets in design, no heat should be transferred across the pinch and no hot and cold utilities are to be used below and above the pinch respectively (Linnhoff, *et al*. 1982). The matching of streams requires the following rules:

- Start the design at the pinch while ensuring that the following inequalities are met;

  Above pinch, $N_H \leq N_C$ (2.8)

  Below pinch $N_{H,} \geq N_C$ (2.9)

  where N_H and N_C are the number of hot and cold streams respectively.

  This condition is known as the number count criterion. For situations in which the number count criterion does not hold one of the hot or cold streams will have to be split.

- Moving away from the pinch, temperature differences become larger. This implies that matches to be selected must also have diverging temperature differences away from the pinch. Matches can be selected based on the following criterion in order to meet this condition.

  Above pinch $CP_H \leq CP_C$ (2.10)

  Below pinch $CP_H \geq CP_C$ (2.11)

- The DFP as mentioned earlier is used to evaluate potential matches on the basis of the degree to which their driving forces approach those on the balanced composite curves. The DFP shows the vertical temperature differences, ΔT, between the hot and cold composite curves. 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 (Linnhoff and Vredeveld, 1984). Each potential match is superimposed on the plot; matches which fit perfectly will transfer heat vertically in the design,

those that use too much or too little driving forces will result in a higher capital cost requirement.

- The RPA is used to evaluate potential matches not only based on temperatures (as it is in DFP) but on heat duty as well. RPA, as the name implies is a tool which can be used to investigate the penalty to be incurred for every individual match relative to the final network meeting the targets without having to complete the network (Ahmad and Smith, 1989). The RPA according to Shenoy (1995) despite being a powerful tool for meeting total capital costs (TCC) in designs requires much computational effort. This is because the efficiency of each match has to be analyzed one after the other and the order in which to go about the matching is not usually known before hand.

It is worth mentioning at this point that the above design rules do produce networks that approach the targets. However for problems having many streams, there are no specifc orders to follow or what streams to give preference in applying the aforementioned rules. Also, the targets do not establish a simultaneous trade-off among the competing costs (such as utility, number of units and heat exchange area) since each step is dependent on the previous ones, therefore networks initiated from such targets can not be guaranteed to be optimum.

2.2.1.5 Multiple Utilities

The temperature enthalpy plot illustrated in Figure 2.1 only shows the total hot and cold utilities required to service the heat load of the network not satisfied by process heat exchange. Linnhoff, *et al*. (1982) developed a tool known as the grand composite curve (GCC) in order to be able to represent utilities not only based on enthalpy but on temperature levels as well. The GCC is a plot of interval temperatures (adjusted by $\frac{1}{2}\Delta T_{min}$) against cumulative heat. Figure 2.5 illustrates steam at two different temperature levels exchanging heat with the process.

The pinch is the point of zero net heat flow as indicated in the figure. 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 can best be used. It is also used for profile matching for total energy integration.

Fraser (1994) proposed using the fraction of a utility used relative to the limit feasible as a parameter while optimising based on ΔT_{min} or minimum flux. This method exposes the inconsistencies in the translation of minimum exchanger area to capital costs and also the fact that linearised cost functions do not perfectly establish the associated costs. Also, the utility capital costs are to be adequately included in the optimisations.

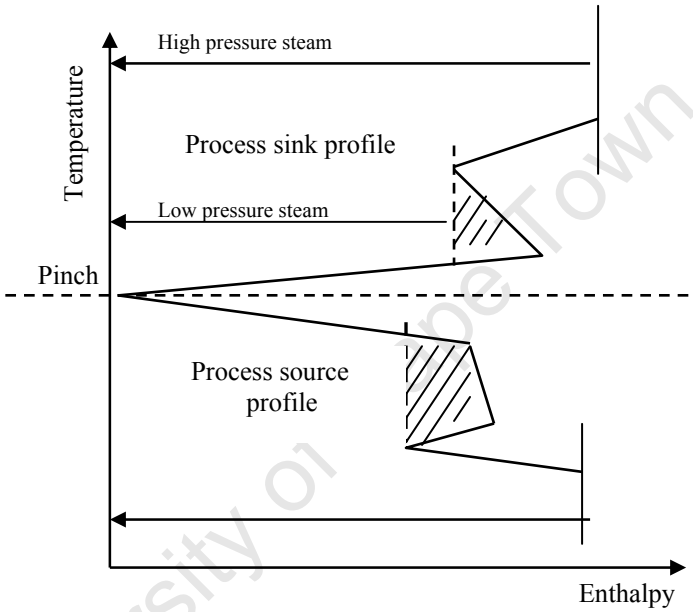


Figure 2.5: The grand composite curve illustrates the temperature levels of utilities relative to the process streams.

Shenoy, *et al*. (1998) developed the cheapest utility principle (CUP) for the targeting of multiple utilities in heat exchanger networks. The CUP is used to determine the optimum loads for multiple utilities based on not only the utility costs but the capital costs as well. The approach requires that the load of the cheapest utility should be increased as the value of the process ΔT_{min} increases while the load of the more expensive utilities should be kept constant. Shenoy, *et al*. (1998) observed that the temperature driving forces at the utility pinches do not change once they are optimised even if the process ΔT_{min} is varied. The utility pinches are optimised in a sequential manner and the best heat load distribution presented on an optimum load distribution (OLD) plot. The OLD is a plot of utility loads against ΔT_{min}. The TAC is further obtained from the OLD plots. The CUP according to Shenoy, *et al*. (1998) gives a good prediction when the capital cost function

is linear. For the non linear cost functions, the approximation is good enough for initialising designs. The pinch design methods discussed earlier are also used to meet the multiple utility targets in designs.

In designing CUP networks, a lower value of exchanger minimum approach temperature (EMAT) can be allowed in order to explore more opportunities for making matches. However there is no specific order in which to make such matches, hence the procedure can be cumbersome. The DFP is also employed in making best use of available driving forces. It is noted that the CUP method is still subject to the problem highlighted above for the pinch target and design methods in HENs problems having single utilities. Also, the targeting becomes more time consuming since the load of each utility has to optimised sequentially. Designing networks having multiple utilities will also be tedious and time consuming because there is no particular order in which to apply the pinch design rules especially for problems with a large number of streams.

2.2.2 Mathematical programming as applied to HENS

Mathematical programming application to the synthesis of HENs has been of two natures: the sequential and the simultaneous. The sequential approach is an automation of pinch technology using mathematical constraints. It also involves decomposition into subtasks. Examples are: the linear programming (LP) transportation model of Cerda, *et al*. (1983), the LP transhipment model of Papoulias and Grossmann (1983). These two models are used to target the minimum utility cost for a heat exchange problem. Papoulias ad Grossmann (1983) also presented a mixed integer non linear programming model (MILP) which can be used to target the minimum number of units. A minimum investment network configuration based on the LP and MILP models can be generated using the non linear programming (NLP) model of Floudas, *et al*. (1986).

Colberg and Morari (1990) developed a pair of transhipment NLP models which can calculate the area and capital cost targets for HEN problems whose heat transfer coefficients differ significantly. This model efficiently handles HENS problems having different capital cost functions for diverse kinds of materials of construction, pressure ratings etc. In addition when areas of matches are constrained, the area and capital cost targets can be determined for retrofit synthesis.

The sequential mathematical programming methods as it applies to the pinch approach do not simultaneously trade-off the different costs which contribute to the TAC. Each decision step for heat recovery approach temperature (HRAT) and partitioning into subnetworks affects the number of exchangers and the areas of exchangers. According to Floudas (1995), networks which are strictly partitioned into subnetworks have the tendency to exclude solutions which might have a minimum TAC through the transfer of heat across the pinch. The task of trading off the competing costs at each value of HRAT in order to get a minimum TAC may be tedious and time consuming.

The MILP minimum number of matches model of Papoulias and Grossmann (1983) can give multiple feasible solutions meeting the minimum number of units criterion. The vertical MILP model of Gundersen and Grossmann (1990) can be used to discriminate among these multiple networks on the basis of approach to vertical heat transfer in each of the solutions. However, vertical transfer of heat on the composite curve does not always give the minimum TAC especially in problems having significantly different heat transfer coefficients.

The shortcomings of the sequential mathematical programming approaches (among others) highlighted above gave rise to synthesis techniques for heat exchanger networks which are simultaneous in nature. The simultaneous techniques involve setting up a superstructure/hyperstructure which is believed to embed all potential configurations of the heat exchange problem. Such networks are subsequently optimised either as an NLP or mixed integer non linear programming (MINLP) model.

The simultaneous synthesis methods can still be divided into those which involve decomposition and those without decomposition. The decomposition in this case does not mean partitioning the problem into subnetworks but solving the problem in steps. The hyperstructure model of Floudas and Ciric (1989) and the extended pseudo-pinch version developed by Ciric and Floudas (1990) are examples of decomposed simultaneous methods. Typical examples of the non decomposed simultaneous models include the hyperstructure models of Ciric and Floudas (1991) as well as that of Papalexandri and Pistikopoulos (1994) (which combines HENS with MENS). The simplified stagewise (SWS) MINLP superstructure of Yee and Grossmann (1990) also falls under the simultaneous methods.

Floudas and Ciric (1989) used the information supplied by the minimum hot and cold utilities and pinch point locations to set up a hyperstructure which embeds all feasible matches and network structures. The feasible matches identification and network generation are carried out for the whole network simultaneously and not for subnetworks. The hyperstructure can be optimised as an MINLP model. The resulting solution gives a minimum investment cost network. The network provides information regarding the matches and their corresponding heat loads, stream flowrates, their interconnections and temperatures and the areas of the heat exchangers. Note that the hyperstructure corresponds to a fixed value of HRAT. Subsequent optimisations have to be carried out over a range of HRAT in order to identify the least investment cost network.

Ciric and Floudas (1990) extended the hyperstructure model of Floudas and Ciric (1989) by allowing heat to flow across the pinch. This method is called Pseudo-Pinch synthesis approach. The amount of heat to be allowed to flow across the pinch is determined for a fixed value of HRAT and the hyperstructure is subsequently optimised simultaneously for matches network configurations. Networks which result from this approach are simpler and do not involve by-pass streams.

Ciric and Floudas (1991) developed a simultaneous synthesis approach which does not involve decomposition in any form. The method involves using the information given just by the stream and equipment data to determine the minimum TAC HEN that provides the hot and cold utility loads, matches that take place, heat exchanger areas and the structure of the HEN. This method simultaneously trades-off the operating and investment costs since the utility loads and exchanger areas are treated as explicit optimisation variables. The hyperstructure which is solved as an MINLP involves the following:

- A pseudo-pinch MILP transhipment model
- A hyperstructure topology model comprising of mass balances for mixers and splitters, energy balances for mixers and exchangers, heat exchange feasibility constraints, and utility, nonnegativity and bound constraints.
- An objective function which minimises the TAC.

The solution of these simultaneous approaches is a local optimum due to the presence of nonconvexities in the models (Floudas, 1995). Also initialisation and setting of bounds may be difficult for problem involving a large number of streams.

Kravanja and Glavic (1997) developed a method for handling large scale industrial problems involving a large number of streams. The technique which is an integrated pinch technology and mathematical programming can be used to simultaneously optimise a process flowsheet and its integrated HEN. The unified technique involves two steps. The first step is a direct search optimisation which is used to simultaneously trade-off costs associated with the process and HEN. The second step entails the use of an NLP for the HEN design.

The SWS of Yee and Grossmann (1990) is reviewed in the next section extensively because the proposed IBMS method uses a framework similar to the SWS framework.

2.2.2.1 Simplified stage-wise superstructure (SWS)

As the name implies the SWS comprises of temperature stages. The number of stages can be fixed by the designer. However Yee and Grossmann (1990) recommended setting the number of stages as:

$$\text{Max}\{N_H, N_C\} \tag{2.12}$$

where N_H and N_C are the number of hot and cold streams respectively.

The SWS for a heat exchange problem having two hot and two cold streams is illustrated by Figure 2.6. In the SWS, all hot process streams (and/or hot utilities) start at the first temperature location, k =1, and end at the last temperature location, $k = NK+1$, where NK is the total number of stages. All cold process streams (and/or cold utilities) start at the last temperature location, $k = NK+1$ and end at k =1. All streams are made to participate in every stage and each stream can split into the number of streams of the opposite kind in the superstructure. Heat can be exchanged between streams of opposite kind in each stage. Note that for simplicity, the utilities can be placed at the first and last temperature locations of the superstructure as illustrated by Figure 2.6 above.

Using Figure 2.6 for illustration, the temperature of H_1 is $T^s_{H1,1}$ in temperature location $k=1$, which is its supply temperature. H_1 can split into two streams because there are two process cold streams, C_1 and C_2 present in the superstructure. If H_1 splits, then each of the split branches will exchange heat with C_1 and C_2 in exchangers H_1-C_1 and H_1-C_2 in stage 1. The split streams from exchangers H_1-C_1 and H_1-C_2 are assumed to be mixed at equal temperatures. The exit temperature of the mixer becomes the temperature of H_1 in temperature location, k = 2, this is $t_{H1,2}$ in Figure 2.6. $t_{H1,2}$ is treated as a variable to be optimised in the SWS model. H_1 whose temperature is now $t_{H1,2}$ in temperature location, k = 2, enters into stage 2 and splits again in the same manner as in stage 1.

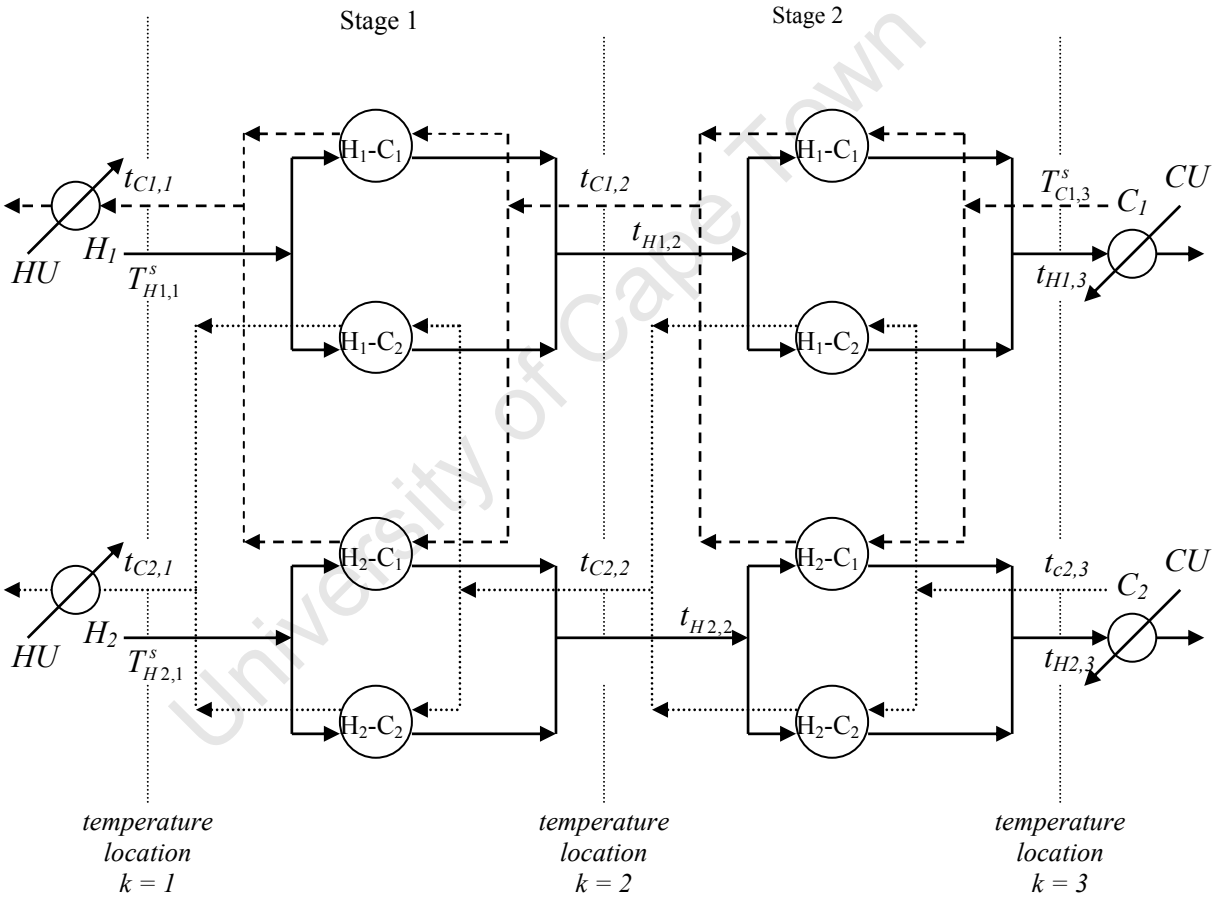


Figure 2.6: Simplified stagewise heat exchange superstructure of Yee and Grossmann (1990)

The heat exchange and mixing pattern of stage 1 is repeated in stage 2. Note that the temperature of H_1 at each temperature location is dependent on how much heat it exchanged with cold streams in previous stages. If H_1 does not get to its target

temperature at the last stage, a cold utility is used to accomplish this; this applies to SWSs that have the utilities placed at the superstructure boundaries. Cold streams also exchange heat in the manner discussed for hot streams. In order to obtain the minimum total costs, the superstructure is optimised as an MINLP model.

Due to the isothermal mixing assumption, Yee and Grossmann (1990) did not include non linear heat balance equations in the superstructure model. This helps to simplify the model since the set of constraints become linear. The SWS can handle streams having significantly different heat transfer coefficients because the stage temperatures are not fixed. This is unlike the balanced composite curves of pinch technology where enthalpy intervals are fixed so as to allow for vertical heat transfer. Restrictions can also easily be placed on matches. However, the shortcomings of the SWS approach include the following;

- Structures which are only feasible with nonisothermal mixing may be excluded from consideration (e.g. by-pass streams) (Floudas, 1995)
- Splits streams cannot go through two or more exchangers in series (Floudas, 1995)
- An NLP sub-optimisation step will be needed in order to determine the split flows and exchanger exit temperatures (Isafiade & Fraser, 2007a)
- Special initialisation techniques may be needed for large heat exchange problems especially those involving multiple utilities or multiple periods (Isafiade & Fraser, 2007a).

The last two shortcomings of the SWS will be addressed in this study by defining the temperature locations of the superstructure using the supply and target temperatures of either the hot or cold set of streams i.e. an interval based approach. This interval based method is described in Chapter 3 of this thesis. The equations of the SWS model of Yee and Grossmann (1990) are described next, note that hot and cold utility streams have been treated as process streams in this description.

Overall stream heat balance

In order for a stream to get to its target temperature, it needs to exchange heat with the streams of the opposite kind in the superstructure stages. Note that a stream does not need to exchange heat in every stage in order for it to get to its target temperature. The

sum of heat exchanged in stages with streams of the opposite kind is set equal to the heat load of the stream concerned. This is described by Equations 2.13 and 2.14 below:

$$\left(T_i^s - T_i^t\right) F_i = \sum_{j \in C} \sum_{k \in K} q_{i,j,k} \qquad i \in H \tag{2.13}$$

$$\left(T_j^t - T_j^s\right) F_j = \sum_{i \in H} \sum_{k \in K} q_{i,j,k} \qquad j \in C \tag{2.14}$$

where T_i^s, T_i^t are the supply and target temperatures of hot stream *i* while T_j^s and T_j^t are for the cold stream *j*. Index *k* corresponds to a temperature location. $q_{i,j,k}$ and *F* are continuous variables, they represent the heat exchanged between hot stream *i* and cold stream *j* in interval *k* and the heat capacity flow rate of each stream respectively. *H* and *C* represent the set of hot and cold streams respectively.

Stage heat balance

Stage enthalpy balances are used to determine the temperature of each stage boundary for each stream. This is shown below:

$$\left(t_{i,k} - t_{i,k+1}\right) F_i = \sum_{j \in C} q_{i,j,k} \qquad i \in H \quad k \in K \tag{2.15}$$

$$\left(t_{j,k} - t_{j,k+1}\right) F_j = \sum_{i \in H} q_{i,j,k} \qquad j \in C \quad k \in K \tag{2.16}$$

where $t_{i,k}$ and $t_{j,k}$ are continuous variables, they correspond to the temperatures of hot stream *i* and cold stream *j* in temperature location *k* (or at stage boundary *k*).

Assignment of superstructure inlet temperatures

Temperature location, $k = 1$, is assigned the supply temperatures of the hot streams while temperature location, $k = NK + 1$ is assigned the supply temperatures of the cold streams. These are described in the following equations:

$$T_i^s = t_{i,1} \qquad i \in H \tag{2.17}$$

$$T_j^s = t_{j,NK+1} \qquad j \in C \tag{2.18}$$

Feasibility of temperatures

Hot streams run from the left to the right while cold streams run from the right to the left in the superstructure. The set of constraints shown in Equation 2.19 and 2.20 are used to ensure that there is a monotonic decrease in stage temperatures from left to right.

$$t_{i,k} \geq t_{i,k+1} \qquad k \in K,\ i \in H \tag{2.19}$$

$$t_{j,k} \geq t_{j,k+1} \qquad k \in K,\ j \in C \tag{2.20}$$

Logical constraints

The existence of a match, *i,j*, in stage *k* is modelled using logical constraints and binary variables, $z_{i,j,k}$. An integer value of '1' indicates the existence of a match in the optimal network and '0' if otherwise. The equations representing this are:

$$q_{ijk} - \Omega_h z_{i,j,k} \leq 0 \qquad i \in H,\ j \in C,\ k \in K \tag{2.21}$$

where Ω_h is an upper bound on the amount of heat that can be exchanged between stream *i* and *j*. It can be set as the smaller heat load of the two streams participating in the match.

Heat exchange area calculation

The heat exchange areas were included in the objective function in the SWS of Yee and Grossmann (1990), this restricts the non linearities in the overall model to just the objective function equation. The approach temperatures, dt_{ijk}, were calculated as follows:

$$dt_{i,j,k} \leq t_{i,k} - t_{j,k} + \Gamma_h\left(1 - z_{i,j,k}\right) \qquad k \in K,\ i \in H,\ j \in C \tag{2.22}$$

$$dt_{i,j,k+1} \leq t_{i,k+1} - t_{j,k+1} + \Gamma_h\left(1 - z_{i,j,k}\right) \qquad k \in K,\ i \in H,\ j \in C \tag{2.23}$$

The binary variables, $z_{i,j,k}$, are also used in the approach temperature calculation so as to ensure feasible driving forces for the exchangers selected in the optimal network. The upper bound, Γ_h, inactivates the equation if a match does not exist. An exchanger minimum approach temperature (EMAT), is used to avoid the inclusion of exchangers with infinite areas in the optimal network, this is represented as:

$$dt_{i,j,k} \geq \delta \tag{2.24}$$

where δ is a small positive number.

Objective function

The objective function simultaneously minimises the utility costs and exchanger capital costs (i.e. fixed charges and area cost of each exchanger). The Chen's first approximation (Chen, 1987) was used to calculate the logarithmic mean temperature difference (LMTD).

$$LMTD_{i,j,k} = \left[\left(dt_{i,j,k}\right) \cdot \left(dt_{i,j,k+1}\right) \cdot \left(dt_{i,j,k} + dt_{i,j,k+1}\right) / 2 \right]^{1/3} \tag{2.25}$$

The objective function:

$$\min \sum_{i \in H} \sum_{k \in K} CUCq_{ijk} + \sum_{j \in C} \sum_{k \in K} HUCq_{ijk} + \sum_{i \in H} \sum_{j \in C} \sum_{k \in K} CF_{ij} z_{ijk} + \sum_{i \in H} \sum_{j \in C} \sum_{k \in K} AC_{ij} \left[q_{ijk} / U_{ij} (LMTD_{ijk}) \right]^{AE_{ij}} \tag{2.26}$$

where *HUC* and *CUC* are the per unit cost of hot and cold utilities respectively, *CF*, *AC*, *AE* are the fixed charge for an exchanger, area cost coefficient and area exponent costs respectively. *U* is the overall heat transfer coefficient. Due to the assumption of isothermal mixing for split streams the SWS model maybe easily solved because non linear equations are only present in the objective function.

The temperature locations which comprise the stage boundaries helps to ensure that only parallel match sequences takes place in each stage. This is usually accomplished in the optimisation through the splitting of streams depending on the heat load of the streams of the opposite kind present in such stages. However there can not always be an automatic equal temperature mixing of split streams in intermediate stages (i.e. stages which are not bounded on any side by either the first or last temperature location of the superstructure). This is because the constraints (such as Equations 2.15, 2.16, 2.19 & 2.20) which determine the intermediate temperatures, are not set using coefficients such as the inlet or exit temperatures of streams. Such parameters are only present in constraints (such as Equation 2.13, 2.14, 2.17 & 2.18) which refer to the first and last temperature locations of the superstructure. This is the reason for which SWS models are easily adapted to different heat exchange problems.

The framework of the SWS of Yee and Grossmann (1990) has been applied to the synthesis of flexible and multiperiod heat exchanger networks (Aaltola, 2003 and Verheyen & Zhang, 2006); this is discussed next.

2.2.2.2 Synthesis of multiperiod heat exchanger networks

Changes in operating parameters of processes such as temperatures and stream flows should be adequately accounted for in designs. Such networks should still be optimal in energy usage as well as keeping to the respective stream temperature targets.

Aaltola (2003) defines the flexible HEN problem as follows:

> *Given are a set of hot and cold streams to be cooled and heated respectively which include multiperiod stream data having supply and target stream temperatures, heat capacity flowrates and heat transfer coefficients. Also, available are a set of hot and cold utilities. The task is to establish within the range of the operating conditions, the heat exchanger network for energy recovery between the given set of hot and cold streams, so as to minimise the annualised cost of equipments and annual cost of hot and cold utilities.*

Aaltola (2003) adapted the SWS MINLP model of Yee and Grossmann (1990) to the synthesis of multiperiod heat exchanger networks. The solution of the multiperiod SWS MINLP model was improved through the use of an NLP model where the configuration of the HEN is fixed while the heat exchange areas are restricted by setting the upper bound of each to correspond to that given by the MINLP model. The NLP model which does not include the isothermal mixing assumption imposed on the MINLP model takes account of maximum areas in order to get the actual area investment cost.

Chen and Hung (2004) presented a method which can be used for the synthesis of HENs that will handle uncertainties in stream temperatures and flowrates in three iterative steps which include the following:

- The use of the SWS model of Yee and Grossmann (1990) to determine a network with a minimum TAC
- Testing of the TAC network obtained in the first step for feasibility of operation over the full variation range using flexibility analysis
- The use of integer cuts to eliminate those networks that do not meet the feasibility test in step two.

Verheyen and Zhang (2006) modified the multiperiod SWS MINLP model of Aaltola (2003) through the use of maximum area per period for the calculation of the area cost and the removal of slack variables and weighed parameters from the NLP improvement models.

The multiperiod approach modelling requires that a set, '*P*', which comprises of different time periods, '*p*', be included for each potential match, *i,j*, in stage, *k*. This approach has also been used in MENS problems involving multiple components (Szitkai, *et al*. 2006) where the set of components, *CM*, which comprises different components, *cm*, is included for every potential mass exchanger in a stage.
The multiperiod MINLP models of both Aaltola (2003) and Verheyen & Zhang (2006) involve the following model equations for each period *p*;

- Overall heat balances for hot and cold streams
- Stage heat balances for hot and cold streams
- Superstructure inlet temperatures
- Feasibility of temperatures along the superstructure
- Utility energy balances which ensure that process streams get to their target temperatures
- Logical constraints for match existence
- Approach temperature equations
- An objective function which minimises the TAC of the problem

The optimisation stages in the multiperiod SWS MINLP approach of Aaltola (2003) entails the following steps;

- The use of LP transhipment model of Papoulias and Grossmann (1983) to estimate the hot utility upper bounds (HU^{UP}) for each period in an MILP and the MINLP models
- The MILP which is also a multiperiod stagewise model is used to set initial bounds for the allowed number of units (MinNU) and the minimum number of stages (MinNST) in the MINLP model

- The multiperiod SWS MINLP model is solved using initial periodical data and bounds based on HU^{UP} and MinNU.
- An LP feasibility test is used to establish the key conditions that limit the flexibility of a design
- Data for additional periods signifying the worst temperature approach violations is used to resolve the multiperiod MINLP model so as to get feasible solutions for the whole specified range of parameter violations
- The final step which is the NLP improvement model is used to take account of maximum areas and non-isothermal mixing assumption in the MINLP model.

The area of one match in a period in the multiperiod SWS MINLP model of Aaltola (2003) is the average of the areas in that period. This according to Verheyen and Zhang (2006) was done so as to avoid the introduction of non-linearities in the set of constraints or non-linearities with discontinuous derivatives into the objective function. Aaltola (2003) and Verheyen & Zhang (2006) used the Paterson (1984) LMTD calculation, as shown below:

$$LMTD_{i,j,k,p} = \frac{2}{3}\cdot\left[\left(t_{i,k,p}-t_{j,k,p}\right)\cdot\left(t_{i,k+1,p}-t_{j,k+1,p}\right)\right]^{\frac{1}{2}} + \frac{\left(t_{i,k,p}-t_{j,k,p}\right)+\left(t_{i,k+1,p}-t_{j,k+1,p}\right)}{6} \quad (2.27)$$

The objective function of Aaltola (2003) which comprises of the unit costs for all exchangers, average area costs for all matches (including hot and cold utility matches) and weighed utility costs is shown as:

$$\begin{aligned}\min\ TAC = {} & AF\left[\sum_{i\in H}\sum_{j\in C}\sum_{k\in K} CF_{i,j}z_{i,j,k} + \sum_{i\in H}\sum_{CU} CF_{i,cu}z_i^{cu} + \sum_{j\in C}\sum_{hu} CF_{j,hu}z_j^{hu}\right] \\ & + AF\sum_{p\in P}\frac{1}{NOP}\sum_{i\in H}\sum_{j\in C}\sum_{k\in K} AC_{i,j}\left[\frac{q_{i,j,k,p}}{LMTD_{i,j,k,p}U_{i,j}}\right]^{AE_{i,j}} \\ & + AF\sum_{p\in P}\frac{1}{NOP}\sum_{i\in H} AC_{i,cu}\left[\frac{q_{i,p}^{cu}}{LMTD_{i,cu,p}U_{i,cu,p}}\right]^{AE_{i,cu}} \\ & + AF\sum_{p\in P}\frac{1}{NOP}\sum_{j\in C} AC_{j,hu}\left[\frac{q_{j,p}^{hu}}{LMTD_{j,hu,p}U_{j,hu,p}}\right]^{AE_{j,hu}} \\ & + \sum_{p\in P}\frac{DOP_p}{NOP}\sum_{i\in H} CUCq_{i,p}^{cu} + \sum_{p\in P}\frac{DOP_p}{NOP}\sum_{j\in C} CUHq_{j,p}^{hu}\end{aligned} \quad (2.28)$$

where AF is the annualisation factor, NOP, the number of periods and DOP_p is the duration of period p. The DOP is defined so that the MINLP model will take into account the weighted periods. This enables the most common operating conditions to dominate while the less common ones are still considered.

Verheyen and Zhang (2006) introduced new area variables into the multiperiod SWS MINLP model of Aaltola (2003) in order to account for the maximum area per period. The area variables which include $A_{i,j,k}$ (maximum area of match i,j in stage k), $A_{j,hu}$ and $A_{i,cu}$ (maximum areas of hot and cold utility matches respectively) restrict the area variable A, to be greater than or equal to each of the previously defined areas. This approach has the following benefits;

- The minimisation of the objective function forces the areas towards the minimum possible values, which is the maximum area per period
- The use of the inequality constraints also enables the solver to find feasible solutions.

Verheyen and Zhang (2006) used the Paterson approximation for the LMTD calculations in the area variables. The area equations are described below:

$$A_{i,j,k} \geq \frac{q_{i,j,k,p}}{LMTD_{i,j,k,p} U_{i,j}} \tag{2.29}$$

$$A_{j,hu} \geq \frac{q_{j,hu,p}}{LMTD_{j,hu,p} U_{j,hu}} \tag{2.30}$$

$$A_{i,cu} \geq \frac{q_{i,cu,p}}{LMTD_{i,cu,p} U_{i,cu}} \tag{2.31}$$

The objective function which comprises the sum of the capital costs (fixed charges for heat exchangers and maximum heat exchanger area costs) and operating costs (hot and cold utility) is shown next:

$$\begin{aligned} \min\ TAC = AF \cdot & \left[\sum_{i \in H} \sum_{j \in C} \sum_{k \in K} CFz_{i,j,k} + \sum_{i \in H} \sum_{cu} CFz_{i,cu} + \sum_{j \in C} \sum_{hu} CFz_{j,hu} \right] \\ & + AF \sum_{i \in H} \sum_{j \in C} \sum_{k \in K} AC_{i,j,k} A_{i,j,k}^{AE_{ij}} + AF \sum_{j \in C} AC_{j,hu} A_{j,hu}^{AE_{j,hu}} + AF \sum_{i \in H} AC_{i,cu} A_{i,cu}^{AE_{i,cu}} \\ & + \sum_{p \in P} \frac{DOP_p}{NOP} \sum_{j \in C} CUHq_{j,hu} + \sum_{p \in P} \frac{DOP_p}{NOP} \sum_{i \in H} CUCq_{i,cu} \end{aligned} \tag{2.32}$$

The maximum areas have been included in the above objective function instead of average areas per period as used by Aaltola (2003) in Equation 2.28.

It has been observed by the current author that the weighting terms included in the utility terms of the objective functions of Aaltola (2003) and Verheyen and Zhang (2006) in Equations 2.28 and 2.32 respectively will only give an accurate AOC per period for situations in which the duration of the periods are equal to one another.
A multiperiod simultaneous synthesis model for heat exchange networks will also be developed in this study using the proposed interval based superstructure model. This approach will use the maximum area per period model equations of Verheyen and Zhang (2006). However a new utility weighting approach which is more general will be used in the objective function. In addition, the proposed multiperiod model will not include an NLP step since the flows of split streams would have been determined in the MINLP step.

The current author believes that since intermediate temperature locations of the SWS model are not set based on fixed temperature parameters as earlier mentioned, special initialisation techniques may be needed so as to obtain an optimal solution in shorter times especially in problems involving multiple utilities and multiperiod operations. Based on these shortcomings of the SWS model, a simplified approach which relies on fixed intervals needs to be developed for superstructures which will simultaneously trade-off the competing costs in heat exchange problems with little or no initialisations. This will be illustrated in the examples to be presented in Chapter 3.

2.3 Mass Exchanger Network Synthesis, MENS

The different kinds of mass exchange operations include: absorption, stripping, adsorption, ion exchange, leaching and extraction. Mass exchanger network synthesis (MENS) unlike HENS has not received much attention. Many 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), later mathematical programming found applications too (El-Halwagi and Manousiouthakis, 1990a; Papalexandri, *et al*., 1994).

The MENS problem 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 MSAs are to be selected, what should be the optimal flow of such MSAs, what stream pairings should be selected and what should be the optimal system configuration?

2.3.1 Pinch Technology as applied to MENS

Pinch technology application to MENS also involves targeting before actual design. The targets in MENS using pinch technology include minimum mass separating agent (MSA) targets, minimum number of units targets (El-Halwagi, 1997), minimum capital cost targets (Hallale and Fraser, 2000a & b) and total annual cost targets using supertargeting for MENS (Hallale and Fraser, 2000c & d). These targets are discussed next.

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 to recover mass from the process before calling on external MSAs. The more mass is removed with process MSAs, the less the

external MSAs that will need to be purchased. Therefore the constraint to maximum mass separating agent recovery lies with the characteristics of each of the process MSAs which are: its available flowrate and process temperature on site (which determines its equilibrium characteristics). The maximum amount of mass that a process lean stream can recover is limited by the pinch composition.

There are two methods of targeting the minimum MSA, these are the graphical (pinch diagram) and algebraic approaches (El-Halwagi, 1997). The graphical approach will be reviewed in this thesis. The algebraic approach is like the problem table of HENS (El-Halwagi, 1997).

Analogies are established between heat and mass pinch so as to target for the minimum MSA cost. However 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. This is essential because equilibrium relations come to play in mass exchange unlike heat exchange. El-Halwagi and Manousiouthakis (1989) overcame the problem of one-to-one correspondence posed by equilibrium relations in mass exchange by establishing the concept of a "minimum allowable composition difference, ε" which is analogous to the minimum temperature difference, ΔT_{min}, in HENS. The authors also used the '*corresponding composition scale*' which is discussed under the pinch diagram.

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 removed against its supply and target compositions. El-Halwagi and Manousiouthakis (1989) had to use the *corresponding composition scale* to establish the same basis for thermodynamic feasibility between the rich and lean streams and hence form a composite of the lean streams. This is necessary since there is no direct relationship between every rich and lean stream unlike hot and cold streams in HENS. The mass exchange composite curves are shown in Figure 2.7.

The point at which the rich and lean composite curves touch each other is known as the *mass transfer pinch.* The two curves touch each other because the ε is built into the lean

stream compositions unlike the hot and cold composite curves in HENS which do not touch at any point. The pinch 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. 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 process gives the MSA cost targets.

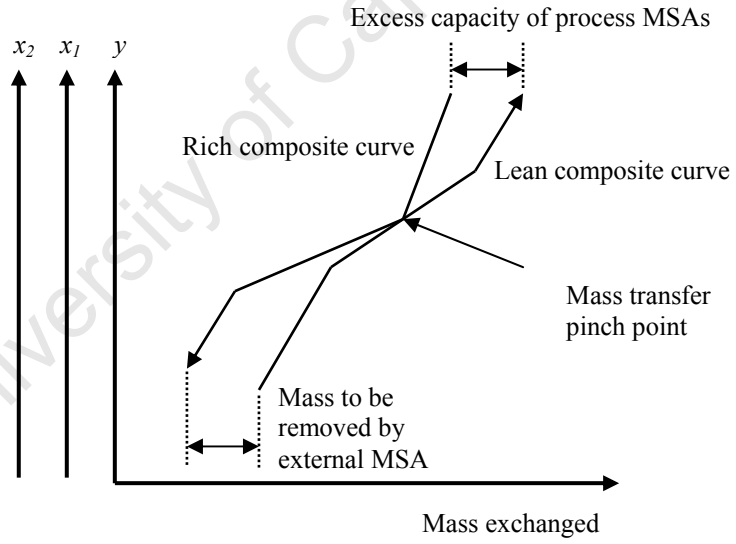


Figure 2.7: Construction of the rich and lean composite curves on the same axes locates the mass transfer pinch and MSA targets.

No mass should be transferred across the pinch, just as it applies in HENS because this will result in a 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.

2.3.1.2 Capital Costs Targets

In predicting the capital cost of a mass exchanger network, factors like the number of mass exchangers, the size (or number of stages) of the exchangers, and the material of construction have to be accounted for as these contribute to the capital cost of a mass exchange network (Hallale, 1998). Staged and continuous contact absorbers will be focused on in this study. The number of units target is reviewed next.

Number of Units targets

The minimum number of units targets for MENS is done as established for HENS. The target is determined 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 (El-Halwagi and Manousiouthakis, 1989).

$$N_{\text{units, pinch}} = (N_{St} - 1)_{\text{Above pinch}} + (N_{St} - 1)_{\text{Below pinch}} \quad (2.27)$$

N_{St} is the total number of streams (rich and lean streams).

Mass Exchange Number of Stages and Height Targets

Hallale and Fraser (2000a & b) developed targeting techniques for factors that contribute to the capital cost of mass exchange networks. Such factors (for both stagewise and continuous contact exchangers) include: total number of real stages (for stagewise exchangers), total height (for continuous contact exchangers), exchanger diameters, tray spacings, inactive heights, distribution of units between streams and distribution of stages and height between streams.

Hallale and Fraser (2000a) developed a new tool known as the *y-y* composite curve plots* for targeting the minimum capital cost for MENs. *y-y** plot represents the *x* composition of each of the MSAs (in the *y-x* plot of Hallale and Fraser, 2000a) as the rich stream composition with which it is in equilibrium, *y**, hence it's a more general approach unlike the *y-x* plot. The minimum composition difference, ε, is now expressed in terms of the rich stream through the following relation:

$$\Delta y_{min} = m_j \varepsilon \quad (2.28)$$

where Δy_{min} is the composition difference in the rich phase and m_j the equilibrium constant.

The mass transfer curve of El-Halwagi and Manousiouthakis (1989) had to be reconstructed in terms of y^* by Hallale and Fraser (2000a). The resulting mass transfer composite curve (Figure 2.8a) 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.

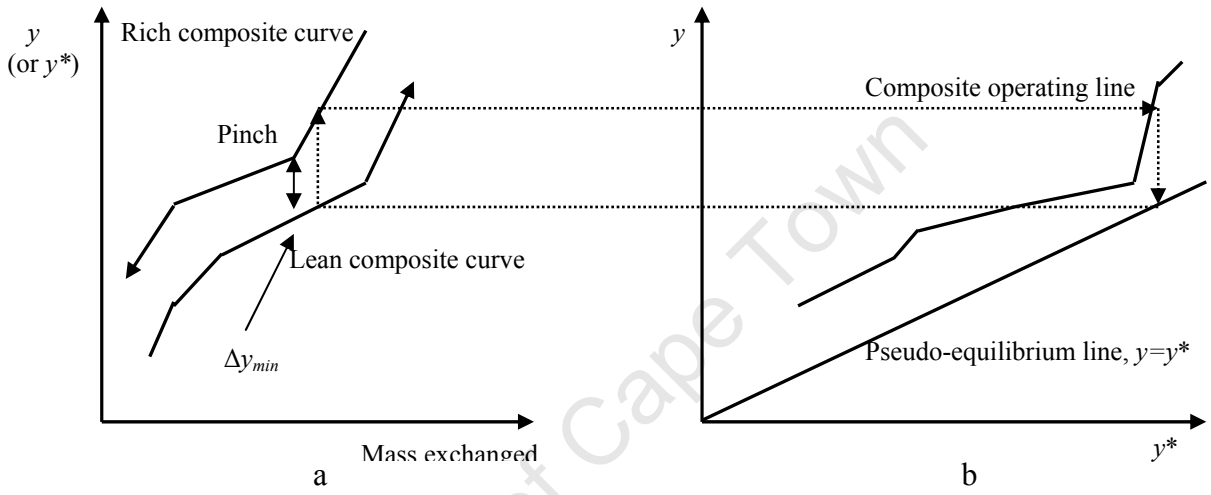


Figure 2.8: Construction of the *y-y** composite curve plot from the balanced mass transfer composite curve plots (*Hallale, 1998*).

Figure 2.8a & b illustrate the construction of the *y-y* composite curve plot* from the modified *mass transfer composite curve plot.* The vertical distance between the rich and lean composite curves is the driving force for mass transfer and the point of closest approach is the $\Delta y_{\min}$. The $\Delta y_{\min}$ (i.e. the pinch) divides the network into two distinct regions: above and below the pinch. The *y-y* composite curve plot* can be used for stages and height targeting. Figure 2.8b 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 major difference is that Figure 2.8b is a composite of more than one MSA. The diagram shows the profile for perfect countercurrent or vertical mass transfer.

This *y-y** composite curve presents the analogy between HENS and MENS using pinch technology. It can be demarcated into composition intervals and each interval treated as

an imaginary mass exchanger for targeting purpose. The composition intervals can also be represented on a grid as is the case with HENS.

For staged columns, the number of stages can be determined in each composition interval (fictitious mass exchanger) using the graphical approach or Kremser equation (when written in terms of y and y^*). Height targets for continuous contact columns can also be established since Δy values are shown.

For staged columns, the number of stages is targeted for each interval to get the equilibrium number of stages: overall column efficiency is then 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:

$$N_{\text{real, total}} = \sum_{i}^{\substack{\text{Rich}\\ \text{streams}}} \left[N_{\text{real},i}\right]_{\text{Above pinch}} + \sum_{i}^{\substack{\text{Rich}\\ \text{streams}}} \left[N_{\text{real},i}\right]_{\text{Below pinch}} \tag{2.33}$$

The number of equilibrium stages divided by column efficiency gives N_{real}. The number of equilibrium stages can be calculated graphically by stepping off on the y-y^* curve or analytically by using the Kremser equation (Treybal, 1981). Note that Kremser has numerical singularities, see section 2.4 for how to overcome them.

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 stages is achieved in the minimum number of units. According to Hallale and Fraser (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 after which a unit distribution pattern is set for the gas steams.

Targeting for continuous contact columns requires accounting for the total packed height, and distribution of packed height between streams. Hallale and Fraser (2000b) used the transfer unit approach for the height targeting. The intervals on the composite

operating line (Figure 2.8b) are also considered as fictitious continuous contact exchangers. The minimum network height, H_{min}, is targeted for each interval as given by:

$$H_{\min} = \sum_{k}^{\text{Intevals}} \frac{1}{\Delta y_{lm,k}} \left(\sum_{i}^{\text{Rich streams}} \frac{w_i}{K_y a DS_i} \right)_k \tag{2.34}$$

where w_i is the mass load of stream i

Δy_{lm} is the logarithmic mean composition difference in interval k

$K_y a$ is stream overall mass transfer coefficient based on rich streams

DS is column cross sectional area

Equation 2.34 will predict to a good extent the minimum height requirement if $K_y aDS$ do not vary significantly. $K_y a$ 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. Note as with $\Delta T_{\min}$, $\Delta y_{\min}$ calculation leads to numerical problems, approximations are discussed in Section 2.4.

Equation 2.34 could also be written as:

$$H_{\min} = \sum_{k}^{\text{Intervals}} \text{NTU}_k \left(\sum_{i}^{\text{Rich streams}} \text{HTU}_i \right)_k = \sum_{k}^{\text{Intervals}} H_k \tag{2.35}$$

where NTU and HTU are number and height of theoretical units respectively. NTU is a function of $\Delta y_{\min}$ in Equation 2.34 while HTU is represents the term in brackets in Equation 2.34.

The column diameter and $K_y a$ are estimated based on the gas streams. Note that the distribution of units among the streams during targeting still remains a challenge as it is not all that straightforward and this can lead to the TAC of designs either being higher or lower than that TAC target, Hallale (1998).

Equation 2.35 can be stated in terms of the streams so as to be able to distribute the total packed height among the streams.

$$H_{\min} = \sum_{i}^{\text{Rich streams}} \text{HTU}_i \sum_{k=\alpha_i}^{\beta_i} \text{NTU}_k = \sum_{i}^{\text{Rich streams}} H_i \tag{2.36}$$

where R_i starts in the interval α_i and ends in β_i on the composite curve.

In keeping with the pinch division, each rich stream's contribution above the pinch is added to that below the pinch (i.e. Equation 2.36 for above and below the pinch) to give the total target which is:

$$H_{\min} = \sum_{i}^{\text{Rich streams}} \left(H_{i,\text{above pinch}} + H_{i,\text{below pinch}} \right) \tag{2.37}$$

Capital Cost Estimation

The procedure for estimating capital cost according to Hallale and Fraser (2000a & b) 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 contributions of each rich stream to the units, diameters, height, and stages are taken into account. Rich streams which cross the pinch are accounted for twice.

2.3.1.3 Supertargeting

With the development of capital cost targeting tools for MENS, TAC targets can be established for MENs before design using pinch technology. Designs can subsequently be initiated based on ε or Δy_{min}. This implies that TAC targets can be determined for a range of ε or Δy_{min} values and design initiated based on the ε or Δy_{min} which gives the least TAC. This procedure is known as supertargeting for MENS (Hallale and Fraser 2000c & d) which is analogous to supertargeting for HENS. Designs based on such optimal ε or Δy_{min} are anticipated to need little or no evolution in order to meet the targets.

2.3.1.4 Network Design

In order to meet the MSA cost targets in design, stream matching should start at the pinch since this is the most constrained part of the network (El-Halwagi and Manousiouthakis, 1989). For capital cost targets, 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-y** composite curve). The two feasibility criteria of El-Halwagi and Manousiouthakis (1989) are first presented 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,

$$N_{R,\text{ above pinch}} \leq N_{S,\text{ above pinch}} \tag{2.38}$$

where N_R and N_S are the number of rich and lean streams respectively.

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

$$N_{\text{R, below pinch}} \geq N_{\text{S, below pinch}} \tag{2.39}$$

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:

$$\frac{L_j}{m_j} \geq G_i \tag{2.40}$$

L_j and G_i are the flowrates of lean stream j and rich stream i respectively, m is the equilibrium relation constant for lean stream j.

Immediately below the pinch the following inequality must hold:

$$\frac{L_j}{m_j} \leq G_i \tag{2.41}$$

Stream splitting may be required 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 and Fraser (1998, 2000a-b) show that the minimum number of units is not always compatible with achieving the minimum TAC.

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

The driving force (y-y) plot*

The driving force plot for MENS is constructed from the *y-y** composite curve plot of Hallale and Fraser (2000a) and it serves about the same purpose as the DFP for HENS (Linnhoff and Ahmad, 1990). The goodness of selected matches is evaluated on the *y-y** composite curve by comparing the operating line of each potential match with the composite operating line. This method makes for a quick screening of potential matches.

Remaining problem analysis

The concept behind remaining problem analysis (RPA) for MENS is exactly as it applies to HENS RPA where the goodness of a match is evaluated based on the penalty incurred when the remaining problem is analysed (Linnhoff and Ahmad, 1990). When a match, *M*, is selected, the remaining stages/height for the problem is denoted $N_{\text{real,remaining}}$. The number of stages/height of the actual match, $N_{\text{real,M}}$ is added to $N_{\text{real,remaining}}$ to give the minimum number of stages/height now possible. The difference between the original target for the whole problem, N_{real} and $N_{\text{real, }M} + N_{\text{real,remaining}}$ gives the penalty incurred by placing the match, *M*. This penalty implies the use of more stages/height above the target in design. The efficiency, α_{match} is used by Hallale (1998) to evaluate the penalty similar to that in HENS as:

$$\alpha_{match} = \frac{N_{real}}{\sum_{M}^{\text{Matches}} N_{real,M} + N_{real,remaining}} \tag{2.42}$$

It should be noted that no specific order to follow has been reported in making matches using the above set of rules in pinch technology for MENS.

2.3.1.5 Multiple External MSAs

Fraser, *et al*. (2005) developed techniques for selecting between alternative MSAs including the minimum flowrate requirement for the selected MSAs. Prior to their study, MSA selection using pinch technology had been based on choosing the external MSA with the lowest cost per unit mass. Fraser, *et al*. (2005) argued that selection criteria should be based on the MSA with the lowest overall cost of removal of mass which

depends on both the cost of the MSA and its allowable concentration range. This approach targets the set of MSAs to use without considering the capital cost implications. The authors suggested that the CUP of Shenoy, *et al*. (1998) can be adapted in order to account for the capital costs of the network.

Implementing the MENS GCC of Fraser, *et al*. (2005) will be a tedious and time consuming task because it involves a series of steps. Firstly, the GCC is constructed using the optimal Δy_{min} value obtained from supertargeting. The second step involves adjusting the flows of the process MSAs so as to establish the mass to be absorbed by the external MSAs on the GCC. The last step is ranking the external MSAs based on their ability to remove mass while considering their composition ranges. The pinch design method as usual follows the targeting stage. The level of tediousness in the synthesis will only increase if the MENS analogue of the CUP of Shenoy, *et al*. (1998) for HENS is combined with the MENS GCC of Fraser *et al*. (2005) in order to select between multiple external MSAs.

Recently, Bandyopadhyay, *et, al*. (2006) developed the source composite curve which can be applied to problems that involve the flow of water, hydrogen and material recycle. Shenoy and Bandyopadhyay (2007) extended this source composite curve to the targeting of multiple resources for the purpose of minimising the operating cost of the whole process. Shenoy and Bandyopadhyay (2007) made a similar observation with Fraser, *et al*. (2005) in terms of the best resource to use. They reported that the best resource to use is not the one with the minimum cost. The authors developed a cost priotising technique in order to select the proper resources that minimise operating cost subject to the availability of the resource. However none of these approaches which are based on the source composite curve includes capital costs.

It is worthwhile to mention that the decomposition of a mass exchange problem at the pinch does not allow for a simultaneous trade-off among the costs which contribute to the TAC. Each step of the pinch synthesis method is based on the previous ones. The sequential nature of the pinch method makes the optimisation of multiple variables a difficult task to accomplish especially for large mass exchange problems. Such problems include: those involving multiple MSAs, those that have multiple periods of operation and those that need to be combined with heat exchange networks. In addition, problems

involving significantly different mass transfer coefficients will not always be perfectly predicted using the targeting equations just discussed.

Hallale (1998) developed targets for mass exchange networks based on exchanger mass or volume because targets based on exchanger number of stages can be beaten in design. The current author observed that such discrepancies are more pronounced in mass exchange problems which involve multiple process MSAs. The pinch synthesis approach requires that at least one of the process MSAs be used up to the thermodynamically feasible capacity before bringing in external MSAs. Such process MSAs create the pinch. The simultaneous mathematical approaches which are discussed in the next section do not decompose at the pinch or give preference to any MSA. Networks which do not partition process MSA usage at the pinch but still give good solution networks are presented in Chapter 4.

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 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 methods.

The task of mass exchange network synthesis using mathematical programming has been tackled through the decomposition method just as has been done for HENS. The sequential approach entails the following steps:

- Minimum MSA cost
- Minimum number of matches
- Minimum investment cost network configurations

El-Halwagi and Manousiouthakis (1990a) established analogies between the transhipment model and the MENS problem just as was done by Papoulias and Grossmann (1983) for the HENS problem. They formulated as a mathematical

optimization model the problem of determining the mass exchange pinch point and hence the minimum MSA cost requirement using LP. These authors went on to use MILP to determine the minimum number of matches that meet the MSA cost target.

Lee and Park (1996) used Process Graph Theory to synthesize mass exchange networks. This method entails two steps: all feasible MEN flowsheets are evaluated in the first step while their operating conditions are determined in the second step. The process graph theory involves the use of material and operating nodes. Lee and Park converted rich and lean stream information into the material set of the P-graph theory while mass exchanger unit information is transformed into an operating unit set. A maximal structure which comprises of all the possible network structures is subsequently generated. Each of the networks generated is optimised as an NLP model in order to determine the optimal operating conditions.

Comeaux (2000) formulated an NLP superstructure for MENS which combines insights from the vertical mass transfer concept of pinch technology with reducible superstructure. This approach is good in that mathematical constraint and hence optimisation can then be used to conquer the dimensionality problems encountered in pinch technology while approaching vertical mass transfer. The method finds the minimum total costs by simultaneously trading off the different costs involved in mass exchange problems.

The NLP superstructure of Comeaux (2000) is generated by creating composition intervals using the supply and targets compositions of the rich streams and the equilibrium equivalents of the lean streams in the problem. The composition intervals are ordered in a descending order from right to left and each stream is made to participate in composition intervals which fall within its composition range. Every lean stream is then extended beyond its target composition to the right in order to make it participate in at least one interval with every rich stream in the problem. Such extension is feasible thermodynamically and Comeaux (2000) called this the ‘stream extension rule’.

The concept upon which the NLP superstructure is generated is the vertical mass transfer of pinch technology. However it is different from the pinch technology approach in the following ways. Firstly, it does not partition the network at the pinch. Secondly, no

preference is given to any of the MSAs in terms of how much of its capacity is to be used. Thirdly, the intermediate compositions of streams are variables to be optimised. The superstructure despite being generated using supply and target compositions of streams can have parallel and series exchanger match configurations through the use of stream bypass constraints.

The superstructure consists of the following constraints:

- Rich stream total mass balances which are written over every interval where the streams exist
- Lean stream total mass balances (including branch flows) also written over every interval where the streams exist
- Splitter component mass balances for rich streams at the inlet of the first interval where the streams exist
- Splitter component mass balances for the starting interval of lean streams (this includes exchanger and bypass branches)
- Splitter/mixer interval component mass balances for calculating interval inlet compositions for rich streams
- Splitter/mixer interval component mass balances for calculating interval compositions for lean streams (this includes bypass streams)
- Rich and lean stream final composition component balances
- Mass exchanger component mass balances (including bypass)
- Bounds for lean stream flows and target compositions
- Driving force equations
- Mass exchanger sizing equations
- An objective function which minimises the TAC of the network

The NLP reducible superstructure of Comeaux (2000) and the P-graph synthesis approach of Lee and Park (1996) both have the advantage that binary variables are not involved in the model, hence the size of the model is reduced since only an NLP model needs to be solved. The presence of binary variables requires that multiple NLP be solved in order to find the best solution. Comeaux (2000) argued that the presence of branch flows through exchangers can be used to ascertain whether an exchanger exists or not. It should be noted that the exclusion of binary variables may not necessarily simplify

the initialisation and bound setting required for the model since the presence of non linear mass balances and mixing equations introduce non linearities and non convexities into the model. Also the absence of integer variables makes it difficult to synthesise MENs having non linear functions with installation costs.

Szitkai, *et al*. (2006) developed a mass exchange analogue of the simplified SWS MINLP Model of Yee and Grossmann (1990). The mass exchange SWS model also simultaneously optimises the competing costs in a mass exchange problem. The model equations of this superstructure are discussed next.

2.3.2.1 Fairly Linear MINLP (FLM) Model for MENS

Similar to the SWS model of Yee and Grossmann (1990) for HENS, the FLM model of Szitkai, *et al*. (2006) relies on flexible stages whose composition boundaries are variables to be optimised. The model does not require partitioning at the pinch; also, it does not discriminate among the MSAs in terms of their flow usage. A simultaneous trade-off among the different costs is established since the objective function comprises all the costs which contribute to the total costs. The superstructure for a two rich and two lean stream problem is shown in Figure 2.9.

Note that this superstructure is similar to the SWS of Yee and Grossmann (1990) for HENS. The rich streams are shown in Figure 2.9 with each starting from the first composition location, b =1, and running to the last composition location, b = 3. The lean streams run countercurrent to the rich streams starting from the last composition location, b = 3, and ending in the first location, b = 1. The number of stages can also be determined based on $\max\{N_R, N_S\}$ where N_R is the number of rich streams while N_S the number of lean streams in the problem.

Using Figure 2.9 for illustration, the composition of R_1 is $Y_{1,1}^{S}$ in composition location, b=1, which corresponds to its supply composition. R_1 can split into two streams because there are two lean streams, S_1 and S_2 present in the superstructure. If R_1 splits, then each of the split branches will exchange mass with S_1 and S_2 in exchangers R_1-S_1 and R_1-S_2 in stage 1. The split streams exiting from exchangers R_1-S_1 and R_1-S_2 are assumed to be

mixed at equal compositions. The exit composition of the mixer becomes the composition of R_1 in composition location, $b = 2$, i.e. $y_{1,2}$ in Figure 2.9. $y_{1,2}$ is treated as a

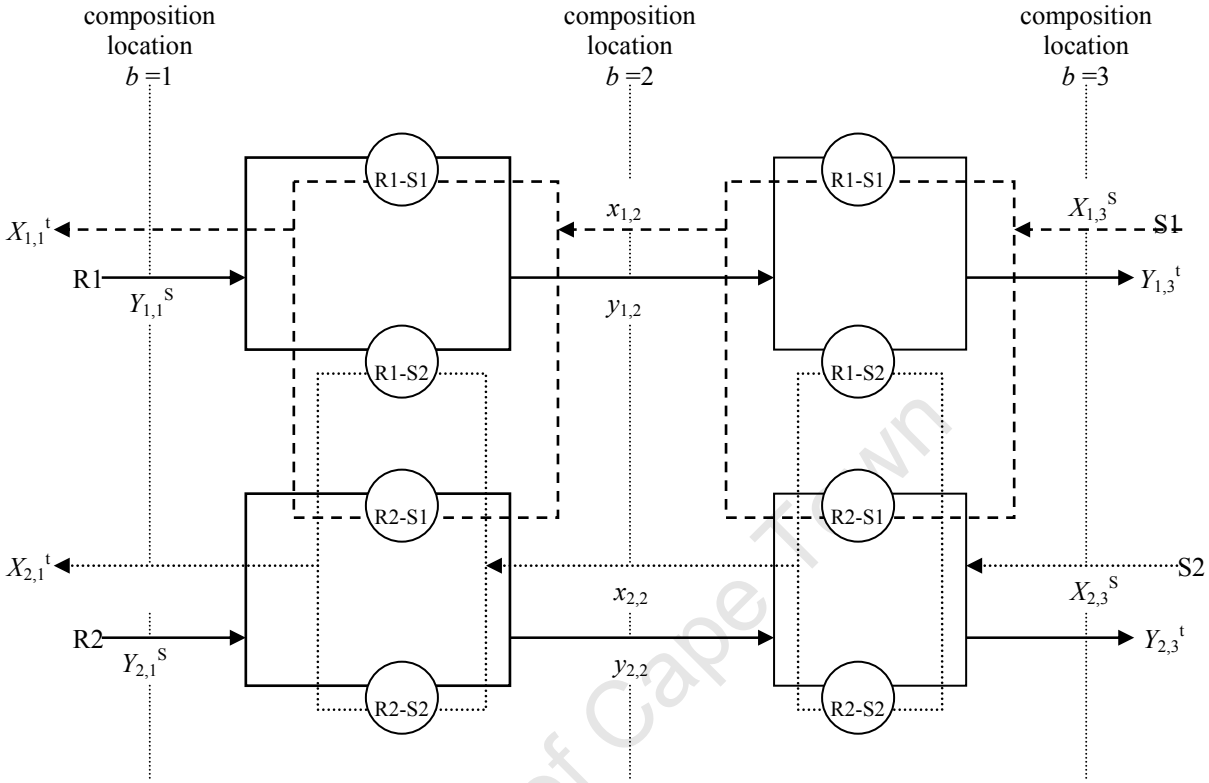


Figure 2.9: Two stage superstructure of Szitkai, *et al*. (2006)
for two rich streams and two lean streams.

variable to be optimised in the FLM model for mass exchange. R_1 whose composition is now $y_{1,2}$ in composition location, $b = 2$, enters into stage 2 and splits again in the same manner with stage1. The mass exchange and mixing pattern of stage 1 is repeated in stage 2. Note that the composition of R_1 in each composition location is dependent on how much mass it exchanged with lean streams in previous stages. The lean streams also exchange mass in the same manner as discussed for rich streams.

Szitkai, *et al*. (2006) as mentioned earlier also assume equal composition mixing for split streams which are recombining. Hence the authors did not include the non linear mass balance and mixing equations in the superstructure model. This assumption has the advantage of simplifying the model because non linear equations are restricted to just the objective function. The FLM superstructure composition stages are flexible because every composition location is a variable to be optimised; hence there is no strict vertical

mass transfer. Streams and matches can easily be restricted in terms of which stream pairings to allow and the associated mass loads. The shortcomings of the FLM model for MENs are similar to those of HENs and they include the following;

- Structures which are only feasible with nonisocomposition mixing may be excluded (e.g by-pass streams) from consideration in the optimisation
- Split streams cannot go through two or more exchangers in series (Floudas, 1995)
- An NLP sub-optimisation step will be needed in order to determine the split flows and exchanger exit compositions (Isafiade & Fraser, 2007a)
- Special initialisation techniques may be needed for large mass exchange problems especially those involving multiple process and external MSAs or multiple periods of operations.

A new fairly linear interval based MINLP superstructure (IBMS) model for MENS is developed in this study. This method overcomes the last two shortcomings of the FLM model of Szitkai, *et al*. (2006). The composition locations of the new superstructure model are defined using the supply and target compositions of either the rich or lean set of streams while the other stream set compositions are allowed to float across the defined composition intervals. The ability of the floating stream set to exchange mass in any interval is dependent on thermodynamic feasibility. The IBMS method for MENS is described in detail in Chapter 4 of this thesis. The equations of the FLM model are similar to those of the SWS model of Yee and Grossmann (1990) except that in the SWS model the utilities are positioned outside the superstructure while in the FLM, the external lean streams are made to run across the superstructure. The FLM model equations are described next.

Overall stream mass balance

In order for a stream to get to its target composition, it needs to exchange mass with the streams of the opposite kind in the stages. Note that a stream does not need to exchange mass in every stage in order for it to get to its target composition. The sum of masses exchanged in stages with streams of the opposite kind is set equal to the mass load of the stream concerned. This is described by Equations 2.43 and 2.44 below:

$$\left(Y_r^s - Y_r^t\right)\cdot G_r = \sum_{b\in B}\sum_{l\in S} M_{r,l,b} \qquad r\in R \tag{2.43}$$

$$\left(Y_l^{*t} - Y_l^{*s}\right)\cdot L_l = \sum_{b\in B}\sum_{r\in R} M_{r,l,b} \qquad l\in S \tag{2.44}$$

where, Y_r^S and Y_r^t are the supply and target compositions of rich stream *r* while Y_l^{*s} and Y_l^{*S} are the equilibrium compositions of lean stream *l* in the rich phase. $M_{r,l,b}$, and L_l are continuous variables, they represent the mass exchanged between rich stream, *r,* and lean stream, *l,* in interval *b* and the flow rate of lean stream, *l*, respectively. G_r is the flowrate of rich stream, *r*, while *R* and *S* represent the set of rich and lean streams respectively.

Stage mass balance

Stage mass balances are used to determine the composition of each stage boundary for each stream. This is shown below:

$$\left(y_{r,b} - y_{r,b+1}\right)\cdot G_r = \sum_{l\in S} M_{r,l,b} \qquad r\in R \quad b\in B \tag{2.45}$$

$$\left(y^*_{l,b} - y^*_{l,b+1}\right)\cdot L_l = \sum_{r\in R} M_{r,l,b} \qquad l\in S \quad b\in B \tag{2.46}$$

where $y_{r,b}$ and $y^*_{l,b}$ are continuous variables, they correspond to the composition of rich stream *r* and lean stream *l* (equilibrium composition in the rich phase) in composition location *b*.

Assignment of superstructure inlet compositions

Composition location, $b = 1$, is assigned the supply composition of the rich streams while composition location, $b = NB + 1$ is assigned the supply compositions of the lean streams. These are described in the following equations:

$$Y_r^S = y_{r,1} \qquad r\in R \tag{2.47}$$

$$Y_l^{*S} = y_{l,NB+1} \qquad l\in S \tag{2.48}$$

Feasibility of compositions

Rich streams run from the left to the right while lean streams run from the right to the left in the superstructure. The set of constraints shown in Equations 2.49 and 2.50 are used to ensure that there is a monotonic decrease in stage composition from left to right.

$$y_{r,b} \geq y_{r,b+1} \qquad b \in B,\ r \in R \tag{2.49}$$

$$y^*_{l,b} \geq y^*_{l,b+1} \qquad b \in B,\ l \in S \tag{2.50}$$

Logical constraints

The existence of a match, *r,l*, in stage *b* is modelled using logical constraints and binary variables, $w_{i,j,k}$. An integer value of '1' indicates the existence of a match in the optimal network and '0' if otherwise. The equations representing this are:

$$M_{r,l,b} - \Omega_m w_{r,l,b} \leq 0 \qquad r \in R,\ l \in S,\ b \in B \tag{2.51}$$

where Ω_m is an upper bound on the amount of mass that can be exchanged between stream *r* and *l*. It can be set as the smaller mass load of the two streams participating in the match.

Mass exchange driving force calculation

The approach compositions, $dy_{r,l,b}$, were calculated as follows:

$$dy_{r,l,b} \leq y_{r,b} - y^*_{l,b} + \Gamma_m\left(1 - w_{rlb}\right) \qquad b \in B,\ r \in R,\ l \in S \tag{2.52}$$

$$dy_{r,l,b} \geq y_{r,b} - y^*_{l,b} - \Gamma_m\left(1 - w_{rlb}\right) \qquad b \in B,\ r \in R,\ l \in S \tag{2.53}$$

$$dy_{r,l,b+1} \leq y_{r,b+1} - y^*_{l,b+1} + \Gamma_m\left(1 - w_{r,l,b}\right) \qquad b \in B/last,\ r \in R,\ l \in S \tag{2.54}$$

$$dy_{r,l,b+1} \geq y_{r,b+1} - y^*_{l,b+1} - \Gamma_m\left(1 - w_{r,l,b}\right) \qquad b \in B/last,\ r \in R,\ l \in S \tag{2.55}$$

The binary variables, w_{rlb}, are also used in the approach composition calculation so as to ensure feasible driving forces for the exchangers selected in the optimal network. The upper bound, Γ_m, inactivates the equation if a match does not exist. The following equation gives numerical stability to the solution; it is the integer infeasible path MINLP (IIP-MINLP) formulation of Sorsak and Kravanja (2002):

$$w_{rlb} = dw_{rlb} + ew_{rlb} - fw_{rlb} \quad r \in R \ \ l \in S \ \ b \in B \tag{2.56}$$

where dw_{rlb} is the real binary variable while w_{rlb} is the relaxed version. ew_{rlb} and fw_{rlb} are positive and negative tolerances respectively.

Logarithmic mean concentration differences (LMCD)

Chen's first approximation for LMCD is used to calculate the LMCD of the exchangers (Chen, 1987).

$$LMCD_{r,l,b} = \left[(dy_{r,l,b}) \cdot (dy_{r,l,b+1}) \cdot (dy_{r,l,b} + dy_{r,l,b+1})/2 \right]^{1/3} \qquad r \in R \;\; l \in S \;\; b \in B \qquad (2.57)$$

The capital cost estimation based on exchanger mass for packed columns by Hallale (1998) is used in the FLM model of Szitkai *et al*. (2006) for calculating capital cost of the exchangers. However, an example was also presented that requires conventional exchanger costing and it was solved using the FLM model. The equation relating mass exchanged, M_{rlb} to exchanger mass, $mass_{rlb}$ is shown in Equation 2.58.

$$mass_{rlb} K_W LMCD_{rlb} = M_{rlb} \qquad r \in R \;\; l \in S \;\; b \in B \qquad (2.58)$$

where $mass_{rlb}$ is the estimated mass of exchanger in kg, K_w is the lumped mass transfer coefficient.

Objective function

The objective function simultaneously minimises the MSA costs and the annualized capital cost of exchangers which is a function of exchanger masses $fn(mass_{rlb})$.

$$\text{TAC} = \sum_{r \in R} \sum_{l \in S} \sum_{b \in B} fn(mass_{rlb}) + \sum_{l \in S} AC_l L_l + o \sum_{r \in R} \sum_{l \in S} \sum_{b \in B} \left(ew_{rlb} + fw_{rlb} \right) \qquad (2.59)$$

where AC_l is the cost per unit of the lean stream, the last term in Equation 2.59 is the penalty term based on Equation 2.56, the o in this term is the weighting factor, which can be an arbitrarily large number.

When the costing equations are included in the objective function, the model becomes fairly linear since Equations 2.44, 2.46 and 2.59 would be the only non linear equations in the model. In order to maintain the fairly linear nature of the FLM model in its application to staged columns, the costing equations have to be made linear as well. According to (Szitkai *et al*., 2006), the use of the Kremser equation will increase the number of non linear equations in the model.

Chen and Hung (2005) also used the stagewise approach of Yee and Grossmann (1990) to generate a superstructure for MENS. The technique of these authors is different from that of Szitkai, *et al*. (2006) based on the fact that they included non linear mass balance and mixing equations in order to calculate the split stream flows and exchanger exit compositions. This helps to eliminate the need for an NLP suboptimisation step which is needed in order to determine the split flows and exchanger exit compositions. A second benefit of the inclusion of the non linear mass balance and mixing equation is that MENs problems involving multiple components can be handled. On the other hand, initialisations, setting of bounds and optimal solution generation in short times may be difficult due to the presence of the non linear mass balance and mixing equations. Szitkai, *et al*. (2006) extended their FLM model to handle multiple components problems based on the following conditions: using just one set of integer variables for all component subnetworks, using the same lean stream flowrates in all subnetworks and including additional composition constraints for the matches so as to ensure the same stream splits in the subnetworks.

The COG sweetening example of El-Halwagi and Manousiouthakis (1989) which involves multiple compatible components was solved by both Szitkai, *et al*. (2006) (using the extended FLM model) and Chen & Hung (2005). The extended model of Szitkai, *et al*. (2006) gave a network with a TAC of 436,289 $/yr and five units while that of Chen and Hung (2005) gave a network with a TAC of 429,700 $/yr and four units.

Emhamed, *et al*. (2007) in trying to overcome the problems associated with the stagewise FLM of Szitkai, *et al*. (2006) developed a hybrid approach which involves the use of integer cuts and bounds. The process starts by using the DFP of a supertarget solution from pinch technology to construct an initial flowsheet. Just one of the external MSAs is used to construct the flowsheet which is then optimised using the stagewise FLM model. The following scenario is then observed in order to know when to stop the iteration;

- Feasible solution obtained and TAC is less than or equal to $1.1*TAC_{target}$, iteration is stopped and the final solution is gotten
- Feasible solution obtained and TAC not less than or equal to $1.1*TAC_{target}$, integer cut and bound applied

- Infeasible solution, new initial structure is constructed and a relaxed binary variable used in the stagewise FLM model.

This approach does not give a guarantee of the optimum because the pinch technology TAC_{target} which is used to set bounds is itself fraught with shortcomings. In addition going through the procedure stated above can be tedious and time consuming because it involves pinch technology and the stagewise FLM model.

It is worth mentioning once again that the problems associated with the SWS of Yee and Grossmann (1990) for HENS also applies to the FLM of Szitkai, *et al*. (2006). The composition locations which form the boundaries of the stages in the FLM helps to split streams in stages so that they can exchange mass before entering into the next stage. Such approach only allows parallel match sequences.

Another shortcoming of the FLM model is that there cannot always be an automatic equal composition mixing of the split streams in stages because the composition locations (i.e. stage boundaries) are variables to be optimised. Only the first and last composition boundaries of the superstructure are fixed by the problem specifications. Hence only splits which occur in the first or last stage of the superstructure can be guaranteed of having isocomposition mixing. Examples which illustrate this and how it can be overcome is presented in Chapter 4 of this thesis. Solutions which involve split streams might need to be solved in a suboptimisation step in order to determine the split flows and their exchanger exit compositions. The FLM model of Szitkai, et al. (2006) and the SWS model of Chen and Hung (2005) may require intervention in the optimisation process in order to get good solutions in reasonable times.

Based on these shortcomings of the FLM model, an approach which is still fairly linear but relies on fixing the composition locations of the superstructure needs to be developed. Such a method will still simultaneously trade-off the competing costs in mass exchange problems with little or no initialisations. This method is presented in Chapter 4 of this thesis.

2.4 Logarithmic mean

Equal temperature differences on both sides of exchangers introduces numerical difficulties in the logarithmic mean temperature difference (LMTD) calculation due to division by zero, This led to a series of approximations proposed by different authors for overcoming such difficulties. Similarly for mass exchange networks, equal composition differences on both sides of exchangers introduce the same numerical problems. The analogues of the logarithmic mean temperature difference (LMTD) approximations have also been used in mass exchange problems. The mass exchange logarithmic mean composition difference (LMCD) is shown in Equation 2.60 while the approximations are presented in Equations 2.61 to 2.64.

$$\frac{\left[y_{r,b}-y_{l,b}^{*}\right]-\left[y_{r,b+1}-y_{l,b+1}^{*}\right]}{\ln\left[\frac{\left(y_{r,b}-y_{l,b}^{*}\right)}{\left(y_{r,b+1}-y_{l,b+1}^{*}\right)}\right]} \tag{2.60}$$

Average LMCD

$$\frac{\left[y_{r,b}-y_{l,b}^{*}\right]+\left[y_{r,b+1}-y_{l,b+1}^{*}\right]}{2} \tag{2.61}$$

Underwood (1970) LMCD approximation

$$\left[\frac{1}{2}\left(\left(y_{r,b}-y_{l,b}^{*}\right)^{1/3}+\left(y_{r,b+1}-y_{l,b+1}^{*}\right)^{1/3}\right)\right]^{3} \tag{2.62}$$

Paterson (1984) LMCD approximation

$$\frac{2}{3}\cdot\left[\left(y_{r,b}-y_{l,b}^{*}\right)\cdot\left(y_{r,b+1}-y_{l,b+1}^{*}\right)\right]^{\frac{1}{2}}+\frac{\left(y_{r,b}-y_{l,b}^{*}\right)+\left(y_{r,b+1}-y_{l,b+1}^{*}\right)}{6} \tag{2.63}$$

First Chen (1987) LMCD approximation

$$\left[\left(y_{r,b}-y_{l,b}^{*}\right)\cdot\left(y_{r,b+1}-y_{l,b+1}^{*}\right)\cdot\frac{\left(\left(y_{r,b}-y_{l,b}^{*}\right)+\left(y_{r,b+1}-y_{l,b+1}^{*}\right)\right)}{2}\right]^{\frac{1}{3}} \tag{2.64}$$

Second Chen (1987) LMCD approximation

The second Chen (1987) approximation is a modification of the Underwood (1970) approximation. It is given as:

$$\left[\frac{1}{2}\left(\left(y_{r,b}-y_{l,b}^{*}\right)^{0.3275}+\left(y_{r,b+1}-y_{l,b+1}^{*}\right)^{0.3275}\right)\right]^{1/0.3275} \tag{2.65}$$

The presence of singularities in the Kremser equations results in difficulties when applied in a mathematical programming environment. This led Shenoy and Fraser (2003) to develop a new formulation of the Kremser equation for the sizing of mass exchangers. Their formulation involves the use of the logarithmic mean approximations of Underwood (1970) and the second Chen (1987) for the ratio of logarithmic mean terms in the Kremser sizing formular. Shenoy and Fraser (2003) presented Equation 2.66 for the sizing of mass exchangers.

$$N_{r,l,b}=\left(\frac{\Delta y^{n}+\Delta y^{*n}}{\Delta y_{1}^{n}+\Delta y_{2}^{n}}\right)^{1/n} \tag{2.66}$$

where Δy^{n} = rich stream concentration difference,

Δy^{*n} = lean stream equilibrium concentration difference

Δy_{1}^{n} = rich end of the exchanger driving force

Δy_{2}^{n} = lean end of the exchanger driving force

n = 1/3 (Underwood, 1970) and 0.3275 (Chen, 1987).

Shenoy and Fraser (2003) applied their formulation of the Kremser equation to 71 different mass exchangers in eight different networks presented by Hallale (1998). The authors did some comparisons using the actual logarithmic mean and the each of the logarithmic mean approximations. They tabulated the worst results (i.e. those with the largest deviations from the actual logarithmic mean) for each of the approximations and also averaged deviations over all 71 networks. The first Chen (1987) approximation gave the largest average deviation, an error of 4.67% which is an overestimation of the number of stages. Chen's second approximation performed best (0.53%), followed by Underwood (1970) and Patersen (1984) with 0.76% and 1.55% respectively. Nevertheless Chen's first approximation is used in sizing heat and mass exchangers in this study because most of the literature examples which were worked also used this approximation.

2.5 Synthesis of Combined Heat and Mass Exchange Networks

Absorption and stripping are improved at lower and higher mass exchange temperatures respectively (Seader and Henley, 1998). Also, temperature dependent equilibrium relations may be strongly non linear relations; hence it would be beneficial to combine the synthesis of heat and mass exchange networks. Process streams needing heating or cooling on site can be used to enhance absorption/stripping in mass exchange networks. This requires that the different costs involved have to be optimised simultaneously in order to obtain minimum total costs. Such costs include heating/cooling costs, MSA costs and heat and mass exchanger capital costs. However very little attention has been given to the study of combined heat and mass exchange network synthesis (CHAMENS).

The few studies have used pinch technology (Hallale, 1998; Isafiade & Fraser, 2007b) and mathematical programming (Srinivas & El-Halwagi, 1994; Srinivas, 1994 and Papalexandri & Pistikopoulos, 1994). Figure 2.10 is a presentation of combining the synthesis of heat and mass exchange networks.

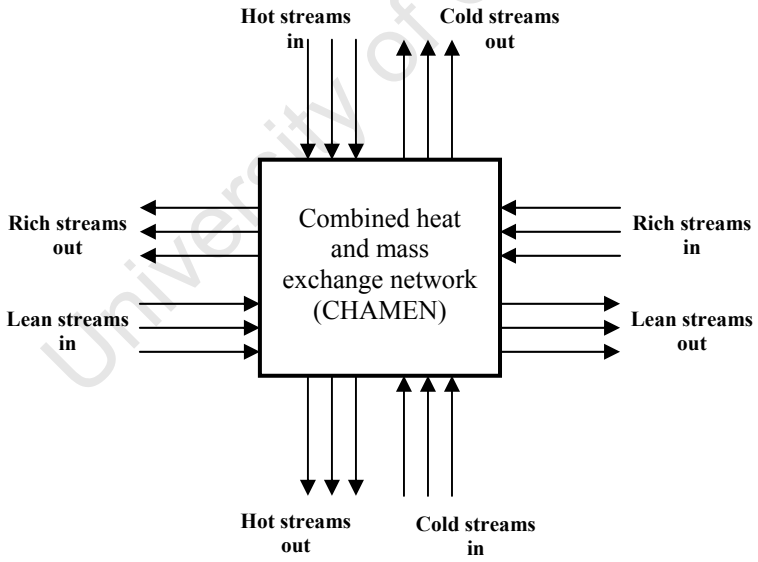


Figure 2.10: Schematic representation of the combined heat and mass exchange network synthesis problem (after Srinivas and El-Halwagi, 1994).

Srinivas and El-Halwagi (1994) used a two stage MINLP decomposition approach to combine the synthesis of heat and mass exchange networks. The first stage involves targeting the minimum operating cost (MOC) of the problem. The MOC comprises the costs of heating/cooling and the costs of MSAs. The minimum number of heat and mass

exchangers which corresponds to the targeted MOC in the first step is determined in the second step. The MOC MINLP model is initialised using a shortcut linear formulation.

In order to optimise the mass exchange temperatures, the authors used the concept of lean substreams where each of the lean streams is assumed to split into a number of substreams. The composition and temperature of each substream can vary between a supply and a target value. The flow of every substream (which is treated as a variable) does not split or mix with any other. Srinivas and El-Halwagi (1994) argued that an MOC solution of a CHAMEN can be obtained when each substream exchanges mass at a particular optimum temperature. The temperature range of the lean substreams is allowed to fall within the working temperature range of the MSA.

Srinivas (1994) used a state space approach to combine the synthesis of heat and mass exchanger networks. The state space technique also gives the same network given by the two stage MINLP approach of Srinivas and El-Halwagi (1994) when applied to a CHAMENS problem.

Papalexandri and Pistikopoulos (1994) developed a MINLP hyperstructure for multiperiod separation processes involving both heat and mass transfer. The hyperstructure is believed to embed all potential configurations of mass (including regeneration) and heat exchange alternatives where stream flowrates and their supply compositions and temperatures may vary according to a set of discrete values. Initial splitting, mixing of inlet and outlet streams respectively 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. The authors applied the MINLP hyperstructure model to a problem involving just one distillation column.

The MINLP model of Papalexandri and Pistikopoulos (1994) comprises of the following equations:

- Splitter mass balances in each period for each stream
- Splitter mass balances in each period prior to and after each mass and heat exchange units

- Mixer mass balances in each period for the total stream flowrate and prior to every mass and heat exchanger
- Mixer component mass balances in each period and mixer for every component and prior to every mass and heat exchanger, this also includes the superstructure final mixer
- Mixer energy balances in every period prior to each mass and heat exchanger and after every heat exchanger
- Component mass balances in every mass exchanger in each period
- Energy balances for every heat exchanger in each period of operation
- Driving forces to ensure feasibility of the transfer of mass and energy in every exchanger and period
- Mass and heat exchanger sizing equations
- Logical constraints which relate continuous variables (mass and heat loads, stream flowrates, areas and number of stages) in every period to discrete variables (existence of pipes and units)
- Integer constraints describing the connectivity and logic of the network
- An objective function which simultaneously minimises the TAC consisting of utility and external lean stream costs and the equipment (heat and mass exchanger) costs.

Isafiade and Fraser (2007b) used pinch technology to combine the synthesis of heat and mass exchange networks. Pinch technology TAC targeting methods for mass exchange were used to analyse the total cost of the mass exchange problem at discrete values of substream temperatures. The thermal needs at each of these mass exchange temperatures were optimised using pinch technology TAC targeting methods for heat exchange. The costs of the two networks at each of the mass exchange temperatures were added and the least chosen as the best.

The concept of the lean substream of Srinivas and El-Halwagi (1994) is a good way of discretising the lean stream where each substream is associated with a mass exchange temperature which is to be optimised. However the decomposition approach might miss the optimal solution because there is no simultaneous trade-off among the multiple competing costs. Synthesizing combined heat and mass exchange networks with the sole

aim of minimizing the heating/cooling, MSA cost and number of units will fail to exploit to the fullest the potential in combining the synthesis. The MINLP method of Srinivas and El-Halwagi (1994) also requires a special initialisation technique (the near minimum MOC solution). This initialisation method serves the operating cost part of the CHAMENS problem while leaving out the capital cost aspect.

There is no guarantee of optimality in the solutions of the hyperstructure model of Papalexandri and Pistikopoulos (1994) due to the presence of non linear heat and mass exchange equations in the model. These non linear equations also makes developing an initialisation technique difficult.

The pinch technology approach of Isafiade and Fraser (2007b) has the following shortcomings: firstly, the problems associated with pinch technology targeting and design steps for heat and mass exchanger networks synthesis discussed in previous sections are carried over into CHAMENS when pinch technology is used to synthesise both networks. Secondly, the pinch method becomes tedious to implement for large CHAMENs problems involving regeneration since supertargeting needs to be done at each option of mass exchange temperature for the two networks.

The effect of mass exchange temperatures on the rich streams will be neglected in this study as has been done by other workers. On the basis of such assumption, the mass exchange network interacts with the heat exchange network through the lean streams whose equilibrium relations are temperature dependent. A systematic technique of simultaneously trading off the economic objectives involved in CHAMENS will be developed in Chapter 5 of this study. The approach will involve using the lean substream concept of Srinivas and El-Halwagi (1994) to simultaneously optimise the variables. The mass exchange operation of each substream will be analysed using IBMS for MENS. The thermal requirements of each of the substreams will be determined using the IBMS for HENS.

2.6 Conclusions and Thesis Contributions

Synthesis methods for heat and mass exchange network problems have been reviewed in this chapter. Pinch technology, which is an insight based approach, relies strictly on the

vertical transfer of heat/mass within composite curve intervals. The pinch method does not have initialisation problems due to its sequential synthesis nature. Intervals which are in enthalpy/mass load balance are defined using temperatures/compositions of the problem at hand. This allows the designer to be in full control of the synthesis.

The simultaneous mathematical approaches that have been applied to the synthesis of heat and mass exchange networks were also discussed in this chapter. Partitioning superstructures on the basis of a key variable such as temperature for HENs or compositions for MENs has the tendency to increase the chances of getting good solutions in shorter times and less difficulty in initialising such superstructures. This is because intermediate temperature/composition partitioning serves to simplify the initialisation while simultaneously optimizing the competing variables. Also, such a partitioning approach helps to exclude the need for non linear heat/mass balance and mixing equations in the model thus reducing the solution time. The SWS for HENS by Yee and Grossmann (1990) and the FLM for MENS by Szitkai *et al*. (2006) are based on this concept. However such partitioning excludes some configurations such as split streams going through exchangers in series from consideration in the optimisation. Also MINLP model solutions which involve split streams might have to be solved in a suboptimisation step in order to calculate the split flows and exchanger exit temperatures.

The current author is also concerned that since the intermediate temperatures/compositions locations in the SWS and FLM models are not defined using the supply and target temperatures/compositions of the streams in the problem, special initialisation techniques may be required in large problems so as to get an optimal solution in shorter times. This is because large problems have the tendency to involve large number of stages in which the intermediate ones will not be bounded on either side by fixed temperature/composition values. Instead both boundaries of such stages are temperature/composition variables to be optimised. This implies that much expertise would be needed in order to give initial points which lie within the neighbourhood of the optimum to such stages. Evidence for this concern is that Shenoy (1995) and Verheyen & Zhang (2006) solved HENS problems with the SWS model of Yee and Grossmann (1990) by running the model several times at different values of maximum available hot utilities and different values of minimum allowable temperature difference (ΔT_{min}).

The hyperstructure approach of Papalexandri and Pistikopoulos (1994) does not have any kind of partitioning, hence the name 'hyperstructure'. All possibilities for stream and exchanger configurations are considered simultaneously in the optimisation. However such level of simultaneity and non linearities makes it difficult to give appropriate initialisations to the model thus increasing the solution times.

A new method known as the interval based MINLP superstructure (IBMS) for the synthesis of heat and mass exchange networks is presented in this study. The IBMS method involves defining the superstructure stage (or interval) boundaries using the supply and target temperature/compositions of either the hot/rich or cold/lean set of streams. This method is different from the SWS and FLM in that the temperature/composition locations in the IBMS are not all treated as variables.

Superstructure model equations of the SWS and FLM which involve calculating the intermediate temperatures/compositions e.g. the stage heat/mass balance equations and logical constraints are modified in this study by including existence coefficients. Such a model approach is beneficial in that split streams can be mixed at equal temperature/composition and no special initialisation techniques are needed. Another benefit is that intermediate temperature/compositions of streams along the superstructure are optimised as variables while still simultaneously trading-off the competing costs.

The application of the IBMS method is extended to more complex process synthesis problems which involve the following;

- Multiperiod heat exchange problems
- Mass exchange problems involving regeneration
- Mass exchange problems having non-linear equilibrium relations
- Combined heat and mass exchange networks problems involving regeneration.

CHAPTER 3

INTERVAL BASED MINLP SUPERSTRUCTURE (IBMS) FOR THE SIMULTANEOUS SYNTHESIS OF HEAT EXCHANGE NETWORKS

3.1 Introduction

This chapter presents a new superstructure for the simultaneous synthesis of heat exchange networks. The construction of the superstructure which is interval based is first presented followed by the model equations which describes the superstructure. The new interval based superstructure is also compared with the stagewise superstructure (SWS) of Yee and Grossmann (1990).

The application of the newly developed interval based superstructure to the synthesis of heat exchange network problems involving single and multiple utilities will be presented. The solutions will be compared with those in the literature.

3.2 Interval Based MINLP Superstructure for HENS

Motivation

The calculation of area in heat exchange networks is strongly dependent on the driving forces. Driving forces are calculated using supply, intermediate and target temperatures of the hot and cold streams. Hence partitioning a superstructure and defining the superstructure model equations (which involve calculating these intermediate temperatures) on the basis of the temperatures is advantageous. The benefits include the following:

- There may be no need to include non linear heat balance and mixing equations in order to get near minimum total costs in reasonable time. This is because these equations increase the degree of non linearity as well as the number of equations and variables in the model.
- Since the intermediate temperatures of the superstructures are treated as variables, competing costs and the effect on area and costs of streams which have significantly different heat transfer coefficients can be optimised simultaneously.
- The multidimensional nature of heat exchange problems such as those involving multiple utilities, multiperiod operations, etc, can easily be overcome.

Simplifying superstructures in this manner however has shortcomings; some of these have been discussed in Chapter 2 for the SWS of Yee and Grossmann (1990). Nevertheless those to be addressed in this study are discussed below:

- Problems with large numbers of streams and multiple utilities would require a large number of temperature partitions. This implies that intermediate temperatures of streams in potential exchangers which are variables to be optimised will follow one another in a sequence along the superstructure. Initialising and setting of bounds for superstructures with many temperature stages may be difficult for problems which have the inclination to have stream splits in stages whose boundaries do not correspond to either the first or last temperature location of the superstructure.
- For problems with large numbers of streams, the possibility for split stream branches to be mixed at equal temperatures becomes reduced for splits occurring in stages not bounded by fixed temperature parameters. This implies that the calculation of the split streams branch flows and temperatures will require an NLP suboptimisation step. Such NLP models would be generated from the optimal flowsheet of the MINLP optimisation step.

The SWS of Yee and Grossmann (1990) partitions superstructures using stages in the manner just described. The number of stages chosen in the SWS can be $\max\{N_H, N_C\}$, where N_H and N_C are the number of hot and cold streams in the problem respectively.

This study aims to generate superstructures for HENS by partitioning the superstructure (i.e. setting the interval boundaries or temperature locations) using the supply and target temperatures of either the hot or cold set of streams. If the hot streams are used (i.e. a hot stream based superstructure) then the cold streams are allowed to participate (float) in all the intervals created by the hot streams. The ability of the cold streams in the hot stream based superstructure to exchange heat in each interval of the superstructure is however subject to thermodynamic feasibility. The reverse would be the case for a cold stream based superstructure.

Within each interval of the interval based MINLP superstructure (IBMS), each hot and each cold stream has the potential of exchanging heat (by splitting) with each of the streams of the opposite kind present in the interval. Also, the exit temperatures of exchangers involved with split streams in the IBMS are equal and such temperatures form the temperature of the next interval boundary. The intermediate temperatures of

streams at temperature locations (i.e. interval boundaries) other than those which they define are variables to be optimised. This implies that the intermediate temperatures may be less than, equal to or greater than the temperature defining such locations.

This approach was chosen because defining the interval boundaries of a HEN superstructure with fixed temperature values automatically mixes split streams (in every interval where such splits occur) at equal temperatures. This is unlike the SWS of Yee & Grossmann (1990) where it is just assumed that the split streams will be mixed at equal temperatures. But split streams will not always be mixed at equal temperatures in the SWS for superstructure stages not bounded on either side by fixed temperature parameters. This will be illustrated in one of the example problems to be considered. Each temperature interval boundary in the IBMS is defined by a fixed temperature parameter, therefore initialisation and setting of bounds for the IBMS model is simplified.

The IBMS approach to be presented in this study does not include non linear heat balance, mixing and bypass equations in the model. A shortcoming of excluding these equations in the model are that series exchangers for split stream branches and structures with non isothermal mixing configurations would be excluded from the search for the optimum. Nevertheless the examples where the IBMS have been applied which are presented in this study show that good solutions can still be obtained in reasonable times for problems with relatively few streams and significantly different heat transfer coefficients. The model also performs reasonably well for problems involving multiple utilities and multiperiod operations.

The fixed temperature interval boundary defining approach allows the superstructure to simultaneously optimise the utility costs and capital costs (i.e. heat exchange areas and exchanger fixed charges). This is because the intermediate temperatures of streams while crossing an interval boundary (which is defined by the supply or target temperature of some other stream) are treated as variables to be optimised. This implies that there is no strict adherence to vertical heat transfer; hence matching of streams which have significantly different heat transfer coefficients and at the same time require different exchanger specifications can be effectively optimised.

3.2.1 Construction of the IBMS

The interval based superstructure for an illustrative heat exchange problem having two hot and two cold streams is shown in Figure 3.1.

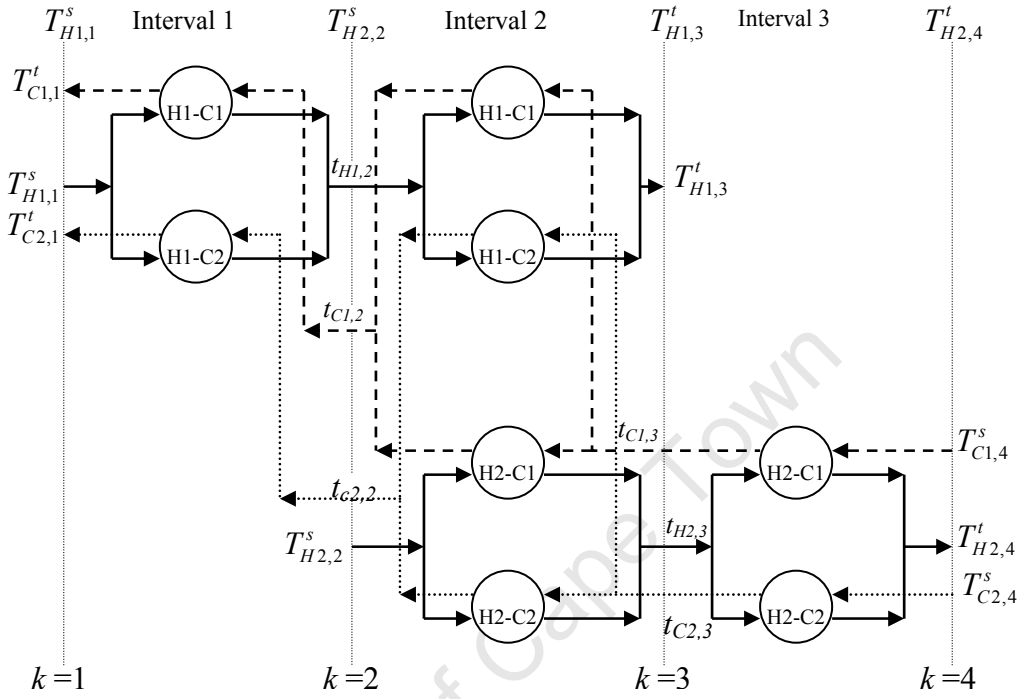


Figure 3.1. Hot stream based interval superstructure.

It should be noted that the hot and cold utilities are treated as process streams in the IBMS. In the illustrative problem which is hot stream based, the supply temperature, T^s_{H1} of H_1 (hot stream 1) is higher than the supply temperature, T^s_{H2} of H_2 (hot stream 2). The target temperature, T^t_{H1} of H_1 is also higher than the target temperature, T^t_{H2} of H_2 but lower than T^s_{H2}. Sorting these temperatures in a descending order and using each to define a temperature location, k, gives the superstructure shown in Figure 3.1. In this superstructure, T^s_{H1} defines k =1, T^s_{H2} defines k = 2, T^t_{H1} defines k = 3 while T^t_{H2} defines k = 4, the last temperature location. Note that the supply/target temperatures of two or more streams that coincide are represented just once.

The cold streams, C_1 and C_2, are assumed to participate in all the intervals. It should be noted that H_1 has a temperature of T^s_{H1} in temperature location, k = 1, its temperature in temperature location, k = 2, is a variable ($t_{H1,2}$) to be optimised. The value of this variable

can be less than, greater than or equal to T^s_{H2}, the supply temperature of H_2. This condition applies to other streams (hot and cold) in temperature locations which are not defined by their supply or target temperatures (i.e. their intermediate temperatures). The model equations that involve the calculation of the intermediate temperatures (e.g. that of H_2, $t_{H1,2}$, in temperature location, k = 2) are constrained using existence coefficients in form of conditionals. These coefficients are defined in terms of stream existence in an interval and the temperature (supply or target) of the stream defining the temperature location. Defining the model equations in such a manner helps to ensure that streams which are split in the hot side of such temperature locations (e.g. interval 1 for the split of H_1 in Figure 3.1) are mixed at equal temperatures in temperature location, k =2. With this approach, there is no need to include the non linear heat balance and mixing equations in the superstructure model, hence the model is easily solved in shorter times.

It should be noted that the reverse would apply if a cold stream based superstructure is constructed, the hot streams including hot utilities would be allowed to participate in all the intervals. Their ability to exchange heat in any interval is also subject to thermodynamic feasibility.

3.2.1.1 IBMS Model Formulation

After constructing the interval based superstructure, it is then modelled as a mixed integer non linear program (MINLP) in order to minimise the total annualised cost. The necessary sets, indices, parameters and variables which are used in the model formulation are presented next.

Sets

H hot process and utility streams

C cold process and utility streams

K temperature intervals in superstructure

Indices

i hot process or utility stream

j cold process or utility stream

k index for temperature interval location (k = 1,….. NOK)

Parameters

AC area cost coefficient

AE area cost index

CF fixed charge for exchangers

CUC cost per unit of cold utility

HUC cost per unit of hot utility

h_c stream heat transfer coefficient

T_k temperature of location or interval boundary k

T_i^s supply temperature of hot stream i

T_i^t target temperature of hot stream i

T_j^s supply temperature of cold stream j

T_j^t target temperature of cold stream j

$U_{i,j}$ overall heat transfer coefficient

Ω_h upper bound for heat exchanged in match i,j

Γ_h upper bound for driving force in match i,j

Binary variables

z_{ijk} variable indicating the existence of match i,j in interval k in the optimal network

Positive variables

dt_{ijk} driving force for match i,j in interval k

F_i flow rate of hot stream i

F_j flow rate of cold stream j

q_{ijk} heat exchanged between hot stream i and cold stream j in temperature interval k

$t_{i,k}$ temperature of hot stream i at hot end of interval k

$t_{j,k}$ temperature of cold stream j at hot end of interval k

Model Equations

Before presenting the equations used to model the IBMS, it is necessary to state that two types of stream existence conditionals have to be defined as mentioned earlier. The first conditional states that; ‘a hot stream in a hot stream based superstructure will only be considered for the calculation of its variables in interval k if it exists in the interval being considered, the same condition applies to cold streams in a cold stream based

superstructure. The conditionals are described below for hot and cold stream based superstructures respectively.

$$H_{i,k}\,\$\left(T_i^s \geq T_k \text{ and } T_i^t \leq T_{k+1}\right)=1 \tag{3.1}$$

$$C_{j,k}\,\$\left(T_j^t \geq T_k \text{ and } T_j^s \leq T_{k+1}\right)=1 \tag{3.2}$$

where \$ is the operator used to check whether a condition is true or not. Note that T_k represents the supply and target temperatures of the streams defining the superstructure intervals which were ordered in a descending order; hence T_k is a parameter which is problem specific.

Equation 3.1 implies that H_i either starts at temperature location k or crosses it and that it either ends at temperature location k+1 or crosses it. If these two conditions are not met, then H_i will not be considered as existing in interval k and its variables will not be calculated in interval k, hence the right hand side of Equation 3.1 will be equal to '0'. The same description applies to Equation 3.2 for cold streams in a cold stream based superstructure. Note that Equations 3.1 will also apply in some of the model equations for cold streams. This enables the heat exchanged between the hot stream and potential cold streams to be considered as well in the variable calculations. The reverse will be the case for a cold stream based superstructure, i.e. Equation 3.2 applies to hot streams equations.

The second conditional (stream supply and target temperature recognition conditionals) specifically recognises the supply and target temperatures of the set of streams which define the temperatures of the superstructure interval boundaries.

$$HS_{i,k}\,\$\left(T_i^s = T_k\right)=1 \tag{3.3}$$

$$HE_{i,k}\,\$\left(T_i^t = T_k\right)=1 \tag{3.4}$$

$$CS_{j,k}\,\$\left(T_j^s = T_k\right)=1 \tag{3.5}$$

$$CE_{j,k}\,\$\left(T_j^t = T_k\right)=1 \tag{3.6}$$

where *HS*, *HE*, *CS* and *CE* represent hot start, hot end, cold start and cold end respectively. Equations 3.3 and 3.4 imply that temperature location *k* is defined by the supply or target temperature of hot stream *i* in a hot stream based superstructure. The same condition applies to Equations 3.5 and 3.6 for a cold stream based superstructure. The conditionals are discussed in the model equations where they need to be used.

Overall stream heat balance

In order for a stream to get to its target temperature, it needs to exchange heat with streams of the opposite kind. The heat exchange can take place in some or all of the temperature intervals. The sum of heat exchanged over the intervals where such heat transfer takes place is equated to the overall energy requirement of the stream concerned. The model equation for hot and cold streams can be represented as;

$$\left(T_i^s - T_i^t\right) F_i = \sum_{j \in C} \sum_{k \in K} q_{i,j,k} \qquad i \in H \tag{3.7}$$

$$\left(T_j^t - T_j^s\right) F_j = \sum_{i \in H} \sum_{k \in K} q_{i,j,k} \qquad j \in C \tag{3.8}$$

Note that stream flowrate, *F*, is modelled as a parameter for the process streams and as a variable for utilities. For a hot stream based interval superstructure, hot stream interval existence conditionals (Equation 3.1) are used to constrain Equations 3.7 and 3.8 so that $q_{i,j,k}$ will be calculated for hot streams in intervals where they exist. This automatically ensures that $q_{i,j,k}$ is also calculated for cold streams in intervals where they can exchange heat with those hot streams. For a cold stream based superstructure, the conditionals are included in the same way using cold stream interval existence conditionals (i.e. Equation 3.2).

Interval heat balance

Interval enthalpy balances are used to calculate the interval boundary temperatures for each stream.

$$\left(t_{i,k} - t_{i,k+1}\right) F_i = \sum_{j \in C} q_{i,j,k} \qquad i \in H \quad k \in K \tag{3.9}$$

$$\left(t_{j,k} - t_{j,k+1}\right) F_j = \sum_{i \in H} q_{i,j,k} \qquad j \in C \quad k \in K \tag{3.10}$$

Note that $t_{i,k}$ and $t_{j,k}$ are both sets of variables to be optimised. The hot stream interval existence conditionals are applied in Equations 3.9 for a hot stream based superstructure. This helps to ensure that intermediate temperatures and heat loads are calculated for hot streams in intervals where they exist. The same set of hot stream interval existence conditionals are also used in Equation 3.10 despite being an equation for the cold streams. This is necessary so that intermediate temperatures and heat loads will be calculated for the cold streams in intervals where they can feasibly exchange heat with a hot stream, i.e. in intervals where hot streams exist. The feasibility equations are dealt with in later equations. Cold stream existence conditionals are also used for both hot and cold stream heat balance equations for a cold stream based superstructure.

Assignment of superstructure interval temperatures

In the interval based superstructure, it is not only the first and last temperature locations that are assigned the supply and target temperatures of the participating streams in the problem (as it is in the SWS of Yee and Grossmann, 1990) but every temperature location. Each temperature location, k, is recognised using both the stream interval existence conditional (Equations 3.1 & 3.2) and the supply/target temperature recognition conditional (Equations 3.3 to 3.6). Using Figure 3.1 as an illustration;

$$k = 1; \quad T^{S}_{H1,1} = t_{H1,1}, \; T^{t}_{C1,1} = t_{C1,1}, \; T^{t}_{C2,1} = t_{C2,1} \tag{3.11}$$

$$k = 2; \quad T^{S}_{H2,2} = t_{H2,2} \tag{3.12}$$

$$k = 3; \quad T^{t}_{H1,3} = t_{H1,3} \tag{3.13}$$

$$k = 4; \quad T^{S}_{H4,4} = t_{H2,4}, \; T^{s}_{C1,4} = t_{C1,4}, \; T^{s}_{C2,4} = t_{C2,4} \tag{3.14}$$

Equations 3.11 to 3.14 are problem specific equations; they relate the supply and target temperatures of the hot and cold streams to the intermediate temperature variables. Using Equation 3.12 as an example, the model will recognise that temperature location k = 2 is defined by T^{s}_{H2} while calculating the intermediate temperature of H_1 in this location. This equation (together with Equation 3.11 and the conditional equations) will automatically ensure that the splits of H_1 in interval 1 are mixed at equal temperatures in k = 2. This equally applies to the calculation of intermediate temperatures for all other streams (hot and cold) in temperature locations which they do not define but cross.

Feasibility of temperatures

The temperature of both hot and cold streams should decrease along the superstructure from left to right. For a hot stream based interval superstructure, the stream interval existence conditionals are used to ensure that the temperature of the hot streams will decrease from left to right only in intervals where such hot streams exist. Note that the existence conditionals do not have to be included for the cold stream feasibility equations because when the hot streams decrease in temperature along the superstructure, the cold streams will automatically decrease based on the other set of constraints.

$$t_{i,k} \geq t_{i,k+1} \qquad k \in K,\ i \in H \tag{3.15}$$

$$t_{j,k} \geq t_{j,k+1} \qquad k \in K,\ j \in C \tag{3.16}$$

Logical constraints

Binary variables, $z_{i,j,k}$, are used to model the existence of a match *i,j* in interval *k* as done by Yee and Grossmann (1990) in the SWS method. The binary variables are included in logical constraints so that it will take on a value of '1' if the match *i,j* exists in interval *k* and '0' if otherwise. An upper bound, Ω_h, is also included in the logical constraints so as to limit the amount of heat that can be exchanged between *i* and *j* to the smaller of the overall heat load of each of the streams involved in the match. This logical constraint can be represented as;

$$q_{ijk} - \Omega_h z_{ijk} \leq 0 \qquad i \in H,\ j \in C,\ k \in K \tag{3.17}$$

Heat exchange area calculation

Approach temperature variables, $dt_{i,j,k}$, are introduced to calculate the driving forces for the LMTD in the heat exchange area (Yee and Grossmann, 1990). The binary variables, $z_{i,j,k}$, are included in the logical constraint equations for the calculation of the approach temperature (driving force) variables. As indicated above, the binary variable, $z_{i,j,k}$, takes on a value of '1' if the match, *i,j,* exists in interval, *k*, in the optimal network and the approach temperature, $dt_{i,j,k}$, will be appropriately calculated. If the match does not exist in the optimal network, the binary variable will take on a value of '0' and in the presence of Γ_h in the approach temperature equation, the equation will be inactivated. This helps to avoid the inclusion of negative approach temperatures for any match.

$$dt_{i,j,k} \le t_{i,k} - t_{j,k} + \Gamma_h\left(1 - z_{i,j,k}\right) \quad k \in K,\ i \in H,\ j \in C \tag{3.18}$$

$$dt_{i,j,k+1} \le t_{i,k+1} - t_{j,k+1} + \Gamma_h\left(1 - z_{i,j,k}\right) \quad k \in K,\ i \in H,\ j \in C \tag{3.19}$$

Γ_h can be set as the maximum of zero and each of the temperature differences between the hot and cold streams in the match (Shenoy, 1995) so as to avoid numerical errors due to negative approach temperatures for matches that do not exist.

An exchanger minimum approach temperature (EMAT) is used to ensure that exchangers of infinite areas are not included in the solution network. This can be represented as;

$$dt_{ijk} \ge \delta \tag{3.20}$$

where δ is a small positive number.

Objective function

The objective function, like that of the SWS of Yee and Grossmann (1990) simultaneously minimises the utility costs and capital costs (i.e. fixed exchanger costs and the area cost of each exchanger). Chen's first approximation is also used to calculate the LMTD (Chen, 1987).

$$LMTD_{i,j,k} = \left[\left(dt_{i,j,k}\right)\cdot\left(dt_{i,j,k+1}\right)\cdot\left(dt_{i,j,k} + dt_{i,j,k+1}\right)/2\right]^{1/3} \tag{3.21}$$

The objective function:

$$\min \sum_{i\in H}\sum_{k\in K} CUCq_{i,j,k} + \sum_{j\in C}\sum_{k\in K} HUCq_{i,j,k} + \sum_{i\in H}\sum_{j\in C}\sum_{k\in K} CF_{i,j} z_{i,j,k} + \sum_{i\in H}\sum_{j\in C}\sum_{k\in K} AC_{i,j}\left[q_{i,j,k}/U_{i,j}(LMTD_{i,j,k})\right]^{AE_{i,j}} \tag{3.22}$$

The interval based MINLP model can easily be solved since the equations (Equations 3.7 to 3.20) defining the feasible space are all linear except for Equations 3.9 and 3.10. However if the utilities are not modelled as process streams then Equations 3.9 and 3.10 will also be linear. The utilities have been represented as process streams in this study so that multiple utilities can easily be traded-off against one another. However, it was found that such non linearties do not have a significant effect on the solution generation.

Matches can easily be restricted (e.g. preferred, forbidden) by fixing the concerned binary variables or restricting the heat to be exchanged by such streams.

3.2.2 Comparison of SWS and IBMS

In the SWS, the first temperature location is defined by the supply temperatures of all the hot streams while the last temperature location is defined by the supply temperatures of all the cold streams. The intermediate temperatures are all variables to be optimised for both hot and cold streams. Hot and cold utilities which will ensure that the cold and hot streams both get to their target temperatures can be placed outside the superstructure or treated as process streams. For the hot stream based IBMS, the first temperature location is defined by the supply temperature of the hot stream with the highest supply temperature. The last temperature location is defined by the hot stream with the lowest target temperature. Intermediate temperature locations are defined by the supply and target temperatures of the hot streams sorted in a descending order. The cold streams start at the last temperature location of the superstructure and end in the first location. The temperatures of hot and cold streams at temperature locations which they do not define but cross are variables to be optimised.

Using Figures 2.6 and 3.1 as illustration, intermediate temperature location $k = 2$ in the SWS (Figure 2.6) is a variable to be optimised for all the hot and cold streams. For the IBMS (Figure 3.1), intermediate temperature location $k = 2$ is a variable to be optimised for H_1 and the two cold streams only since H_2 starts at this location. A similar situation occurs in temperature location, $k = 3$ of IBMS where the intermediate temperatures of H_2 and the cold streams are the variables to be optimised.

3.2.3 Examples

The model equations of the examples presented in this thesis have been solved with the solver DICOPT++, which uses CPLEX for the MILP and CONOPT for the NLP sub problems, all operating in the GAMS environment (Rosenthal, 2007). The results of applying the IBMS to literature problems are in some cases better while they are reasonably close in other cases. The IBMS GAMS code for Example 3.5 is presented in Appendix D1.

3.2.3.1 Example 3.1

This example is the 4S1 problem of Shenoy (1995) which involves two hot and two cold streams and one hot and one cold utility. Stream and capital cost data are presented in Table A1 in Appendix A. Note that this is a simple problem because the heat transfer coefficients, h_c, are equal for all the streams.

Shenoy (1995) solved this problem for a minimum TAC scenario using the simplified SWS of Yee and Grossmann (1990) with the Paterson approximation (1984) for the LMTD calculation. The solution network is shown in Figure 3.2 having two stages and a TAC of 235,400 $/yr.

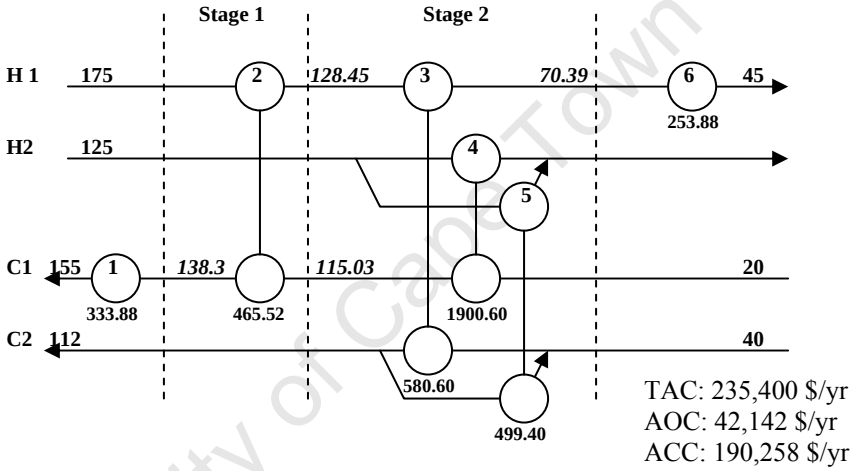


Figure 3.2. Network generated for Example 3.1 at a minimum TAC by Shenoy (1995) using simplified SWS of Yee and Grossmann (1990).

Hot utility and cold utility usage are 333.88 kW and 253.88 kW respectively. The SWS network features six units and two stream splits. Heat exchanger heat loads are shown below the concerned exchangers while stream intermediate temperatures are shown in italics above the streams.

The interval based superstructure for this problem has five intervals and six interval boundary temperature locations which correspond to the supply and target temperatures of the hot set of streams (hot stream based superstructure). The IBMS solution network is similar to that of the SWS; the network is shown in Figure 3.3 with a TAC of 237,800 $yr which is just 1% higher than the TAC of the SWS. The solution was generated in 0.319s of CPU time on an Intel Pentium M, 1.7 GHz machine.

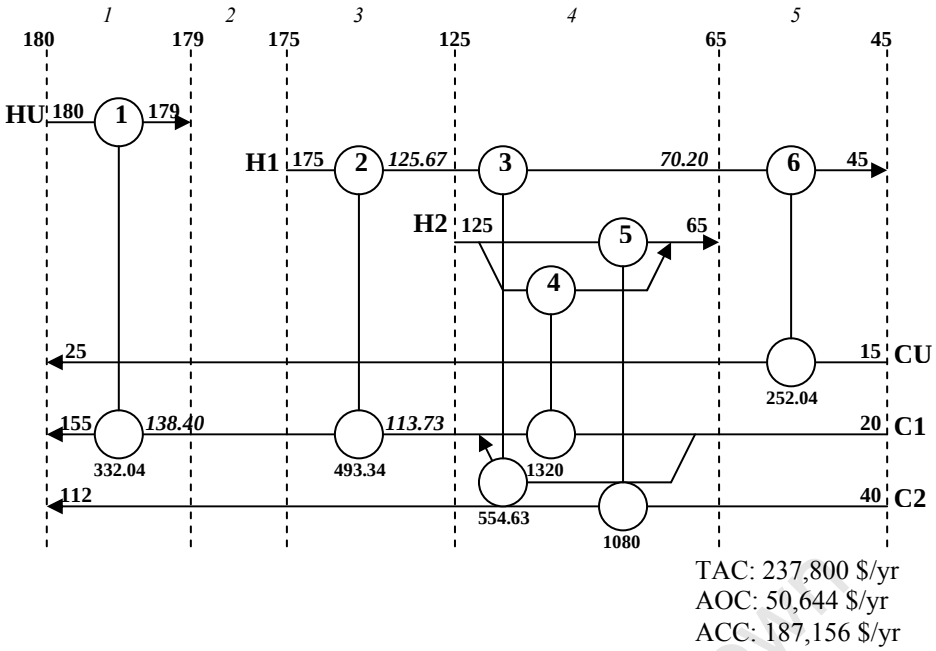


Figure 3.3. Optimal IBMS network for Example 3.1 featuring six units and two stream splits.

The IBMS network in Figure 3.3 also has six units with two stream splits, H_2 and C_1; this is unlike the SWS where H_2 and C_2 are the split streams. The mixing of these split streams in both the SWS and the IBMS are isothermal. The reason the SWS structure gives isothermally mixed temperatures can be observed from Figure 3.2. The two splits occur in streams which possesses some or all of the following characteristics. Firstly, the hot/cold end of the stage where the split occurs is the first/last temperature location of the superstructure. This implies that the stream (C_2 in Figure 3.2) was split because one end of the stage is bounded by a fixed temperature. Secondly the stream involved in the split has not exchanged heat with any stream in any stage prior to the stage involved with the split (H_2 in Figure 3.2). The alternative to this is that the stream will not be exchanging heat with any stream in any stage after the stage involved in the split.

It then becomes evident the reason for which the IBMS splits and mixes streams at equal temperatures. Since the two observations made from Figure 3.2 involve streams mixing at equal temperatures on the condition that they have a fixed temperature (target/supply) at either end of the stage in which the split takes place. This phenomenon of having at least a fixed temperature in an interval) is a key feature that differentiates the IBMS from SWS. This is demonstrated further in Example 3.2.

When the IBMS is generated on a cold stream basis for Example 3.1, a network with a TAC of 239,322 $/yr which is less than 1% higher than the TAC of the hot stream based IBMS is obtained. The structure which is shown in Figure 3.4 was generated in 0.344s of CPU time on an Intel Pentium M, 1.7 GHz machine. This demonstrates that the IBMS works adequately when used on the cold stream basis.

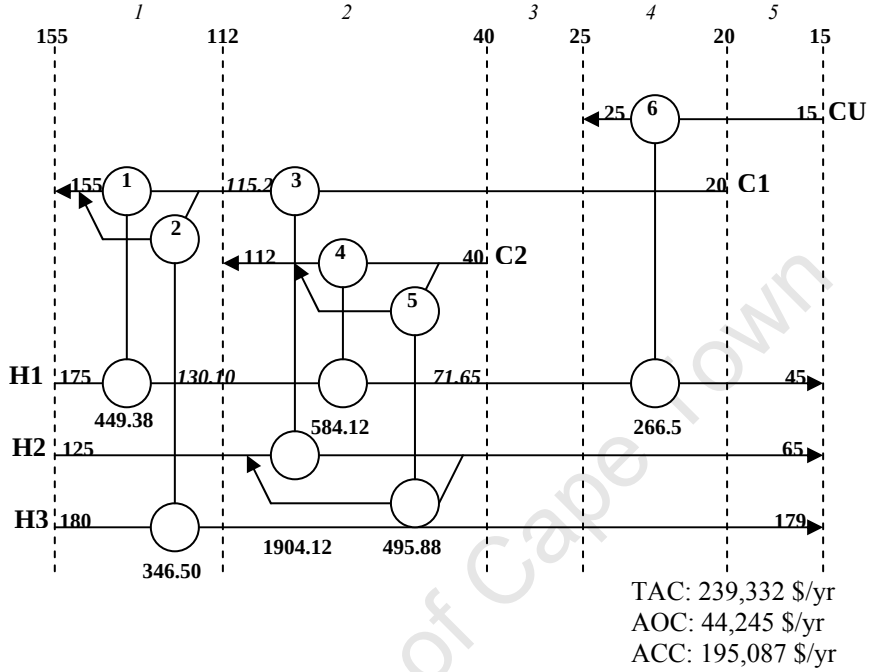


Figure 3.4. Cold stream based IBMS network for Example 3.1 featuring six units and three stream splits.

In order to constrain a match in the IBMS model, the appropriate parameter or variable is simply set to the preferred value. Using Example 3.1 as an illustration, if a match between H_2 and C_2 is not allowed, then existence coefficient conditionals for such a match is set to '0'. When this is applied to Example 3.1, the resulting network solution is shown in Figure 3.5. The network has a TAC of 311,300 $/yr with no stream split. It should be noted that Figure 3.5 is a cold stream based superstructure. This network is the same as that generated by SWS though not shown in this thesis.

3.2.3.2 Example 3.2

The IBMS is applied to Example 3 of Yee and Grossmann (1990) which has five hot streams, one cold stream, steam and cooling water. Due to the large number of hot streams relative to the cold stream, splitting of the only cold stream in the problem becomes unavoidable. The problem will be used to show the ability of the IBMS model

to handle the mixing of split streams. The problem data is presented in Table A2 in Appendix A. The network generated by the SWS model is shown in Figure 3.6.

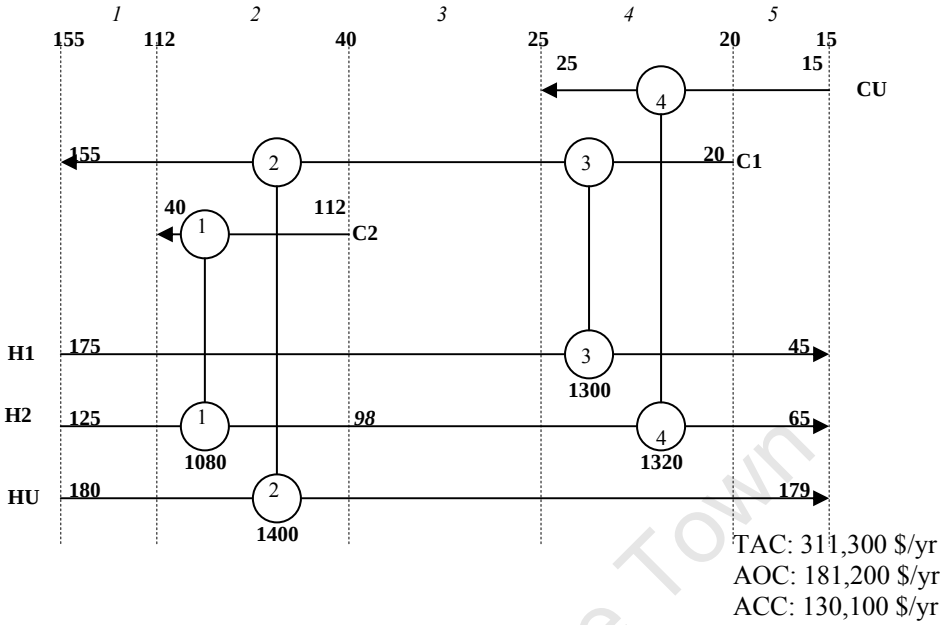


Figure 3.5. IBMS network for Example 3.1 with H_2-C_2 match forbidden.

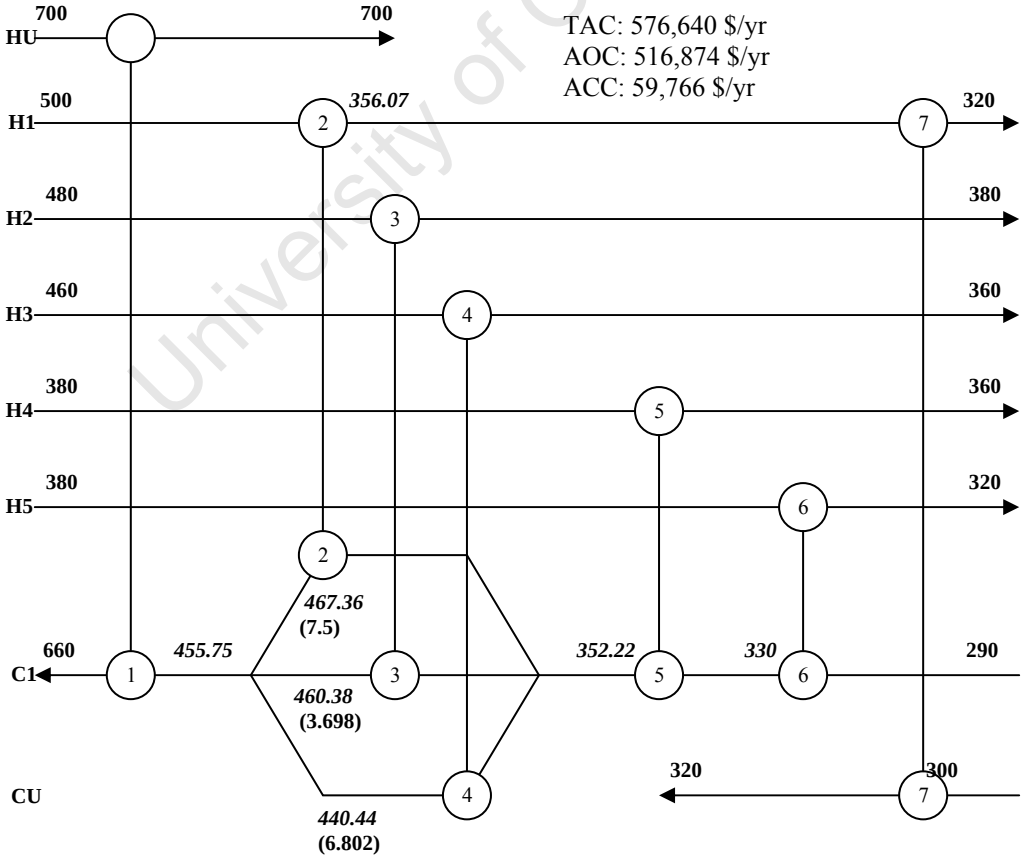
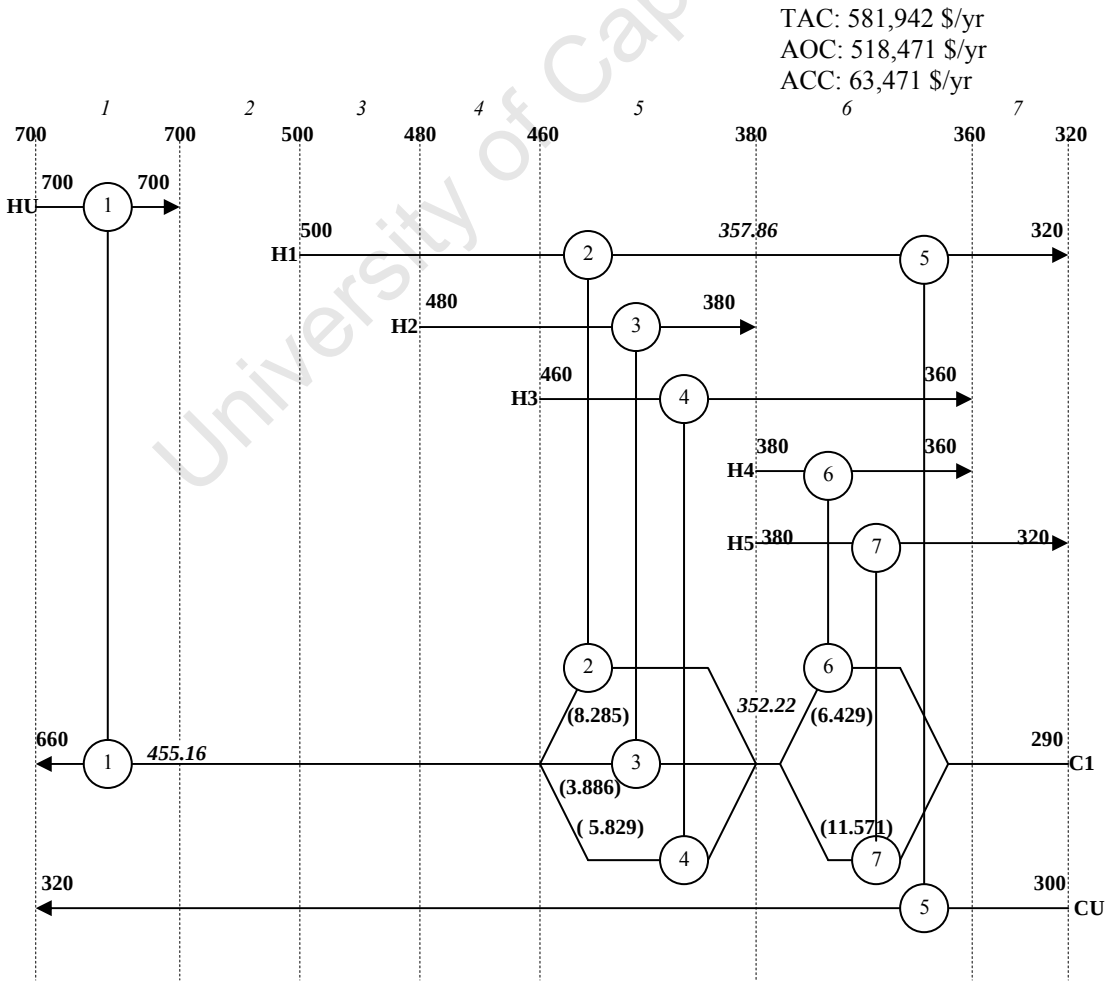


Figure 3.6. Optimal network for Example 3.2, generated by the SWS with seven units and a three-way stream split (Yee and Grossmann, 1990).

Match location within stages in the SWS of Example 3.2 cannot be identified because the configuration presented by Yee and Grossmann (1990) does not show matches within the stages. Hence the grid form is shown in this thesis for the purpose of comparison. This network which is the NLP suboptimisation step has seven units with three way split of stream C_1 and a TAC 576,640 \$/yr. The NLP suboptimisation step had to be solved in order to determine the split stream individual flow rates and exchanger exit temperatures. The SWS MINLP model for the network has nine units and three split streams. Figure 3.6 is the resulting NLP network, the split flow rates are shown in brackets next to the concerned stream in this figure.

The IBMS for this problem has seven intervals and eight temperature locations defined by the supply and target temperatures of the hot set of streams (hot stream based superstucture). The resulting network is shown in Figure 3.7 with a TAC of 581,942 \$/yr which is just 0.9% higher than that of the SWS. The solution was obtained in 0.421s of CPU time on an Intel Pentium M, 1.7 GHz machine.



Exch.	Heat load (kW)	Area (m^2)
1	3687.12	33.1
2	852.86	46
3	400	15.2
4	600	96.9
5	227.15	8.1
6	400	8.8
7	720	24.9

Figure 3.7. IBMS network for Example 3.2 with seven units and multiple stream splits of the cold stream.

The IBMS structure also features seven units and a stream split 3 ways and 2 ways. The MINLP model was solved just in a single step with the two sets of stream splits being mixed at isothermal temperatures.

The splits in Figure 3.7 are automatically mixed at equal temperatures and these temperatures define the temperature of the next interval boundary. C_1 was split and mixed at equal temperatures specifically in intervals 5 and 6 because the intervals have hot stream(s) that create the intervals by either starting or ending in it. Interval 5 has its hot end created by the supply of H_3 and its cold end by the target of H_2. The same scenario is observed in the splits in which H_4 and H_5 are involved in interval 6, though C_1 is still at its fixed (supply) temperature of 290K at the cold end of the interval.

Example 3.2 was solved with a cold stream based superstructure so as to investigate what kind of network this would give. The solution of such model is a structure having a TAC of 595,100 $/yr which is marginally higher than the hot stream based superstructure. This structure which also has seven units is slightly different from that of Figure 3.7; it is shown in Figure 3.8. The figure is inverted because the cold streams are used to define the superstructure intervals.

3.2.3.3 Example 3.3

This example is taken from Colberg and Morari (1990) where they used the NLP transhipment model to solve the problem. The problem involves three hot streams and four cold streams with steam and cooling water as the utilities. The heat transfer coefficients of the streams in this example are significantly different. It will therefore be used to show the ability of the IBMS model to handle streams with significantly different

heat transfer coefficients. The problem data is shown in Table A3 in Appendix A. Yee and Grossmann (1990) also used the SWS model to solve this problem where they used 8600 + 670*(Area)$^{0.83}$ to calculate the capital cost because Colberg and Morari (1990) did not include any capital cost data. The same capital cost data is used in this thesis.

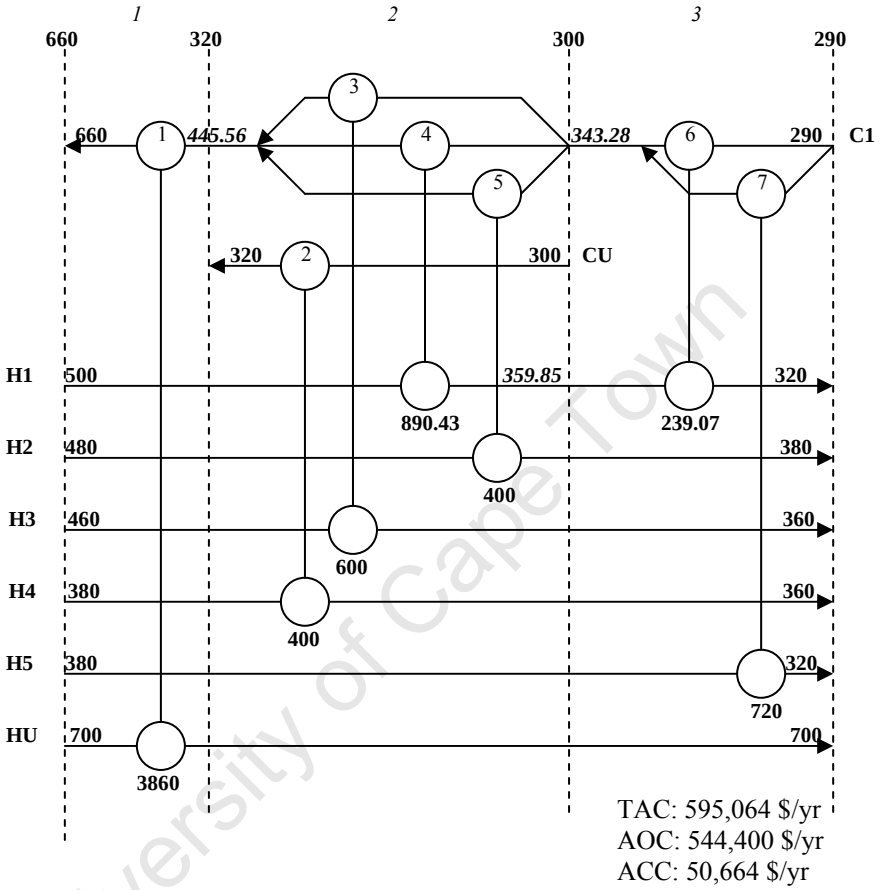
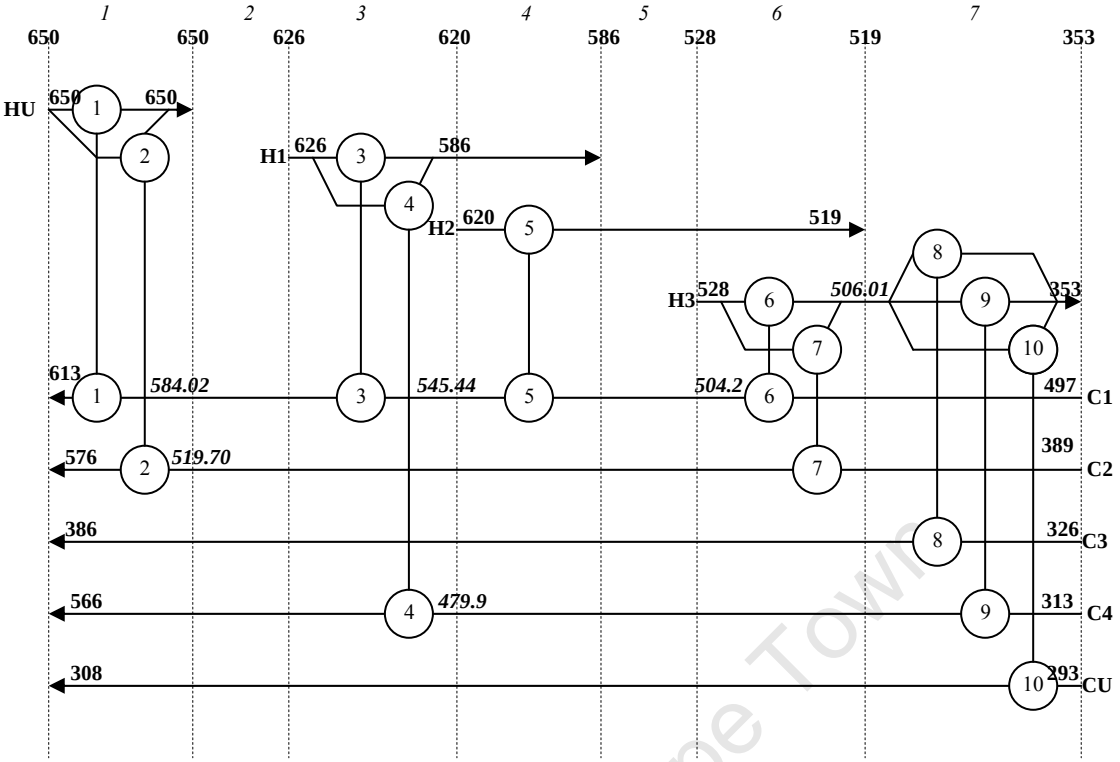


Figure 3.8. Cold stream based IBMS network for Example 3.2.

Colberg and Morari (1990) and Yee and Grossmann (1990) both solved the problem with a fixed heat recovery approach temperature (HRAT) of 20 K. The hot and cold utility consumptions at this approach temperature are 244.2 kW and 172.6 kW respectively.

A hot stream based IBMS for this problem has eight temperature locations. The utilities were fixed at 244.2 and 172.6 kW for the hot and cold utilities respectively. The resulting structure has a total capital cost of $168,700, ten units and an area requirement of 251.5m^2. The network is shown in Figure 3.9 while Table 3.1 compares the number of units, area requirements and total costs of the three methods.



Exch.	Heat load (kW)	Area (m^2)
1	208.03	7.6
2	36.1	1.6
3	277	15.7
4	115.1	1.8
5	296	173.9
6	51.68	6.3
7	83.78	9.2
8	457.62	24.7
9	312.5	9.9
10	172.6	0.9

Figure 3.9. IBMS network for Example 3.3 featuring ten units.

Table 3.1: Comparison of different optimisation methods for Example 3.3

Model	Number of units	Area(m^2)	Total capital cost ($)
NLP Transshipment	12	188.9	177,400
SWS	9	217.8	151,000
IBMS	10	251.5	168,700

The total number of units of the NLP transhipment is higher than the SWS and IBMS networks because the approach of Colberg and Morari (1990) requires partitioning the network at the pinch. However the NLP transhipment model gives the smallest area since the objective of the model is to minimise area.

The network of each method involves split streams: the NLP transhipment model has six, the SWS has one while the IBMS has two. Suboptimisation steps still had to be carried out for the NLP transhipment and SWS models in order to determine their optimal split stream flow rates and exchanger exit temperatures. This is unlike the IBMS which gave the optimal split stream flow rates and exchanger exit temperatures in a single optimisation step.

Utility costs were assumed for this example in order to minimise the TAC of the problem using the IBMS model. The costs are: hot = 110 \$ kW^{-1} yr^{-1}, cold = 20 \$ kW^{-1} yr^{-1}. The resulting IBMS network gives a TAC of 185,090 \$yr/yr with seven units. This cost comprises of a total capital cost (TCC) of 96,549 \$/yr and an AOC of 88,541 \$/yr. This is obviously a better optimum for this problem than fixing the HRAT, as was done by earlier workers.

3.2.4 Application to multiple utilities

The IBMS synthesis method can easily be extended to HENs problems involving multiple utilities. The optimisation may be done in two steps. In the first step, the IBMS model is run with all the available utilities participating as process streams alongside the normal process streams in the superstructure. The hot and cold utility flows, *F*, are set as variables to be optimised. Their initial points and lower bounds can be set to values as low as '1' (since '0' is not a good initialisation point). The upper bounds can be values large enough such that each of the utilities can take care of the total utility requirement of the problem. The second step (run) will only be carried out if one or more of the utilities are not used significantly, i.e. if their flow equals the lower bound or is insignificant relative to other utility flows. This helps to reduce the number of units in the network given in the first step. Two examples are used to demonstrate the capability of the IBMS for handling multiple utilities problems.

3.2.4.1 Example 3.4

Example 3.4 is taken from Shenoy, *et al*. (1998); it involves two hot streams and one cold stream. Three hot utilities and one cold utility are available. The stream data is shown on Table A4 in appendix A.

The IBMS model for this problem has ten temperature locations. Tables 3.2 (for CUP) and 3.3 (for IBMS) show the following: heat load for different combinations (options) of hot utilities, number of units and the TAC for each option.

Table 3.2: Heat load distributions for Example 3.4, for different combinations of hot utilities using CUP (Shenoy, *et al*., 1998)

Options	Cold utility (kW)	HPS Load (kW)	MPS Load (kW)	LPS Load (kW)	N	TAC target (£/yr)	TAC design (£/yr)
1 (3 HU)	725.5	203	53	119.5	9	96,412	98,263
2 (2 HU)	725.5	240	-	135.5	7	96,839	98,699
3 (1 HU)	664	314	-	-	5	100.965	105,027

Table 3.3: Heat load distributions for Example 3.4, for different combinations of hot utilities using IBMS

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

The TAC of Option 2 is the lowest; this TAC is 1% lower than the best of the CUP options. The IBMS solutions were generated at considerably less effort than the CUP technique.

3.2.4.2 Example 3.5

This example which is also taken from Shenoy, *et al*. (1998) involves two hot and three cold streams with three hot and two cold utilities available for use. The stream and capital cost data are shown on Table A5 in Appendix A.

Different combinations of hot and cold utilities and the required number of units are shown on Tables 3.4 and 3.5 for the CUP and IBMS synthesis methods respectively.

Table 3.4: Heat load distributions for Example 3.5, for different combinations of hot and cold utilities for CUP (Shenoy, *et al*., 1998)

Options	HPS Load (kW)	MPS Load (kW)	LPS Load (kW)	CW Load (kW)	Air C Load (kW)	N	TAC Target ($*10^{-3}$)	TAC Design $*10^{-3}$ (£/yr)
1 (2HU, 1CU)	1600	6860	-	7760	-	11	1130.34	1182.94
2 (2HU, 1CU)	1600	6860	-	7760	-	11	1130.34	1212.69
3 (2HU, 2CU)	4885	3575	-	3600	4160	9	1130.34	1158.50
4 (2HU, 2CU)	2730	5730	-	3600	4160	9	1130.34	1163.14

Table 3.5: Heat load distributions for Example 3.5, for different combinations of hot and cold utilities for IBMS

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

TAC targets were first optimised in this example by means of OLD plots for the CUP method. This implies that the evolutions were only carried out on the generated networks. This example is more complex than Example 3.4 because it involves multiple hot and multiple cold utilities. The use of the CUP approach becomes more cumbersome because at each value of ΔT_{min}, air cooling (AC) and cooling water (CW) have to be traded-off against one another. The different levels of steam will also have to be traded-off against one another. Note that Option 1 differs from 2 on the CUP table in that the structure of Option 1 involves a stream split while Option 2 does not. Shenoy, *et al.* (1998) evolved Options 1 and 2 to get Options 3 and 4 respectively.

Different options of the IBMS solutions are shown in Table 3.5 where all the TACs are less than the lowest in the CUP options. Options 1 and 2 of the IBMS on Table 3.5 involve using all the available utilities with LPS being a potential candidate for elimination since its consumption corresponds to the lower bound (1 kW) set for it in the model. But the EMAT of these two options are different. Option 2 gives a network which requires nine units and a higher TAC compared with Option 1.

Options 1 and 2 of the CUP use the same combination of utilities as Option 4 of the IBMS but the TAC of the IBMS is about 3% lower than those of the CUP options. These CUP options have eleven units each while the IBMS option has seven units. Also, these options of the CUP have a higher TAC than Options 1 and 2 of the IBMS despite the fact the IBMS options use all of the available utilities. This shows that the CUP due to its sequential design nature does not establish a simultaneous trade off among the competing costs; hence the search is not exhaustive.

Any of the IBMS options could be chosen as the best depending on other factors which could be site specific: including both availability of utilities and capital cost constraints.

But Options 1 and 2 are not really feasible so Option 4 is the best. The network of Option 4 is shown in Figure 3.10.

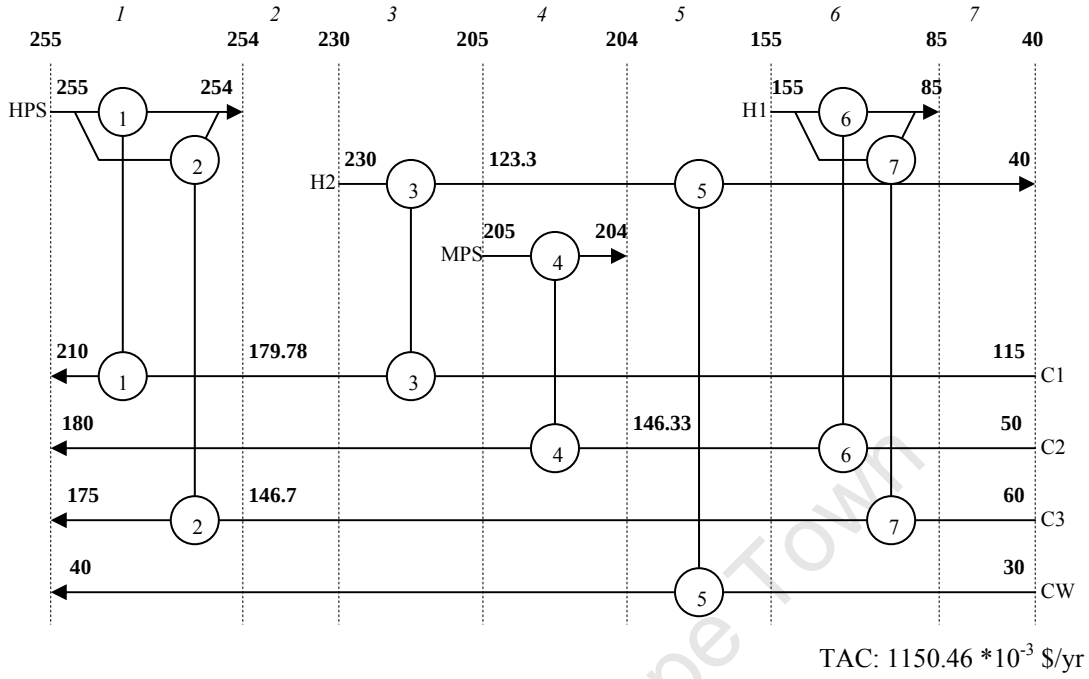


Figure 3.10. Network structure of Option 4 of the IBMS for Example 3.5.

3.3 Conclusion and Summary

The calculation of area in heat exchange problems is strongly dependent on the driving forces. Driving forces are calculated using supply, intermediate and target temperatures of the hot and cold streams. Hence partitioning a superstructure and defining the superstructure model equations (which involve calculating these intermediate temperatures) on the basis of the intermediate temperatures is advantageous. This is because there will be no need to include non linear heat balance and mixing equations in the model thereby reducing the solution generation time. A second advantage is that since the intermediate temperatures are treated as variables, competing costs and streams with significantly different heat transfer coefficients can still be optimised simultaneously. However split streams will not always be mixed at equal temperatures, thus requiring such models to be solved a second time as an NLP in order to calculate spilt flows and exchanger exit temperatures. In addition, setting initial points and bounds for such superstructures will be difficult. These shortcomings are due to the fact that each

of the intermediate temperatures in the stage boundaries are variables which will not always take on the same values in order to determine the optimum network.

This chapter has illustrated a new superstructure generation method which remedies the problems associated with non isothermal mixing and initialisation problems in previous stagewise heat exchange superstructures. The superstructure which is interval based is constructed by defining interval temperature locations with the supply and target temperatures of either the hot or the cold set of streams. The other stream set is allowed to participate in all the intervals defined, and their ability to exchange heat in these intervals is subject to thermodynamic feasibility. The interval based superstructure is able to establish a simultaneous trade-off among competing costs which include energy and capital costs. The model has been demonstrated to effectively handle heat exchange problems whose stream heat transfer coefficients vary significantly. This is possible because there is no restriction of heat transfer in exchangers to be vertical in accordance with pinch composite curve divisions.

The new interval based superstructure automatically mixes split streams at equal temperatures; also, it can easily be initialised and bounded. Intermediate temperatures which are vital to calculating optimal driving forces do not need to be initialised or bounded; only the stream flows are given bounds. This is possible because model equations which involve the calculation of intermediate temperatures are constrained using stream existence conditionals. This implies that the calculation of intermediate temperatures (and the heat load to be exchanged in such intervals) is dependent on the fixed temperatures defining the interval temperature boundaries. This allows the model to be solved in a single step unlike the SWS approach which needs to be solved in an NLP suboptimisation step in order to determine split flows and exchanger exit temperatures.

This chapter has also demonstrated the ability of the interval based superstructure method to optimise heat exchange problems involving multiple utilities. The solutions obtained for heat exchange problems using the IBMS method have been shown to be close to those reported using other methods in the literature, and better in some cases. In all cases, the IBMS involves far less effort than previous multiple utility optimisation methods.

CHAPTER 4

INTERVAL BASED MINLP SUPERSTRUCTURE (IBMS) FOR THE SIMULTANEOUS SYNTHESIS OF MASS EXCHANGE NETWORKS

4.1 Introduction

The mass exchange analogue of the heat exchange IBMS is presented in this chapter. The construction of the interval based superstructure is first illustrated followed by the model equations for optimising the superstructure. The new interval based superstructure for mass exchange networks will also be compared with the stagewise fairly linear MINLP (FLM) model for the simultaneous synthesis of mass exchange networks by Szitkai *et al*. (2006).

This chapter also presents the application of this newly developed interval based MINLP superstructure to the synthesis of mass exchange network problems. The problems to be considered include those that involve stagewise and continuous contact mass exchangers. Problems involving regeneration of the external MSAs will also be considered. The results will be compared with those in the literature.

It should be noted that the IBMS for both HENS and MENS are based on the same concept, which accounts for the references to Chapter 3 which presents the IBMS for HENS.

4.2 Interval Based MINLP Superstructure (IBMS) for MENS

Motivation

Driving forces equally play a key role in determining the optimum sizes for mass exchangers in a network as it applies to temperatures in heat exchanger networks. Hence partitioning a framework for synthesizing a network of mass exchangers on the basis of compositions would be beneficial. The benefits which are similar to those described in Chapter 3 for HENS are highlighted below for MENS:

- Non linear mass balance, mixing and bypass equations may not be needed in such models in order to get near minimum total costs in short times since the overall model would be fairly linear.
- The costs which contribute to the TAC can still be simultaneously optimised since the intermediate compositions are treated as variables.

The fairly linear model (FLM) of Szitkai, *et al*. (2006) partitions mass exchange superstructures on the basis of compositions. The number of composition stages can be $\max\{N_R,N_S\}$, where N_R and N_S are the number of rich and lean streams respectively. All the intermediate compositions of the FLM are treated as variables. The shortcomings associated with such a partitioning approach have been discussed in Chapter 2. However those to be addressed in this study are highlighted below:

- Initialisation and setting of bounds may become difficult especially in problems having superstructures with three or more stages. This is because only the first and the last stages of the superstructure have boundaries that correspond to the supply compositions of the rich and lean streams respectively. The intermediate stage compositions are bounded on both sides with composition locations which are treated as variables.
- The tendency for split stream branches to be mixed at equal compositions for splits occurring within the intermediate stages becomes reduced. This implies that networks involving splits streams may need to be solved in an NLP suboptimisation step for solutions involving split streams in order to determine the branch flowrates and compositions.

This study aims to develop superstructures for MENS by partitioning the superstructure (i.e. setting the interval boundaries or composition locations) using the supply and target compositions of either the rich or lean set of streams. If the rich streams are used (i.e. a rich stream based superstructure) then the lean streams are allowed to participate (float) in all the intervals created by the rich streams. The ability of the lean streams in the rich stream based superstructure to exchange mass in each interval of the superstructure is however subject to thermodynamic feasibility. The reverse would be the case for a lean stream based superstructure. Within each interval of the interval based MINLP superstructure (IBMS), each rich and each lean stream has the potential of exchanging mass (by splitting) with each of the streams of the opposite kind present in the interval. Also, the exit compositions of exchangers through which split streams exchange mass in the IBMS are equal and such compositions form the compositions of the next interval boundary.

This approach was chosen so that each stage (interval) of the superstructure will be bounded on both sides by a fixed composition parameter which corresponds to either a supply or a target composition of streams in the problem. It should be noted that all stream compositions in the same composition location can take on values different from the composition used to define the composition location. The bounding on each side of the interval will help simplify the initialisation and setting of bounds for solving such superstructures. Also, split streams will automatically be mixed at equal compositions thus eliminating the need for non linear mass balance and mixing equations.

In the FLM model, it is assumed that the split streams will be mixed at equal compositions since non linear mass balance and mixing equations are not included in the model. However such assumptions do not always hold. Even if the non linear equations are included as done in the stagewise superstructure of Chen and Hung (2005a), initialisation and setting of bounds may be difficult.

A shortcoming of excluding the non linear equations as done in the IBMS model to be presented in this study are that series exchangers for split stream branches and structures with non isocomposition mixing configurations would be excluded from the search for the optimum. All the same the examples where the IBMS have been applied which are presented in this study show that good solutions can still be obtained in reasonable times for problems with relatively few streams in both stagewise and continuous contact columns. The model also performs reasonably well for problems involving multiple process and external lean streams, regeneration and non-linear equilibrium relations.

Defining composition intervals using the supply and target composition of the rich or lean set of streams in the problem allows the superstructure to simultaneously optimise the MSA and capital costs of mass exchange networks. The capital cost comprises of packed height (for continuous contact columns), number of stages (for stagewise columns) and exchanger fixed costs. The reason for this simultaneous optimisation is that the intermediate compositions of streams at locations where they cross interval boundaries defined by some other streams are modelled as variables to be optimised.

4.2.1 Construction of the IBMS

An illustrative mass exchange problem which involves two rich and two lean streams will be used to describe the construction of the IBMS for MENs. The illustrative superstructure is shown in Figure 4.1.

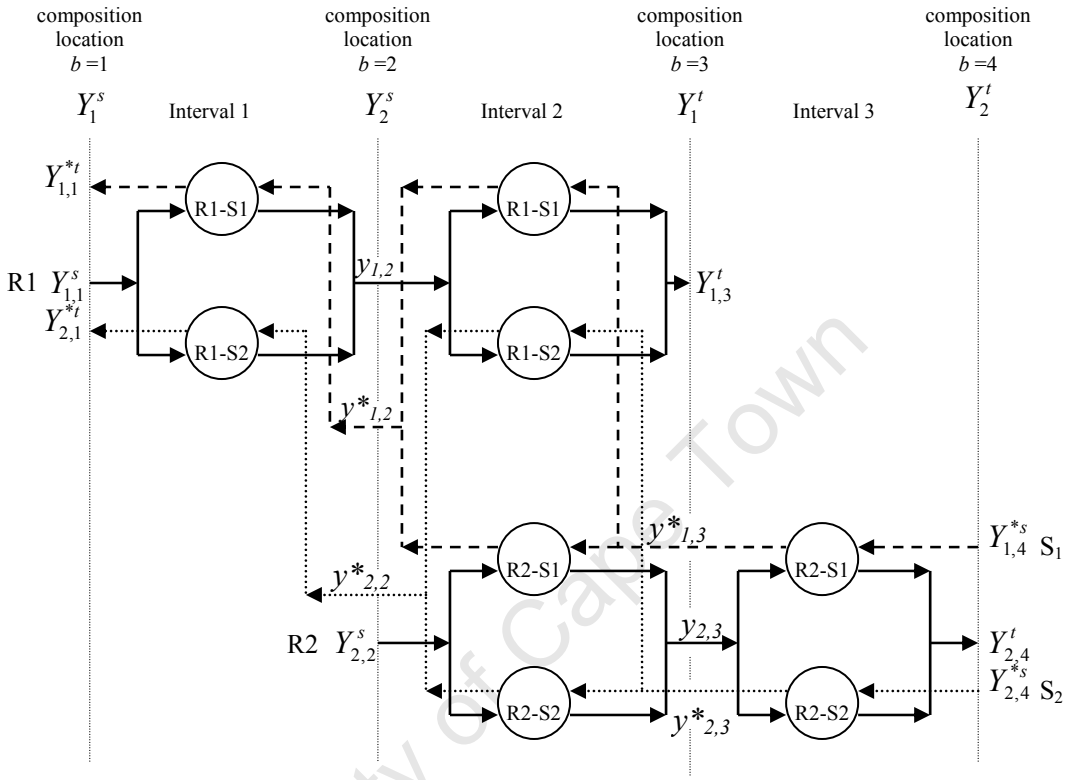


Figure 4.1. Rich stream based interval superstructure.

The composition in the rich phase *Y** (or *y**) in equilibrium with lean stream composition *X* (or *x*) has been used throughout this thesis. However, problems in the appendix and network solutions have been presented with *X* (or *x*) for the lean streams. All compositions may be either mole fractions (normally *x*, *y*) or mole ratios (normally *X*, *Y*) but Capital *Y* (and *Y**) and *X* represent supply and target values while *y* and *x* represent intermediate compositions in this thesis. No distinction is made between process lean streams and external MSAs in terms of how much mass they are allowed to pick up or their location on the superstructure, whether rich or lean stream based.

In the illustrative problem, the supply composition, Y_1^s, of R_1 (rich stream 1) is higher than the supply composition, Y_2^s, of R_2 (rich stream 2). Also, the target composition, Y_1^t of R_1 is higher than that of R_2 (Y_2^t) although lesser than Y_2^s. These compositions are sorted in a descending order and each is used to define a composition location, *b*. This

gives a superstructure with four composition locations as shown in Figure 4.1. If the supply/target compositions of two or more streams coincide, then they would be represented once. The lean streams, S_1 and S_2, are allowed to participate in all the intervals. Note that the composition of R_1 in composition location, $b = 1$, is Y_1^s while in composition location $b = 2$, it is a variable, $y_{1,2}$, to be optimised. $y_{1,2}$ in composition location, $b = 2$, can be less than, greater than or equal to Y_2^s the supply composition of R_2. This situation also applies to other streams (rich and lean) in composition locations not defined by their supply or target compositions.

A key feature of the IBMS model is the use of stream existence and stream supply/target composition recognition coefficients. These coefficients are included in the model equations which directly or indirectly involve the calculation of intermediate compositions. The coefficients can be modelled in the form of conditionals in the model environment. The purpose of the coefficients is to ensure that streams which are split in the rich end of a composition location ($b = 1$ for the split of R_1 in Figure 4.1) are mixed at equal compositions at the lean end of the interval ($b = 2$ for R_1 in Figure 4.1). This implies that there is no need to include non linear mass balance and flow mixing equations in the superstructure model, therefore the model is solved without much difficulty in relatively shorter times.

On the other hand, if a lean stream based superstructure is constructed, the rich streams would be made to participate in all the intervals. As with the lean streams, the ability of the rich streams to exchange mass in any interval in the lean superstructure basis is subject to thermodynamic feasibility.

4.2.1.1 IBMS Model Formulation

Once the interval based superstructure is constructed, it is modelled as a mixed integer non linear program (MINLP) in order to minimise the total annualised cost. Listed below are the required sets, indices, parameters and variables that are used in the model formulation.

Sets

R rich process streams

S lean streams (process and external mass separating agents)

V regenerating streams

B composition intervals in the superstructure

Indices

r rich process stream

l lean stream (process or external mass separating agents)

v regenerating stream

b index for composition interval location (b = 1,……,NOB)

Parameters

AC_l annual operating cost per unit of lean stream l

AC_v annual operating cost per unit of regenerating stream v

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

ACT_{lv} annual cost per stage for staged columns involving lean stream, l and regenerating stream, v

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

ACH_{lv} annual cost per height for continuous contact columns involving lean stream l and regenerating stream, v

CB_{rl} fixed charge or exchanger installation cost for columns involving rich stream, r and lean stream, l

CB_{lv} fixed charge or exchanger installation cost for columns involving lean stream l and regenerating stream, v

D^{rl} area cost exponent for columns involving rich stream, r and lean stream, l

D^{lv} area cost exponent for columns involving lean stream l and regenerating stream, v

m slope of equilibrium line governing the transfer of component from rich stream r to lean stream l

m_v slope of equilibrium line governing the transfer of component from regenerable lean stream l to regenerating stream v

K_w lumped mass transfer coefficient

b_{int} intercept of the equilibrium line

WF weighting function

$X^{S}_{l,b}$ supply composition of lean (process or external) stream l which starts from composition interval b

$X^{t}_{l,b}$ target composition of lean (process or external) stream l which ends in interval b

$Y^{S}_{r,b}$ supply composition of rich process stream r which starts in interval b

$Y^{t}_{r,b}$ target composition of rich process stream r which ends in interval b

$Y^{*S}_{l,b}$ equilibrium supply composition of lean (process or external) stream l which starts in interval b

$Y^{*t}_{l,b}$ equilibrium target composition of lean (process or external) stream l which ends in interval b

Y^{*S}_{v} equilibrium supply composition of regenerating stream v

Y^{*t}_{v} equilibrium target composition of regenerating stream v

Z^{s}_{v} supply composition of regenerating stream v

Z^{t}_{v} target composition of regenerating stream v

Ω_m upper bound for mass exchanged in match r,l in interval b

Ω_r upper bound for mass exchanged in match l,v

Γ_m upper bound for driving force in match r,l in interval b

Γ_r upper bound for driving force in match l,v

ε_{min} minimum composition difference

Binary variables

dw_{rlb} binary variable denoting the existence of match r,l in interval b of the optimal network

w_{lvb} binary variable denoting the existence of match l,v in the optimal network

Positive variables

dy_{rlb} driving force between rich stream r and lean stream l in interval b

dx_{lvb} driving force between lean stream l and regenerating stream v

G_r flowrate of rich stream r

L_l flowrate of lean stream l

M_{rlb} mass exchanged between rich stream *r* and lean stream *l* in interval *b*

N_{rlb} number of stages in staged column *rlb*

N_{lvb} number of stages in staged column *lq*

QR_v flowrate of regenerating stream *v*

$x_{l,b}$ composition of lean (process or external) stream *l* in composition location *b*

$y_{r,b}$ composition of rich process stream *r* in composition location *b*

$y^*_{l,b}$ equilibrium composition of lean (process or external) stream *l* in composition location *b*

w_{rlb} relaxed binary variable representing the existence of match, *r,l*, in interval *b*, in the optimal network

Model Equations

Prior to presenting the equations used to optimise the interval based superstructure, it is essential to state two stream conditionals. The first conditional (described for a rich based superstructure) states that: 'a rich stream will only be considered for the calculation of its variables in composition location *b* if it crosses the location'. It should be noted that this rich stream existence conditional will also need to be included in some of the model equations for lean streams. This ensures that the mass exchanged between the rich stream and potential lean streams is considered as well in the variable calculations. The reverse will be the case for a lean stream based superstructure. The conditional equations may be presented in the following forms for rich and lean stream based superstructures respectively.

$$R_{r,b}\,\$\left(Y_r^s \geq Y_b \;and\; Y_r^t \leq Y_{b+1}\right)=1 \tag{4.1}$$

$$S_{l,b}\,\$\left(Y_l^{*t} \geq Y_b^* \;and\; Y_l^{*s} \leq Y_{b+1}^*\right)=1 \tag{4.2}$$

where \$ is the operator used to check whether a condition is true or not. Note that Y_b (for rich streams) and (Y^*_b for lean streams) represent the supply and target compositions of the streams defining the superstructure intervals which were ordered in a descending order; hence Y_b (or Y^*_b) is a parameter which is problem specific.

Equation 4.1 implies that R_r either starts at composition location *b* or crosses it, and that it either ends at composition location *b*+1 or crosses it. If these two conditions are not

met, then R_r will not be regarded as existing in interval b and its variables will not be calculated in interval b. Hence the right hand side of Equation 4.1 will be equal to '0'. The same description applies to Equation 4.2 for lean streams in a lean stream based superstructure. Note that Equation 4.1 will also apply in some of the model equations for lean streams. This enables the mass exchanged between the rich stream and potential lean streams to be considered as well in the variable calculations. The reverse will be the case for a lean stream based superstructure, i.e. Equation 4.2 applies to rich stream equations.

The stream supply/target composition recognition conditional. This conditional specifically makes the model equations recognise the stream whose supply/target composition defines a composition location in the superstructure. Note that some of the model equations (as will be shown) need to be constrained using both sets of conditionals.

$$RSt_{r,b}\,\$\left(Y_r^s = Y_b\right) = 1 \tag{4.3}$$

$$RE_{r,b}\,\$\left(Y_r^t = Y_b\right) = 1 \tag{4.4}$$

$$SSt_{l,b}\,\$\left(Y_l^{*s} = Y_b^*\right) = 1 \tag{4.5}$$

$$SE_{l,b}\,\$\left(Y_l^t = Y_b^*\right) = 1 \tag{4.6}$$

Where *RSt*, *RE*, *SSt* and *SE* represent rich start, rich end, lean start and lean end respectively. Equations 4.3 and 4.4 imply that composition location b is defined by the supply or target compositions of rich stream r in a rich stream based superstructure. The same condition applies to Equations 4.5 and 4.6 for a lean stream based superstructure. The conditionals are discussed in the model equations where they need to be used.

Overall stream mass balance

Just as it applies in heat exchange IBMS, a stream needs to exchange mass with streams of the opposite kind in order for it to get to its target composition. This mass exchange takes place in some or all of the composition intervals depending on the mass load of the opposite kind of stream. The sum of the mass exchanged over the intervals where mass

exchange takes place is equated to the overall mass requirement of the stream concerned. The model equations for rich and lean streams can be represented as:

$$\left(Y_r^s - Y_r^t\right)\cdot G_r = \sum_{b\in B}\sum_{l\in S} M_{r,l,b}\,, \qquad r \in R \tag{4.7}$$

$$\left(Y_l^{*t} - Y_l^{*s}\right)\cdot L_l = \sum_{b\in B}\sum_{r\in R} M_{r,l,b}, \qquad l \in S \tag{4.8}$$

For a rich stream based interval superstructure, rich stream interval existence conditionals (Equation 4.1) are used to constrain Equations 4.7 and 4.8 so that $M_{r,l,b}$ will be calculated for rich streams in intervals where they exist. This automatically ensures that $M_{r,l,b}$ is also calculated for lean streams in intervals where they can exchange mass with rich streams. For a lean stream based superstructure, the conditionals are included in the same manner using lean stream interval existence conditionals (i.e. Equation 4.2).

Interval mass balance

Interval mass balances are used to calculate the interval boundary compositions for each stream.

$$\left(y_{r,b} - y_{r,b+1}\right)\cdot G_r = \sum_{l\in S} M_{r,l,b}, \qquad r \in R \;\; b \in B \tag{4.9}$$

$$\left(y^*_{l,b} - y^*_{l,b+1}\right)\cdot L_j = \sum_{r\in R} M_{r,l,b}, \qquad l \in S \;\; b \in B \tag{4.10}$$

The rich stream existence conditionals (Equations 4.1 and 4.2) are also included in Equations 4.9 and 4.10 for a rich stream based superstructure because these equations calculate intermediate stream compositions. The conditionals are used to ensure that intermediate compositions and mass loads are calculated for rich and lean streams in composition intervals where they exist. It is worthwhile to mention that rich stream existence conditionals are used in Equation 4.10 despite being a lean stream mass balance equation. This is necessary so that intermediate compositions and mass loads will also be calculated for the lean streams in intervals where they can feasibly exchange mass with a rich stream. Lean stream interval existence conditionals are equally used for both rich and lean stream mass balance equations for a lean stream based superstructure.

Assignment of superstructure interval compositions

The stagewise FLM model of Szitkai, *et al*. (2006) requires that only the first and last composition locations in the superstructure be assigned compositions which correspond to the supply and target compositions of the streams in the problem. However in the IBMS for MENS the supply and target compositions of either the rich or lean set of streams define composition locations in the superstructure. This implies that problem specific equations need to be used to assign the superstructure interval compositions. In order to model this composition assignment approach, the stream supply/target recognition conditionals are employed. These conditionals are used together with the stream interval existence conditionals. This is necessary so as to ensure that the composition intervals are calculated based on Equations 4.7 to 4.10. The equations are described for each composition location of Figure 4.1 below:

$$b = 1; \quad Y_{1,1}^{S} = y_{1,1}, \; Y_{1,1}^{*t} = y_{1,1}^{*}, \; Y_{2,1}^{*t} = y_{2,1} \tag{4.11}$$

$$b = 2; \quad Y_{2,2}^{S} = y_{2,2} \tag{4.12}$$

$$b = 3; \quad Y_{1,3}^{t} = y_{1,3} \tag{4.13}$$

$$b = 4; \quad Y_{4,4}^{S} = y_{2,4}, \; Y_{1,4}^{*s} = y_{1,4}^{*}, \; Y_{2,4}^{*s} = y_{2,4}^{*} \tag{4.14}$$

Equations 4.11 to 4.14 illustrate how the supply and target compositions of the rich streams are used to define the composition locations of Figure 4.1. The lean streams are allowed to participate in all the intervals. The model will recognise Equation 4.12 (as a supply composition) while calculating the intermediate composition of R_1 in composition location, b = 2. Note that R_1 crosses composition location, b = 2. These model constraints (together with Equation 4.11 and the conditional equations) will automatically ensure that any split of R_1 in interval 1 is mixed at equal compositions in b= 2. This also applies to the calculation of intermediate compositions for all other streams (rich and lean) at composition locations which they do not define but cross.

Feasibility of compositions

Along the superstructure, the composition of both rich and lean streams should decrease from left to right. The stream interval existence conditionals are also used here to ensure that the compositions of the streams decrease from left to right starting from the

composition location where the stream enters the superstructure. For Figure 4.1 which is a rich stream based superstructure, rich stream conditionals are used for just the rich stream feasibility equations. These equations are shown next.

$$y_{r,b} \geq y_{r,b+1}, \quad b \in B,\ r \in R \tag{4.15}$$

$$y^{*}_{j,b} \geq y^{*}_{j,b+1}, \quad b \in B,\ l \in S \tag{4.16}$$

The existence conditionals do not have to be included for the lean stream feasibility equations because when the rich streams compositions decrease along the superstructure, the lean streams will automatically decrease as well based on the other set of constraints.

Logical constraints

The existence of a match, *r,l*, in interval *b*, is modelled in the superstructure using binary variables $w_{r,l,b}$, as done by Szitkai, *et al*. (2006) in the FLM model. The binary variables are incorporated into logical constraints. If the match *r,l* exists in interval *b*, the binary variable will take on a value of '1' and '0' if otherwise. The logical constraint contains an upper bound, Ω_m, which is used to limit the quantity of mass that is exchanged between *r* and *l* to the lesser of the total mass load of each of the streams involved in the match. The logical constraint can be represented in the following way;

$$M_{r,l,b} - \Omega_m w_{r,l,b} \leq 0, \quad r \in R,\ l \in S,\ b \in B \tag{4.17}$$

Exchanger driving forces calculation

A continuous variable, $dy_{r,l,b}$, which is the composition difference between rich stream *r* and lean stream *l* in composition location *b*, is used to calculate exchanger driving forces as done by Szitkai, *et al*. (2006). The driving force variable will be included in logarithmic mean composition difference (LMCD) calculation. Logical constraints which involve the binary variable, $w_{i,j,k}$, with an upper bound parameter, Γ_m, are used to calculate the driving forces. If a match *r,l* exists in interval *b*, the binary variable, $w_{i,j,k}$, will take on a value of '1' and the approach composition, $dy_{r,l,b}$, will be properly calculated. But if the match does not exist in the optimal network, then the binary variable will take on a value of '0'. In this case, due to the presence of Γ_m in the logical constraint equation, the equation will be inactivated. This ensures that no negative

approach compositions are included for any match. The logical equations are shown below;

$$dy_{r,l,b} \le y_{r,b} - y^*_{j,b} + \Gamma_m \cdot \left(1 - w_{i,j,k}\right), \quad b \in B,\ r \in R,\ l \in S \tag{4.18}$$

$$dy_{r,l,b} \ge y_{r,b} - y^*_{j,b} - \Gamma_m \cdot \left(1 - w_{i,j,k}\right), \quad b \in B,\ r \in R,\ l \in S \tag{4.19}$$

$$dy_{r,l,b+1} \le y_{r,b+1} - y^*_{j,b+1} + \Gamma_m \cdot \left(1 - w_{i,j,k}\right), \quad b \in B,\ r \in R,\ l \in S \tag{4.20}$$

$$dy_{r,l,b+1} \ge y_{r,b+1} - y^*_{j,b+1} - \Gamma_m \cdot \left(1 - w_{i,j,k}\right), \quad b \in B,\ r \in R,\ l \in S \tag{4.21}$$

Γ_m can be set as the maximum of zero and the composition differences between the rich stream, *r*, and the lean stream, *l*, (Shenoy, 1995) so as to avoid numerical errors due to negative approach compositions for matches that do not exist.

Just as was done for HENS in chapter 3, an exchanger minimum composition difference (EMCD) can be used to give a lower bound to the driving forces at each end of each match. This helps to ensure that exchangers of infinite height/stages are not included in the solution network. This can be represented as;

$$dy_{r,l,b} \ge \alpha \tag{4.22}$$

where α is a small positive number.

The integer infeasible path MINLP (IIP-MINLP) formulation of Sorsak and Kravanja (2002) as used by Szitkai, *et al*. (2006) is also included in the IBMS model equations in order to ensure numerical stability.

$$w_{r,l,b} = dw_{r,l,b} + ew_{r,l,b} - fw_{r,l,b}, \quad r \in R \ \ l \in S \ \ b \in B$$

where $dw_{r,l,b}$ is a real binary variable while $w_{r,l,b}$ is the relaxed version. $ew_{r,l,b}$ and $fw_{r,l,b}$ are positive and negative tolerances respectively.

Objective function

The objective function of the IBMS for MENS simultaneously minimises the MSA costs and capital costs (which comprises installation costs and the costs of the mass exchangers). Chen's first approximation (Chen, 1987) is also used to calculate LMCD.

The LMCD will be included in the objective function as was done in Chapter 3 for heat exchange.

$$LMCD_{r,l,b} = \left[\left(dy_{r,l,b}\right)\cdot\left(dy_{r,l,b+1}\right)\cdot\left(dy_{r,l,b}+dy_{r,l,b+1}\right)/2\right]^{1/3} \tag{4.23}$$

The IBMS model for MENS can handle mass exchange network problems involving both continuous contact and stagewise columns. For continuous contact columns, the capital cost calculation method which is based on exchanger mass by Hallale (1998) is used. For stagewise columns: the per stage costing method of Papalexandri, *et al*. (1994) where the diameter of each column is assumed to be 1m is used. Note that a more detailed costing can be used but none of the comparative examples used it. The stagewise exchangers are sized using the new sizing formula of Fraser and Shenoy (2004). Equations 4.24 and 4.25 describe this for the two types of mass exchange columns.

Continuous contact columns:

$$\min\left\{\sum_{l\in S}(AC_l)\cdot(L_l)+\sum_{r\in R}\sum_{l\in S}\sum_{b\in B}CB_{r,l}\cdot z_{r,l,b}+\sum_{r\in R}\sum_{l\in S}\sum_{b\in B}ACH_{r,l}\cdot\left[M_{r,l,b}/K_W\left\{LMCD_{r,l,b}\right\}\right]^{D_{r,l}}+WT\right\}$$

$$\text{where } WT = WF\cdot\sum_{r\in R}\sum_{l\in S}\sum_{b\in B}(ew_{r,l,b}+fw_{r,l,b}) \tag{4.24}$$

where WF is a weighting coefficient

Stagewise columns:

$$\min\left\{\sum_{l\in S}(AC_l)\cdot(L_l)+\sum_{r\in R}\sum_{l\in S}\sum_{b\in B}CB_{r,l}\cdot z_{r,l,b}+ACT_{r,l}\sum_{r\in R}\sum_{l\in S}\sum_{b\in B}\left[N_{r,l,b}\right]\right\} \tag{4.25a}$$

where $N_{r,l,b}$ which is the number of stages is defined by Fraser and Shenoy (2004) as

$$N_{r,l,b} = \left(\frac{\Delta y^n + \Delta y^{*n}}{\Delta y_1^n + \Delta y_2^n}\right)^{1/n} \tag{4.25b}$$

where Δy^n = rich stream concentration difference,

Δy^{*n} = lean stream equilibrium concentration difference

Δy_1^n = rich end of the exchanger driving force

Δy_2^n = lean end of the exchanger driving force

n = 1/3 (Underwood, 1970) and 0.3275 (Chen, 1987).

Constraints 4.7 to 4.21 define the region of search for the model and they are all linear except for Equations 4.8 and 4.10. Therefore the model can easily be solved with little difficulty. For general mass exchange problems, only the flowrates of the process and external lean streams need to be initialised and bounded when using the IBMS for MENS. However when regeneration is involved, the supply and target compositions of the regenerable lean stream have to be initialised and given bounds as well. The process lean streams flows are initialised and given lower bounds using very small values which depend on the problem specifications. The upper bound flows for these streams should correspond to the upper limit of the available flow of the process lean stream on site. The external MSAs are also initialised like the process lean streams but they are given upper bounds which are big enough just in case any of the external MSA might have to pick up the entire mass alone.

The final compositions of lean streams may need to be bounded for economic reasons. In such instances, the superstructure needs to be generated on a rich stream basis because the compositions of the lean streams become variables to be optimised. Constraints like no stream splits, compulsory or forbidden matches etc, can also easily be included in the interval based superstructure model.

IBMS Model Equations for Mass Exchange Networks involving Regeneration

External MSAs need to be regenerated due to environmental or economic reasons. Regenerating MSAs can help to reduce the TAC of mass exchange networks especially for MSAs that are very expensive. However the benefits can only be exploited if the mass exchange network (primary mass exchange network) is simultaneously synthesised with the regeneration network (secondary mass exchange network). Simultaneously synthesising these two networks is essential since the two networks interact with one another through the regenerable MSA. The MSA flow and its supply and target compositions determine the annual capital and annual operating costs of the primary and secondary networks. Therefore these parameters have to be treated as variables, which lead to an increase in the dimensionality of the mass exchange problem and a resultant

difficulty in initialising and giving bounds to such problems. This calls for the use of a robust simultaneous synthesis technique to tackle regeneration problems.

Figure 4.2 shows the IBMS which involves the regeneration of MSA stream S_2. The regenerating stream V_1 is placed outside the superstructure because it is assumed that regeneration takes place in a single exchanger with full MSA flow from its inlet to outlet composition. It is also assumed that there is no need for make-up of the MSA.

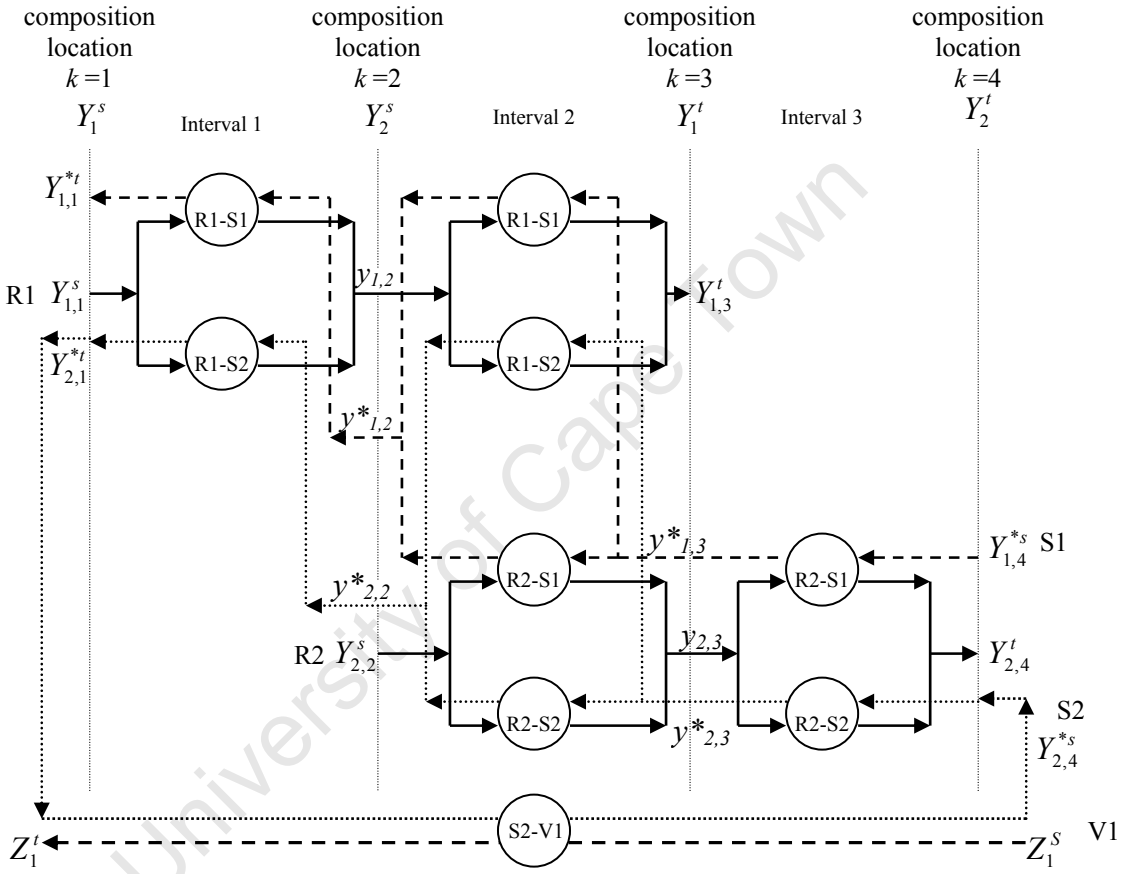


Figure 4.2. Interval-based mass exchanger network superstructure involving regeneration for a rich stream based superstructure.

The additional model equations are described next.

Mass balance for the regenerating stream

An overall mass balance is used to calculate the flow of regenerating agents:

$$\sum_{v \in V} (Z_v^t - Z_v^s) VR_v = \sum_{r \in R} \sum_{b \in B} M_{rlb} \qquad l \in S \tag{4.26}$$

Logical Constraints

Logical constraints are used to denote the existence or otherwise of a match connecting lean stream *l* and regenerating stream *v* in the optimal network. The binary variable, z_{lv}, takes on a value of '1' if the match *l,v* exists and '0' if otherwise. An upper bound, Ω_r can be used to constrain the amount of mass to be exchanged between lean stream *l* and regenerating stream, *v*. Note that Ω can be calculated in a similar way to Equation 4.17:

$$\left(Z_v^t - Z_v^s\right) \cdot VR_v - \Omega_r \, z_{l,v} \leq 0 \tag{4.27}$$

Equation 4.27 allows multiple regeneration with pairing of regeneration and lean streams.

Exchanger driving forces

Approach composition, $dx_{lv,b}$ are introduced in order to calculate the driving forces for matches between the regenerable lean stream, *l*, and the regenerating agent, *v*. Note that the composition in the rich phase is used for the regenerating stream.

$$dx_{l,v,b=1} \leq x_{l,b=1} - Y_v^{*t} + \Gamma_r \cdot (1 - z_{l,v}), \quad b \in B, \;\; l \in S, \;\; v \in V \tag{4.28}$$

$$dx_{l,v,b=1} \geq x_{l,b=1} - Y_v^{*t} - \Gamma_r \cdot (1 - z_{l,v}), \quad b \in B, \;\; l \in S, \;\; v \in V \tag{4.29}$$

$$dx_{l,v,b=last} \leq x_{l,b=last} - Y_v^{*s} + \Gamma_r \cdot (1 - z_{l,v}), \quad b \in B, \; l \in S, \; v \in V \tag{4.30}$$

$$dx_{l,v,b=last} \geq x_{l,b=last} - Y_v^{*s} - \Gamma_r \cdot (1 - z_{l,v}) \quad b \in B, \; l \in S, \; v \in V \tag{4.31}$$

The driving forces for the match between the regenerable lean stream and the regenerating agent is calculated using the composition in the lean phase, $x_{l,b}$. A parameter Γ_r is also applied as an upper bound to either activate or deactivate the equation as it applies in Equations 4.18 to 4.21 for the primary network. The EMCD in Equation 4.22 for the primary network is also used in the secondary network to avoid exchangers with infinitely large sizes. The flow and/or outlet composition of the regenerating stream can be given upper bounds.

Logarithmic mean composition difference (LMCD)

The LMCD is calculated in the same manner with the primary network. The Chen's first approximation (Chen, 1987) is used for continuous contact columns as before:

$$LMCD_{l,v,b} = \left[(dx_{l,v,b=1}) \cdot (dx_{l,v,b=last}) \cdot (dx_{l,v,b=1} + dx_{l,v,b=last}) / 2 \right]^{1/3} \quad (4.32)$$

Objective function

The overall objective function (including the primary network) aims to simultaneously minimise the following: the AOC for the non regenerable MSA in the primary network (process or external), the AOC of the regenerating MSA, the ACC of the primary network mass exchangers and the ACC of the regeneration network exchangers. The TAC equation for the secondary network is shown in the next set of equations. Equation 4.33 describes the TAC for continuous contact columns while Equation 4.34a is for stagewise columns. The necessary equation must be added to the primary network TAC in order to get the TAC for the combined primary and secondary networks.

$$\sum_{v \in V} (AC_v) \cdot (VR_v) + \sum_{l \in S} \sum_{v \in V} \sum_{b \in B} CB_{l,v} z_{l,v,b} + \sum_{l \in S} \sum_{v \in V} \sum_{b \in B} ACH_{l,v} \left[\left(Z^t_{v,b=1} - Z^s_{v,b=last} \right) \cdot VR_v / K_W \left\{ LMCD_{l,v,b} \right\} \right]^{D_{l,v}} \quad (4.33)$$

$$\left\{ \sum_{v \in V} (AC_v) \cdot (VR_v) + \sum_{l \in S} \sum_{v \in V} \sum_{b \in B} CB_{l,v} z_{l,v,b} + ACT_{l,v} \cdot \sum_{l \in S} \sum_{v \in V} \sum_{b \in B} \left[N_{l,v,b} \right] \right\} \quad (4.34a)$$

where N_{lvb} is the number of stages and is defined by Fraser and Shenoy (2004) as;

$$N_{lvb} = \left(\frac{\Delta x^n + \Delta x^{*n}}{\Delta x_1^n + \Delta x_2^n} \right)^{1/n} \quad (4.34b)$$

where Δx^n = lean stream concentration difference of the *l,v* exchanger,

Δx^{*n} = regenerating stream equilibrium concentration difference

Δx_1^n = rich end of the *l,v* exchanger driving force

Δx_2^n = lean end of the *l,v* exchanger driving force

n = 1/3 (underwood, 1970) and 0.3275 (Chen, 1987).

4.2.2 Comparison of Stagewise FLM and IBMS

The superstructure of the FLM model of Szitkai, *et al*. (2006) is similar to the IBMS model for MENS being developed in this study. However there are some differences which are highlighted below:

- The first composition location of the FLM superstructure model is defined by the supply compositions of all the rich streams in the problem while the last composition location is defined by the supply composition of all the lean streams (process and external) in the problem. For the IBMS model, the first composition location is defined only by the rich stream (i.e. for a rich based superstructure) with the highest supply composition while the last composition location of the superstructure is defined by the rich stream with the lowest target composition. All the lean streams start from the last composition location and end in the first composition location. The reverse scenario applies for a lean stream based superstructure.

- The compositions of all the rich and lean streams at intermediate composition locations are variables to be optimised in the FLM superstructure. In the IBMS, the intermediate compositions are defined by the supply and target compositions (when sorted in a descending order) of all the streams upon which the superstructure is based. The intermediate composition of every stream at every composition location is treated as a variable to be optimised.

4.2.3 Examples

Four kinds of MENS problems have been considered in this chapter. The first involves continuous contact columns while the second and third both require stagewise columns. The last problem involves regeneration and mixed types of mass exchangers. Note that the values reported for the lean stream flow initialisations and bounds are those that correspond to the y^* values while the actual flows are shown in the network structures. The IBMS GAMS code for Example 4.1 is presented in Appendix D2.

4.2.3.1 Example 4.1

This example will be used to demonstrate the ability of the IBMS for MENS to minimise the TAC of problems where all exchangers are continuous contact columns. The example is adapted from Hallale (1998) where pinch technology was applied for its synthesis. The problem involves five gaseous streams which are rich in ammonia. Three water based lean streams are available for the ammonia removal. The first two of the leans streams, S_1 and S_2 are process lean streams while S_3, the last lean stream is an external MSA. The capital costing approach of Hallale (1998) which is exchanger mass based is used to cost the columns. The process MSAs are available free of charge. The problem data are shown in Tables B1, B2 and B3 of the appendix.

Two other set of authors have solved this example. The first is Szitkai, *et al*. (2006) which used the stagewise FLM. The second set of workers (Emhamed, *et al*. 2007) used TAC_{target} of pinch technology to set bounds for the solution of the stagewise FLM model. Hallale (1998) solved the problem for a TCC situation while Szitkai, *et al*. (2006) solved it for both TCC and TAC situations. They assumed operating and capital cost data which are also used in this thesis for fair comparison. Equation 4.24 is used as the objective function.

Hallale (1998) got a TCC of 298,000 \$/yr while Szitkai, *et al*. (2006) obtained a TCC of 307,000 \$/yr and a TAC of 134,000 \$/yr. Emhamed, *et al*. (2007) first solved the problem using pinch technology supertargeting of Hallale and Fraser (2000c & d) where they got a TAC of 788,405 \$/yr at a Δy_{min} of 0.0007. Note that this TAC should be 139,000 \$/yr and not 788,405 \$/yr, as recalculated by the current author. Emhamed, *et al*. (2007) further used this solution to set bounds for the stagewise FLM model based on their new hybrid method for MENS where they obtained a final TAC of 134,399 \$/yr. Applying the IBMS model to this example gives a TAC of 133,323 \$/yr which is less than the other TACs. Figures 4.3, 4.4 and 4.5 are the solution networks of Szitkai, *et al*. (2006), Emhamed, *et al*. (2007) and the IBMS method respectively.

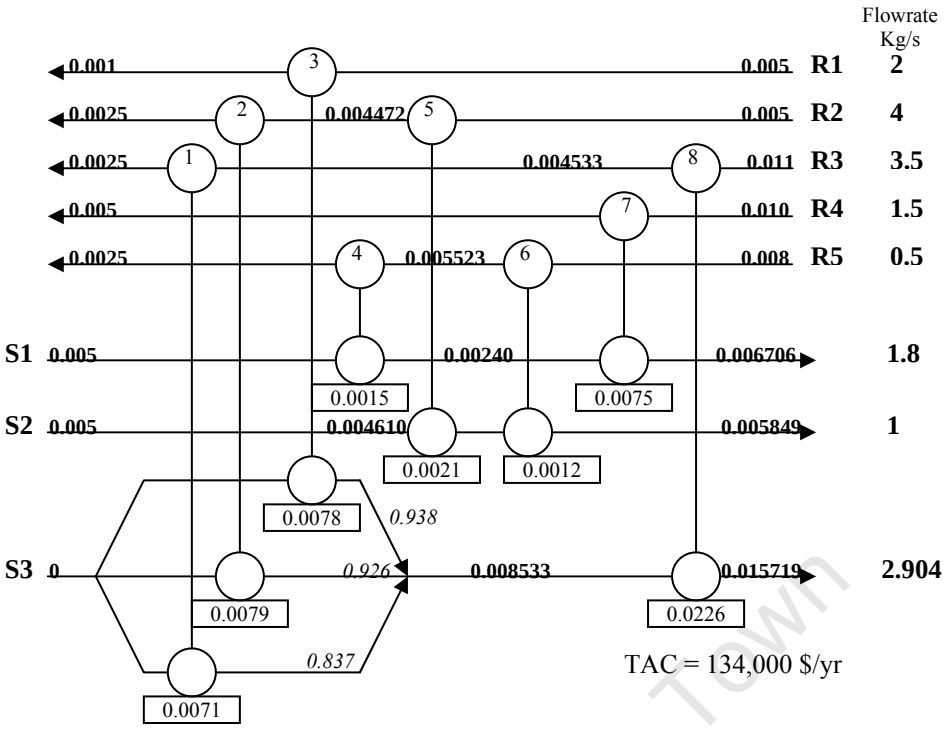


Figure 4.3. Stagewise FLM model network for Example 4.1 as presented by Szitkai, *et al*. (2006) with eight units.

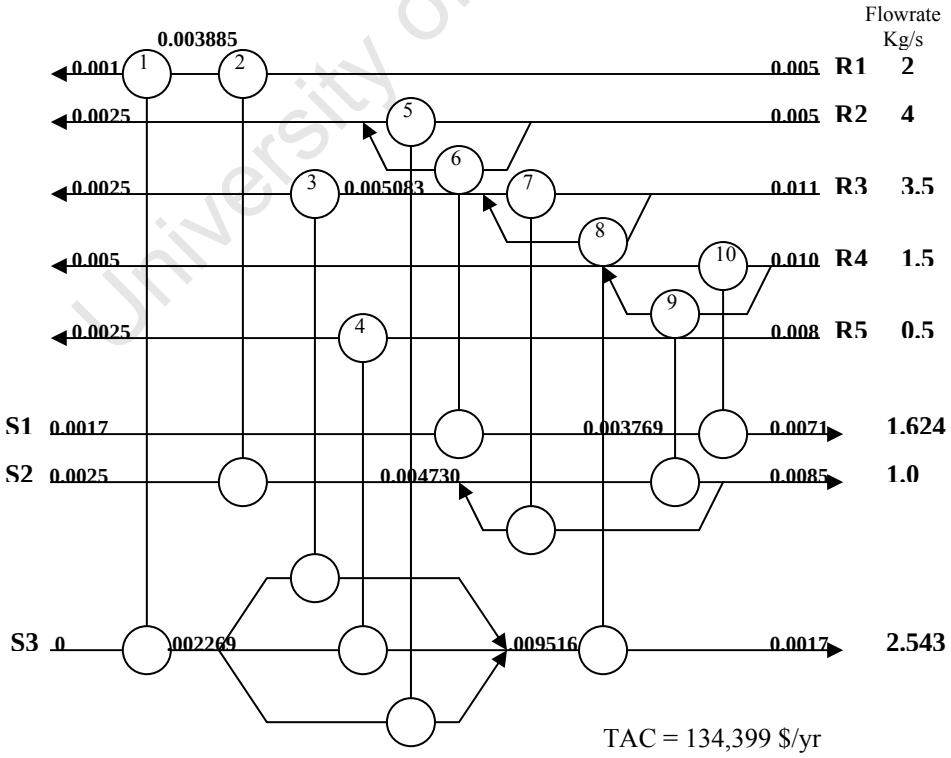


Figure 4.4. Final structure presented by Emhamed, *et al*. (2007) for Example 4.1 featuring ten units and rich and lean stream splits.

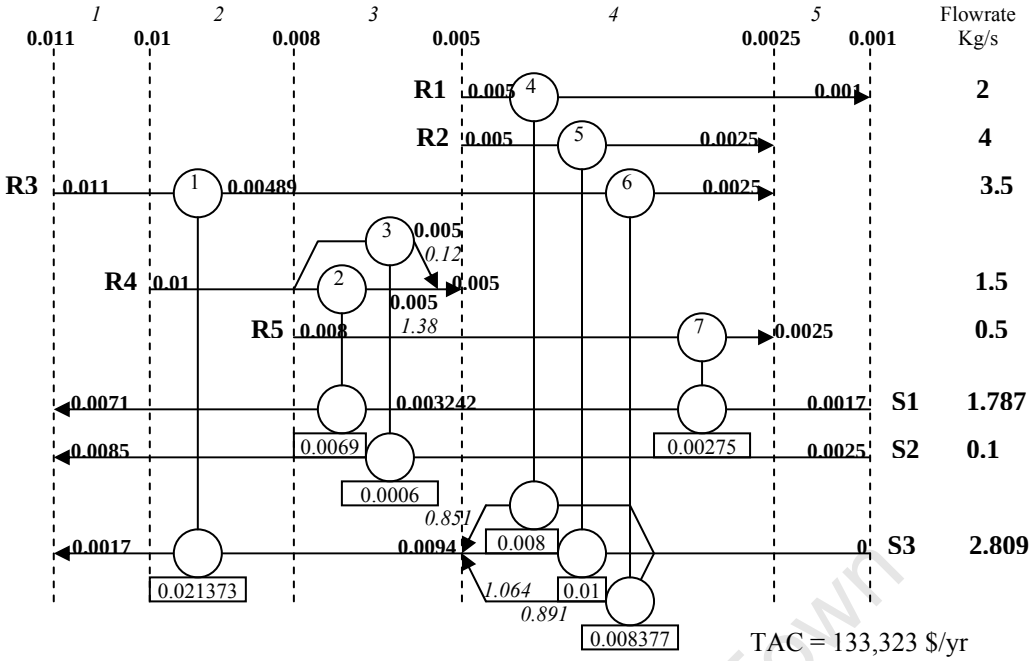


Figure 4.5. IBMS network for Example 4.1 featuring seven units with a 2-way split for a rich stream and a 3-way split for a lean stream.

Note that this solution (Figure 4.5) demonstrates the capability of the IBMS to also split both rich and lean streams as required.

Table 4.1 shows a comparison of the TACs, number of units and splits of the three methods.

Table 4.1: Comparison of the three methods

	FLM model	Hybrid approach	IBMS
Number of units	8	10	7
TAC ($/yr)	134,000	134,399	133,323
Type and number of splits	3-way split of S_3	2-way splits of R_2, R_3, R_4 & S_2 3-way split of S_3	2-way split of R_4 3-way split of S_3

In each of the figures, the intermediate compositions of streams are located at the exit of exchangers on the streams concerned. The mass exchanged in each unit is shown in boxes below the exchangers concerned. S_3 is split three ways in the stagewise FLM network but the individual branch flows were not included by the authors. These have been backcalculated by the current author using the combined outlet composition of 0.008533 and the flows obtained placed next to the splits. The flows do not add up to 2.904 kg/s which is the total flow of S_3 reported. This is due to the isocomposition

mixing assumption of the stagewise FLM model which does not always hold for streams having splits.

The two process lean streams, S_1 and S_2 were used to full capacity in the solution network of the FLM model. This is a feature of the pinch technology method where at least one of the process lean streams is used to full capacity so as to identify the pinch. This kind of solution was still obtained while using the stagewise FLM model in spite of the fact that no distinction was made between the process and external lean streams in terms of flow usage and process/external lean streams positioning in the network. The current author believes that such a solution may have resulted due to an improper initialisation and setting of bounds for the problem.

Another similarity between the networks of the stagewise FLM model in Figure 4.3 and pinch technology networks of Hallale and Fraser (2000a-d) where the conventional costing method is used is that the rich streams are not split. However the exchanger mass targeting method of Hallale (1998) assumes that rich streams can be split in order to meet targets in designs.

Emhamed, *et al*. (2007) got the best solution as 808,986 $/yr in the fourth iteration step of their hybrid approach. This was also recalculated by the current author to give 134,399 $/yr which is shown on Table 4.1. This TAC (134,399 $/yr) is less than 1% higher than that of the stagewise FLM (134,000 $/yr) and 3% less than the pinch TAC_{target}. The hybrid network (Figure 4.4) has a 2-way split on rich streams 2, 3 and 4 and another on S_2, S_3 has a 3-way split.

The IBMS network is shown in Figure 4.5 with a TAC of 133,323 $/yr, which comprises of an AOC of 82,410 $/yr and an ACC of 50,913 $/yr. The IBMS solution is less than 1% lower than the TACs of the stagewise FLM and the hybrid methods. The IBMS network also features the minimum number of units (7) for the problem.

It can be seen that the flow of S_1 was used to full capacity in the hybrid method as well. This is unlike the IBMS network where the onsite capacity of neither of the two process lean streams was used to the fullest. The model which is also fairly linear was easily solved in 0.726 s of CPU time on an Intel Pentium M, 1.7 GHz machine. The

initialisation and setting of bounds was equally straightforward, only the lean stream flows were initialised and given bounds. There was no need initialising or giving bounds to the compositions because the interval based approach for generating the superstructure adequately takes care of this. S_1 and S_3 were given lower bounds of 1 kg/s, S_2 was given 0.1 kg/s since its maximum available flow on site is 1 kg/s. The upper bounds set for S_1 and S_2, the process lean streams was equal to their maximum available flow on site. S_3 on the other hand was given 6 kg/s which is a value large enough for S_3 to take away all the available mass alone.

The split individual flows all add up to the total flow of the parent stream. Note that Figure 4.5 is a rich stream based superstructure. Solving the problem using a lean stream based superstructure gives a similar network with seven units and the same TAC of 133,322 $/yr. The lean stream based interval superstructure is shown in Figure 4.6. The *y** compositions is shown for the lean streams in this figure. The two process lean streams are used to full capacity in this solution. The superstructure is inverted because the lean streams are used to define its intervals.

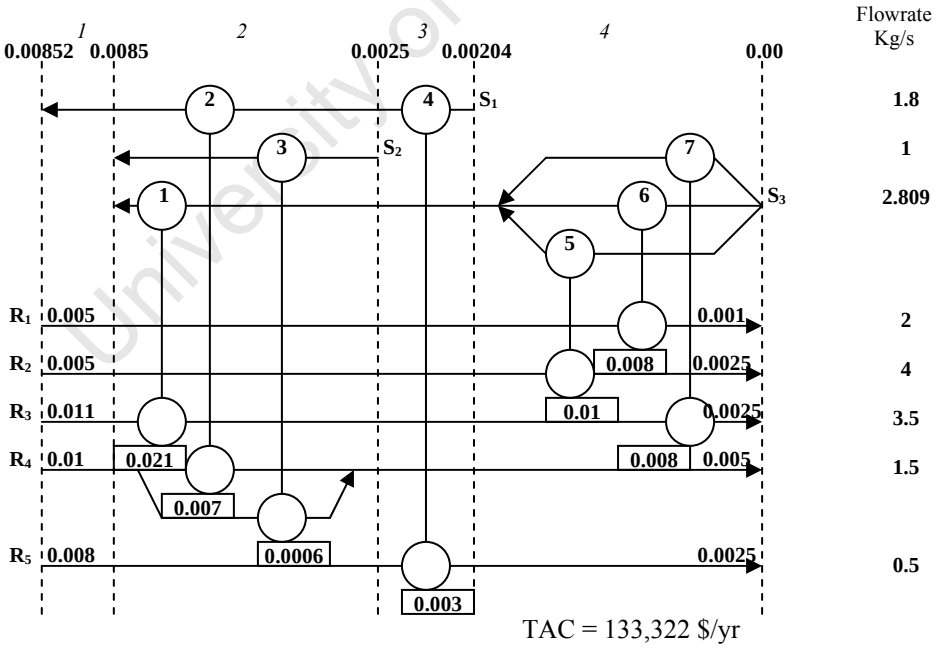


Figure 4.6. Lean stream based IBMS network for Example 4.1 featuring seven units with a 2-way split for a rich stream and a 3-way split for a lean stream.

4.2.3.2 Example 4.2

This example which was first solved by El-Halwagi and Manousiouthakis (1989) by minimising the TAC through minimisation of the number of units is used to demonstrate the ability of the IBMS model for MENS to handle stagewise columns. The problem involves two hydrogen sulphide rich streams (coke-oven, R_1 and tail gas from a Claus unit, R_2). Two MSAs are available for the hydrogen sulphide removal. The first MSA, S_1, which is a process MSA, is aqueous ammonia. The second MSA, S_2, is chilled methanol. S_2 is an external MSA. The stream data are shown in Tables B4 and B5 in Appendix B. The costs of supplying the MSAs have been taken from Papalexandri, *et al*. (1994). The stream flowrates are assumed to be constant (El-Halwagi and Manousiouthakis, 1989). The columns required are stagewise columns and the cost per stage per year ($4552) of Papalexandri, *et al*. (1994) is used to cost these columns.

Hallale and Fraser (2000a) also solved this problem using their MENs capital targeting tools. They also used the $4552 costing to calculate the cost of the columns. The structure generated by Hallale and Fraser (2000a) at the supertargeting optimum minimum composition difference (ε) is shown in Figure 4.7.

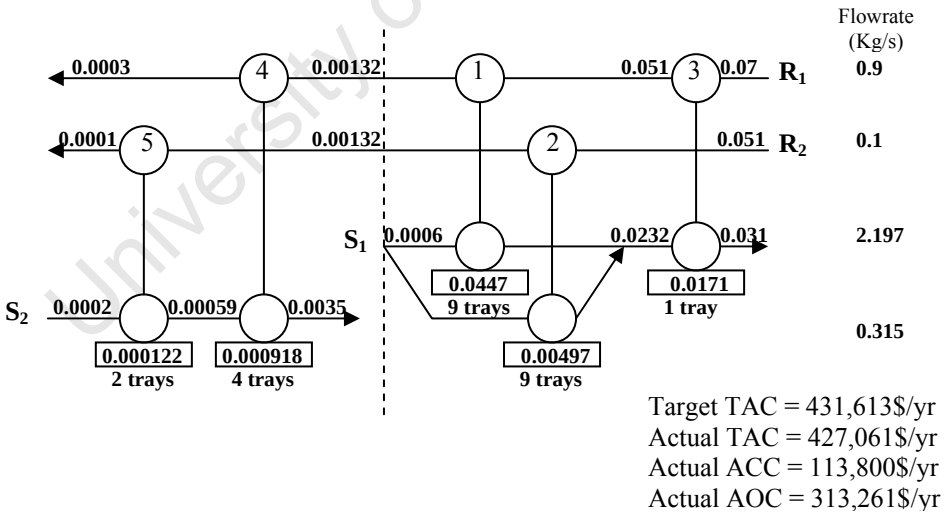


Figure 4.7. Pinch design at the supertarget value of ε for Example 4.2 featuring five units and 2-way split for S_1

The pinch network has a TAC of 427,061 $/yr, five units and a 2-way split of stream S_1.

Applying the IBMS model to this example gives a network with a TAC of 446,840 $/yr, four units and 2-way splits of streams S_1 and S_2. This TAC which was obtained in 3.176s

of CPU time is about 4% higher than the TAC of the pinch method of Hallale and Fraser (2000a). The AOC of the network is 328,488 $/yr while the ACC is 118,352 $/yr. The network is shown in Figure 4.8 using a lean stream based superstructure.

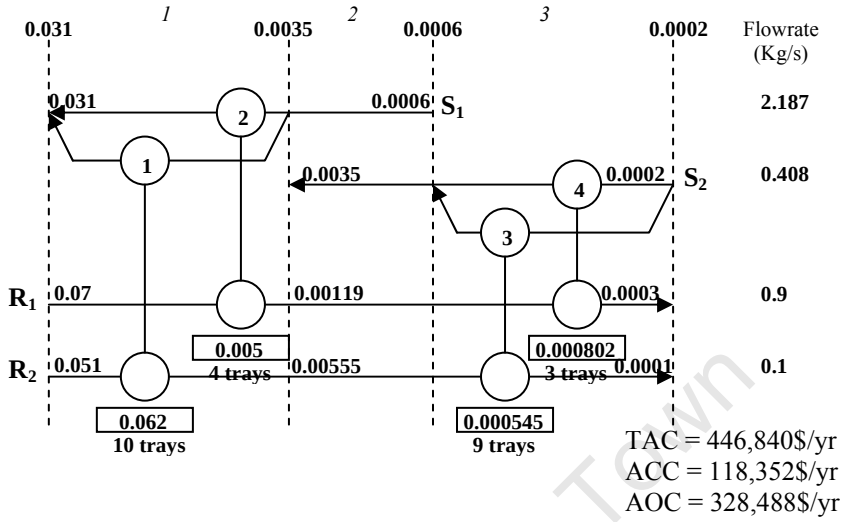


Figure 4.8. IBMS network for Example 4.2 featuring four units with 2-way splits of S_1 and S_2.

Using a rich stream based superstructure gives a network with a TAC of 530,471 $/yr. No explanation can be given as to why the TAC is very different from that gotten with the rich basis. The structure has four units with no stream split. It is shown in Figure 4.9.

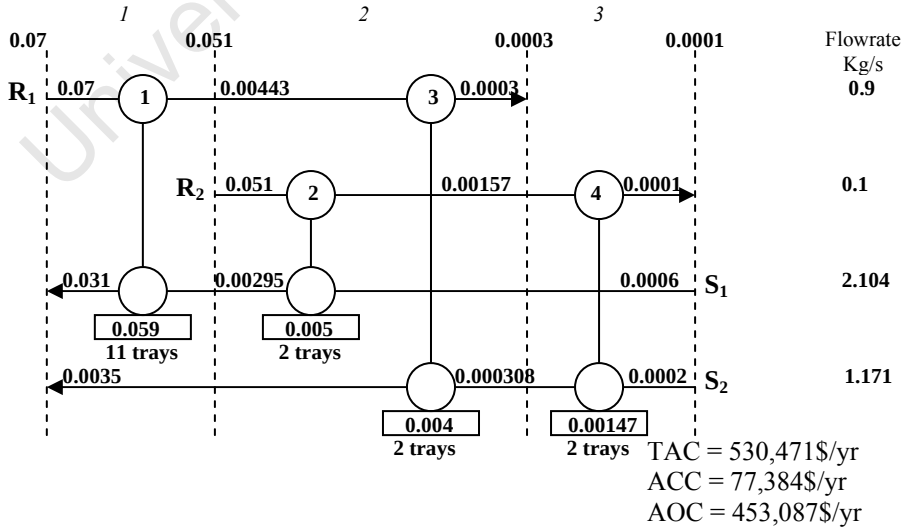


Figure 4.9. Rich stream based superstructure network for Example 4.2 featuring four units with no splits.

4.2.3.3 Example 4.3

This example problem is adapted from El-Halwagi (1997) and it involves two aqueous rich streams, R_1 and R_2 from which phenol has to be absorbed using solvent extraction. Three lean streams, S_1, S_2 and S_3 are available for the phenol removal. S_1 and S_2 (gas oil and lube oil respectively) are process lean streams while S_3 (light oil) is an external MSA. The addition of phenol to the process lean streams is beneficial for them, therefore it is specified that the total flowrate of the gas oil (S_1) should be used. The problem data is presented on Tables B6 and B7 in the appendix. The \$4552 per year per equilibrium stage capital costing method of Papalexandri, *et al*. (1994) has been used for exchanger cost. The annual operating time is 8600 h.

Hallale and Fraser (2000a) applied their MENS capital cost targeting tools to this problem and solved for a TAC scenario. Comeaux (2000) also solved the problem for a TAC with the insight based NLP superstructure. The stream and capital cost data used by Hallale and Fraser (2000a) is also used in this thesis. S_1 and S_2 are available free and the exchanger type is sieve tray columns for all streams.

Hallale and Fraser (2000a) presented a TAC target of 336,312 \$/yr at a Δy_{min} of 0.001. The actual design TAC is 345,416 \$/yr which is 2.6 % higher than the target. The design has seven units and a 2-way split of S_1 immediately below the pinch. The supertarget TAC is 333,716 \$/yr but no design was shown at this target by Hallale and Fraser (2000a). Comeaux (2000) generated two different solutions in terms of structure but similar in terms of TAC. The first network has a TAC of 332,000 \$/yr with eight exchangers while the second network (shown in Figure 4.10) has a TAC of 333,300 \$/yr but has seven exchangers. Comeaux (2000) reported the real number of stages for both solutions.

The IBMS developed in this study was used to solve this example. The model used 2.932 s of CPU time. The values 1kg/s and 0.1 kg/s were given as initial points and lower bounds for S_1 and S_2 while 1 kg/s was used for S_3. The maximum available flows onsite for S_1 and S_2 were used as upper bounds for these streams while 1 kg/s was used for S_3. A lean stream based IBMS model gives a more simplified network having a TAC of 338,168 \$/yr, six units and no stream split. The network is shown in Figure 4.11 with the real number of trays shown. It is worthwhile mentioning that if a big value (as big as

would allow S_3 take away all of the mass load alone) was used as an upper bound to S_3, the TAC will be 358,292 \$/yr. The network in this case will have five units without any stream split.

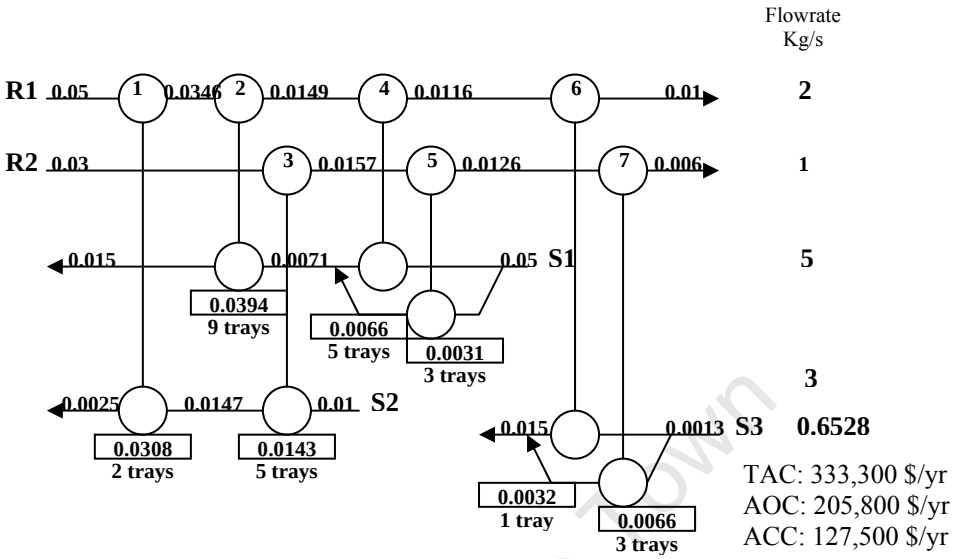


Figure 4.10. Insight based NLP superstructure of Comeaux (2000) for Example 4.3 featuring seven units and 2-way splits for S_1 and S_3.

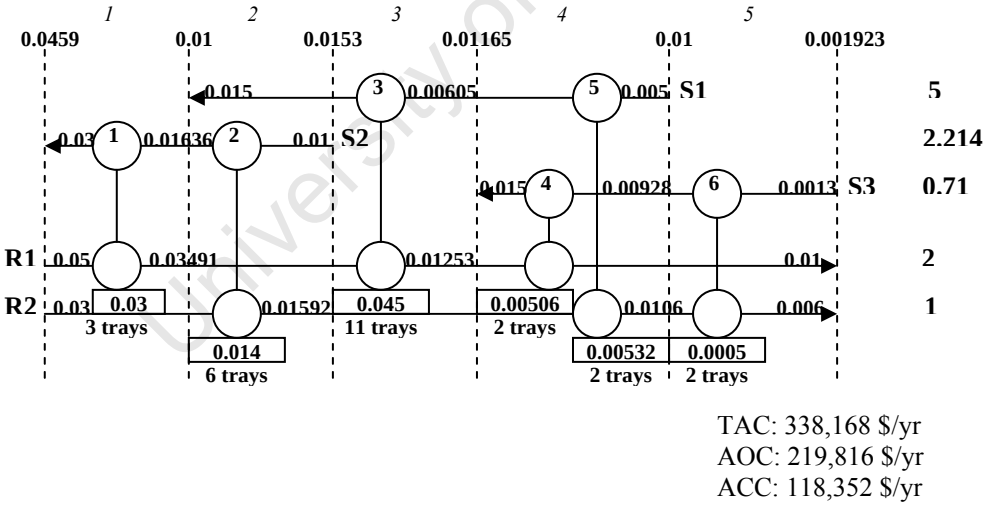


Figure 4.11. Lean stream based IBMS structure for Example 4.3 featuring six units with no stream split.

The IBMS soluiton is just 1.4% higher than the insight based NLP supertsructure of Comeaux (2000) and the pinch supertarget TAC_{target}. The number of units, kinds of splits and TAC of the three methods are shown on Table 4.2.

Table 4.2: Comparison of the three methods for Example 4.3

	Pinch Technology		NLP Superstructure		IBMS	
	Supertarget	Design at Δy_{min}=0.001	Option 1	Option 2	Option 1	Option 2
Units	-	7	8	7	6	5
Splits	-	S_1 split 2-way	S_1 split 2-way twice in series	S_1 & S_3 split 2-way	None	None
TAC ($)	333,312	345,416	332,000	333,300	338,168	358,292

4.2.3.4 Example 4.4

This example involves regenerable MSAs; therefore it will be used to show the applicability of the IBMS model to simultaneously optimise the competing costs in mass exchange regeneration problems. It will also be used to demonstrate the ability of the IBMS model to establish the minimum total costs for problems whose streams require different exchanger types.

The problem, which is taken from Example 3 of Hallale and Fraser (2000d), involves four gaseous phenol rich streams. Light oil S_1 and activated carbon S_2 are available for this phenol removal. S_1 is not regenerable hence it is to be used on a once-through basis while S_2 can be regenerated by stripping it with caustic soda (V_1). The lean streams require different types of exchangers; S_1 requires staged columns while S_2 and V_1 both require continuous contact columns.

The capital costing approach of Papalexandri, *et al*. (1994) for both continuous contact and stagewise columns has been used. 4552 $/yr per equilibrium stage for stagewise columns and 4245 $/yr per height for continuous contact columns. Papalexandri, *et al*. (1994) first solved this problem but did not include the stream mass transfer coefficient. This was backcalculated by Hallale and Fraser (2000d) to give 3.70 kg phenol m^{-3} s^{-1}. The same value has been used in this thesis. The stream data are shown in Tables B8 and B9 in the appendix.

It should be noted that supply (X^s) and target (X^t) compositions for S_2 are not given in the problem data because fixing a value for them prior to the optimisation can lead to a suboptimal solution. This is because the values of X^s and X^t contribute to the flow of regenerant and absorber size to be used based on the compositions Z^s and Z^t for the

regenerant that are however given. The cost presented for S_2 on Table B9 is the cost of using S_2 (notionally represented as cost of regeneration) and not the cost of its flow within the network, unlike the 'once-through' MSAs. This is because the cost of regeneration involves the cost of the regenerating agent and the capital cost of the regenerating column. With the inclusion of regenerant, the S_2 cost equals zero.

Several authors have solved this example (El-Halwagi and Manousiouthakis, 1990b; Papalexandri, *et al*., 1994; Hallale and Fraser, 2000d; Comeaux, 2000 and Chen & Hung, 2005a). Table 4.3 compares the results of the different methods (including the IBMS) that have been applied to solving this problem, while Figure 4.12 illustrates the structure of Comeaux (2000) which is the best in terms of cost and simplicity of layout.

Table 4.3: Summary and comparison of results in Example 4.4.

	Number of units	TAC($/yr)
Papalexandri *et al*. (1994)	6	957 000
Hallale and Fraser (2000d)	8	706 000
Comeaux (2000)	6	688 000
Chen & Hung (2005a)	7	694 000
IBMS	8	689 300

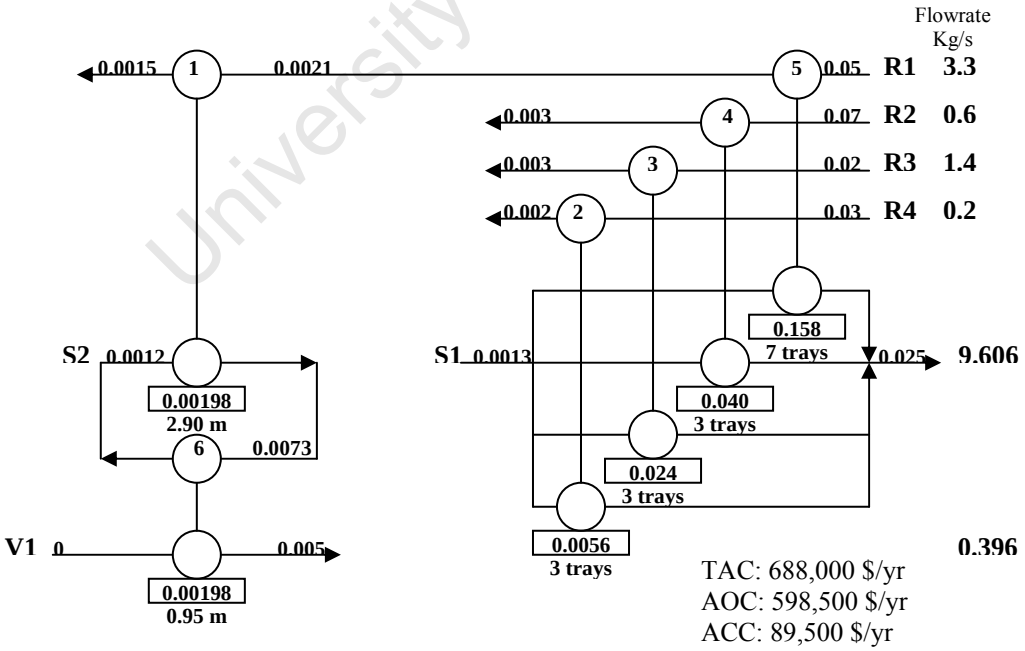


Figure 4.12: NLP solution of Comeaux (2000).

The network of the IBMS method is shown in Figure 4.13. The TAC of the IBMS approach is 689,300 $/yr, the AOC is 609,410 $/yr while the ACC is 79,890 $/yr. The AOC dominates in the problem. Figure 4.13 shows S_1 split in four ways, the flow of each split is shown next to the split concerned. The IBMS solution is within 0.2 % of Comeaux (2000) solution and both networks features a 4-way split of S_1.

4.3 Conclusion and Summary

The interval based MINLP superstructure model partitions a mass exchange network superstructure based on the supply and target compositions of either the rich or lean set of streams. This partitioning approach is unlike the pinch composition partitioning where the network is divided into two thermodynamic independent regions and the intermediate compositions of streams are fixed based on the concept of vertical mass transfer. The intermediate compositions of each stream in the IBMS approach are treated as variables to be optimised. This partitionining approach allows deviation from verticality for the transferred masses in order to establish the minimum total cost network. Defining the entry and exit of the rich or lean streams in the superstructure using stream existence and supply/target composition recognition conditionals helps to eliminate the need to initialise compositions in the model for simple MENS problems.

The stream interval existence and supply/target composition recognition conditionals also ensure that streams are split in intervals where the interval composition boundaries are defined by the supply or target composition of a stream. Due to these conditions in the intervals, such splits are mixed at equal compositions thereby eliminating the need for non linear mass balance and mixing equations.

The IBMS has been demonstrated to give near optimum TAC for mass exchange problems involving continuous contact and stagewise exchangers. The method also efficiently handles problems whose lean streams require different types of columns and those involving regeneration of external MSAs without much difficulty in initialising the MSAs and the regenerating agent.

The solutions presented in this chapter are close to those reported in the literature; they are in some cases better in terms of TAC, number of units or simplicity of the network.

The interval based approach also does not hinder matches from being constrained in terms of preferred or forbidden matches.

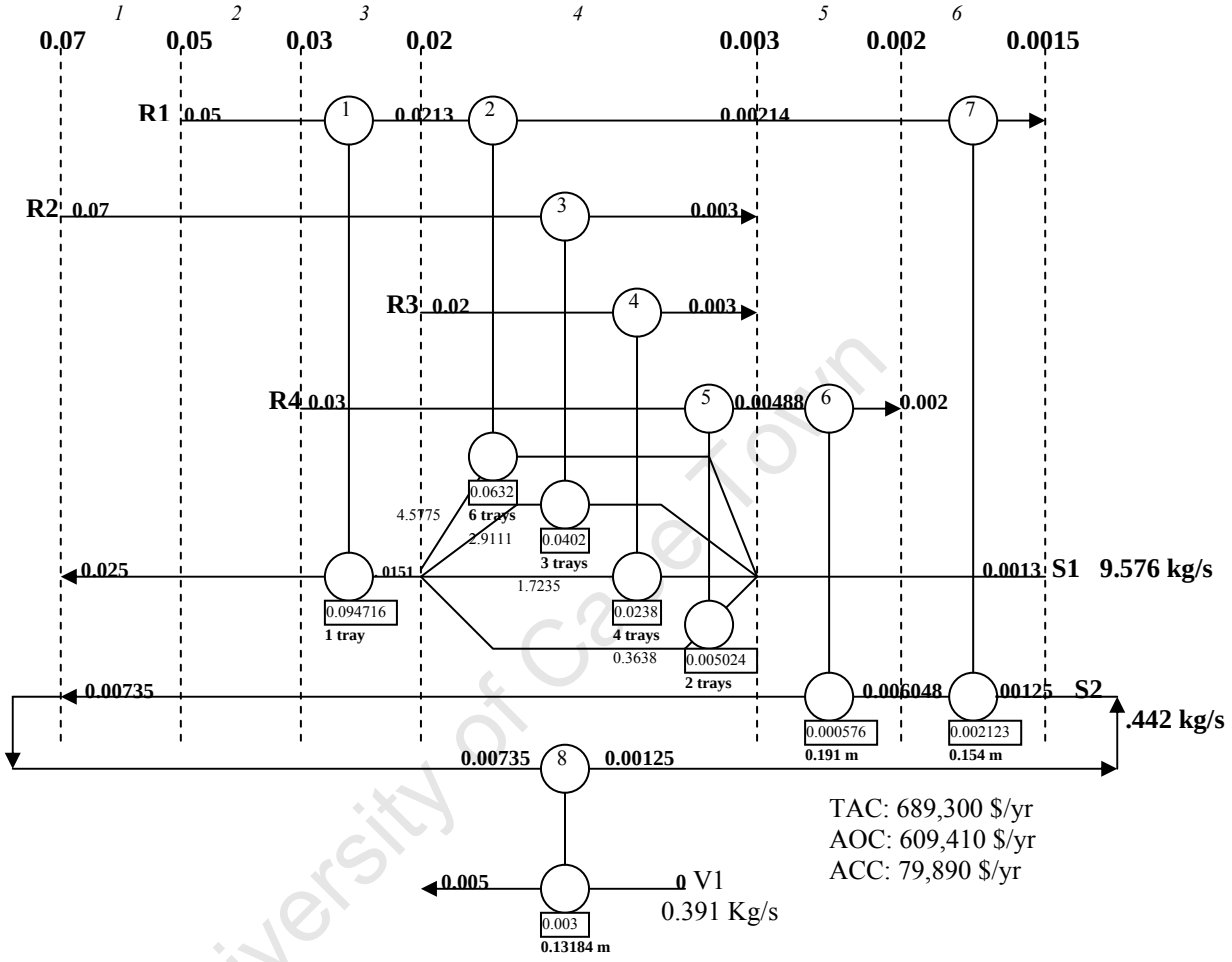


Figure 4.13: IBMS network for Example 4.4 featuring eight units.

CHAPTER 5

EXTENDED APPLICATIONS OF THE HEAT & MASS EXCHANGE IBMS MODELS

5.1 Introduction

Section 5.2 presents the extension of the IBMS method for HENS developed in Chapter 3 to multiperiod heat exchange problems. The model equations as well as an example which demonstrates the applicability of the IBMS model for the synthesis of multiperiod HENs is also presented. The IBMS model for MENS is also extended to problems involving multiple lean streams (process and external) and reactive mass exchange non-linear equilibrium problems in Sections 5.3 and 5.4 respectively. The IBMS equations for both HENS and MENS are combined in Section 5.5 and applied to the synthesis of combined heat and mass exchange network problems. The chapter is concluded in Section 5.6.

5.2 Multiperiod IBMS Framework

The model equations for generating heat exchanger networks that can operate over a specified range of variations in operating parameters are presented in this section. The parameters to be considered in this study include temperatures, flowrates and heat duties. These parameters can be different in each time period. The model equations are an extension of the interval based superstructure framework for nominal conditions to multiperiod scenarios. The extension is accomplished by the inclusion of an index, *p*, which represents each period of operation. The resulting framework is optimised as an MINLP so as to minimise the TAC which includes the annual costs of hot and cold utilities and the annualised cost of the heat exchangers.

5.2.1 Multiperiod IBMS Model Formulation

The following indices, sets, parameters and variables need to be included in the IBMS model for nominal conditions so as to account for the multiple periods of operations.

Sets

P Operation periods

Indices

p index for operation period ($p = 1,\ldots.. NOP$)

Parameters

DOP duration of each period p

NOP number of periods

$T^{s}_{i,p}$ supply temperature of hot stream i for period p

$T^{t}_{i,p}$ target temperature of hot stream i for period p

$T^{s}_{j,p}$ supply temperature of cold stream j for period p

$T^{t}_{j,p}$ target temperature of cold stream j for period p

Ω_{p} upper bound for heat exchanged in match i,j in period p

$\Gamma_{i,j,p}$ upper bound for driving force in match i,j in period p

Positive variables

$A_{i,j,k}$ maximum area of match i,j in temperature interval k

$dt_{i,j,k,p}$ driving force for match i,j in temperature interval k and period p

$F_{i,p}$ flow rate of hot stream i in period p

$F_{j,p}$ flow rate of cold stream j in period p

$q_{ijk,p}$ heat exchanged between hot stream i and cold stream j in temperature interval k and period p

$t_{i,k,p}$ temperature of hot stream i at hot end of interval k in period p

$t_{j,k,p}$ temperature of cold stream j at hot end of interval k in period p

The binary variable for multiperiod operation is the same as that for the nominal condition.

Model Equations

The multiperiod IBMS model equations are presented next, note that the conditionals discussed in Chapter 3 are also included in the same set of equations for the multiperiod scenario.

Overall stream heat balances

An overall heat balance is carried out for each stream so that it will get to its target temperature in each period.

$$\left(T_{i,p}^{s}-T_{i,p}^{t}\right)\cdot F_{i,p}=\sum_{k\in K}\sum_{j\in C}q_{i,j,k,p} \qquad i\in H \quad p\in P \tag{5.1}$$

$$\left(T_{j,p}^{t}-T_{j,p}^{s}\right)\cdot F_{j,p}=\sum_{k\in K}\sum_{i\in H}q_{i,j,k,p} \qquad j\in C \quad p\in P \tag{5.2}$$

Interval heat balance

In order to calculate the temperature for each stream in interval *k* and period *p*, interval enthalpy balances are carried out in each of the intervals and periods.

$$\left(t_{i,k,p}-t_{i,k+1,p}\right)\cdot F_{i,p}=\sum_{j\in C}q_{i,j,k,p} \qquad k\in K,\ i\in H,\ p\in P \tag{5.3}$$

$$\left(t_{j,k,p}-t_{j,k+1,p}\right)\cdot F_{j,p}=\sum_{i\in H}q_{i,j,k,p} \qquad k\in K,\ j\in C,\ p\in P \tag{5.4}$$

Assignment of superstructure interval temperatures

Each temperature location, *k*, in each period, *p*, is recognised using the supply/target temperature recognition conditional and the streams interval existence conditionals presented in Chapter 3. The following conditionals which are problem specific use Figure 3.1 as an illustration but with index *p* included;

$$k=1; \quad T_{H1,1,p}^{s}=t_{H1,1,p},\ T_{C1,1,p}^{t}=t_{C1,1,p},\ T_{C2,1,p}^{t}=t_{C2,1,p} \tag{5.5}$$

$$k=2; \quad T_{H2,2,p}^{s}=t_{H2,2,p} \tag{5.6}$$

$$k=3; \quad T_{H1,3,p}^{t}=t_{H1,3,p} \tag{5.7}$$

$$k=4; \quad T_{H4,4,p}^{s}=t_{H2,4,p},\ T_{C1,4,p}^{s}=t_{C1,4,p},\ T_{C2,4,p}^{s}=t_{C2,4,p} \tag{5.8}$$

Feasibility of temperatures

Temperatures for both hot and cold streams need to decrease from left to right in the superstructure in each temperature location, *k*, and period, *p*. The following equations are used o represent this.

$$t_{i,k,p}\ \geq\ t_{i,k+1,p} \qquad k\in K,\ i\in H \quad p\in P \tag{5.9}$$

$$t_{j,k,p}\ \geq\ t_{j,k+1,p} \qquad k\in K,\ j\in C \quad p\in P \tag{5.10}$$

Logical constraints

Logical constraints are used to relate the existence of a match in interval k and period p with the heat load and its corresponding allowable upper bound heat load (Ω_p). Ω_p can be defined as the smaller of the heat loads of the two streams participating in the match. If a match exists, the binary variable, $z_{i,j,k}$, takes on the value of '1' and the corresponding heat load, $q_{i,j,k,p}$, of the match is restricted based on the Ω_p. If the match does not exist, $z_{i,j,k}$ takes on a value of '0' thereby forcing $q_{i,j,k,p}$ to also be '0'.

$$q_{i,j,k,p} - \Omega_p z_{i,j,k} \le 0 \qquad i \in H,\ \ j \in C,\ \ k \in K \quad p \in P \tag{5.11}$$

Heat exchange area calculation

The approach temperature variables, $dt_{i,j,k,p}$, are introduced to calculate the driving forces at each end of an exchanger in logical constraint equations. If a match i,j exists in interval k and period p, the binary variable z_{ijk} takes on a value of '1' and the corresponding exchanger approach temperature is adequately calculated. If the match does not exist, the binary variable takes on a value of '0' and the equation is inactivated. The presence of Γ_p helps to avoid the inclusion of negative approach temperatures for matches which do not exist. The approach temperature equations are represented as follows;

$$dt_{i,j,k,p} \le t_{i,k,p} - t_{j,k,p} + \Gamma_p \cdot \left(1 - z_{i,j,k}\right) \qquad k \in K,\ \ i \in H,\ \ j \in C \quad p \in P \tag{5.12}$$

$$dt_{i,j,k+1,p} \le t_{i,k+1,p} - t_{j,k+1,p} + \Gamma_p \cdot \left(1 - z_{i,j,k}\right) \qquad k \in K,\ \ i \in H,\ \ j \in C \quad p \in P \tag{5.13}$$

Γ_h can be set as the maximum of zero and each of the temperature differences between the hot and cold streams in the match (Shenoy, 1995).

An exchanger minimum approach temperature (EMAT) is used to limit the approach temperatures on either end of an exchanger in the network. This can be represented as;

$$dt_{i,j,k,p} \ge \varepsilon \tag{5.14}$$

where ε is a small positive number.

The maximum area per period for each exchanger approach of Zhang and Verheyen (2006) is used to calculate the area needed for each exchanger in this study. The continuous variable $A_{i,j,k}$ which was introduced by Zhang and Verheyen (2006)

represents the maximum area of match *i,j* in temperature interval *k*. This area is constrained to be greater than or equal to each of the areas in the periods belonging to temperature interval *k*. The equation is shown below:

$$A_{i,j,k} \geq \frac{q_{i,j,k,p}}{LMTD_{i,j,k,p} \cdot U_{i,j}}, \qquad i \in H, \;\; j \in C, \;\; k \in K, \;\; p \in P \tag{5.15}$$

Aaltola (2003) and Verheyen & Zhang (2006) used the Paterson (1984) LMTD approximation but the Chen's first approximation (Chen, 1987) is used in this study because it gives more accurate predictions of the LMTD and it is shown below:

$$LMTD_{i,j,k,p} = \left[\left(dt_{i,j,k,p}\right) \cdot \left(dt_{i,j,k+1,p}\right) \cdot \left(dt_{i,j,k,p} + dt_{i,j,k+1,p}\right) / 2 \right]^{1/3} \tag{5.16}$$

Objective function

The objective function is the sum of the annual operating costs (hot and cold utility) and capital costs (heat exchanger installation costs and maximum heat exchanger area costs). The equation is shown below having the maximum area per period inequalities included:

$$\begin{aligned} \min \; & \frac{DOP_p}{\sum_{p=1}^{NOP} DOP_p} \sum_{i \in H} CUC \cdot q_{i,j,k,p} + \frac{DOP_p}{\sum_{p=1}^{NOP} DOP_p} \sum_{j \in C} HUC \cdot q_{i,j,k,p} \\ & + \sum_{i \in H} \sum_{j \in C} \sum_{k \in K} CF_{ij} \cdot z_{ijk} + \sum_{i \in H} \sum_{j \in C} \sum_{k \in K} AC_{ij} \cdot A_{i,j,k} \end{aligned} \tag{5.17}$$

Note that the weighting term used in Equation 5.17 is more general because it will give an accurate AOC per period unlike that of Aaltola (2003) and Verheyen and Zhang (2006) shown in Equations 2.28 and 2.32 respectively. The weighting terms of these two sets of authors only accurately gives the AOC per period for problems in which the duration of periods are equal to one another. Also, the inclusion of the maximum area equation (Equation 5.15) which is non linear does not significantly introduce complications involved with solving models having non-linear equations.

5.2.2 Example 5.1

This example is taken from Verheyen and Zhang (2006). It is a HEN problem for a vacuum gas oil (VGO) hydrotreating unit of an oil refinery. The operating data for three periods were presented by Verheyen and Zhang (2006) and they are shown in Table C1 in Appendix C. These periods include: start-of-run (SOR), middle-of-run (MOR) and end-of-run (EOR). Note that the stream heat transfer coefficients were not reported by Verheyen and Zhang (2006), so these were back calculated and an average value of 0.2 $kW^{-1}m^{-2}\ ^0C^{-1}$ was used for all streams in the multiperiod IBMS model. MOR may be greater than SOR and EOR but for this problem, Verheyen and Zhang (2006) assumed that they are equal. However, none of the duration of these periods (*DOP*) was reported by the authors.

The results obtained using the multiperiod IBMS model are shown on Table 5.1 while the network which was generated in 39.813s of CPU time is shown in Figure 5.1. The IBMS GAMS is presented in Appendix D3. Verheyen and Zhang (2006) solved this problem using their model and that of Aaltola (2003). The Verheyen and Zhang (2006) model gives a TAC of 6,320,508 €/yr with twelve units while that of Aaltola (2003) gives a TAC of 6,353,888 €/yr with ten units. It is worth mentioning that since Verheyen and Zhang (2003) did not indicate the duration of each period an assumed value of '1' was used in this study.

The TAC of the network is 7,182,675 €/yr (15.6% above that of Verheyen and Zhang, 2006). The area shown beneath each exchanger in the figure is the maximum area which can transfer heat in all the periods. It can be seen in Table 5.1 that almost all the exchangers in each period use 100% of the maximum area which implies that redundancy is very low in the exchangers (only two are operating below 100% in period 3).

5.3 Multiple process and multiple external lean streams problem: Example 5.2

This example will be used to illustrate the ability of the IBMS for MENS to handle multiple external MSAs and multiple process lean streams. The problem is taken from El-Halwagi (1997) and it involves two rich streams, R_1 and R_2 which are rich in phenol.

Available for the phenol removal are two process lean streams (S_1 and S_2) and four external MSAs (S_3, S_4, S_5 and S_6). The external MSAs are activated carbon, ion exchange resin, air and light oil respectively. El-Halwagi (1997) specified S_3, S_4 and S_5, while S_6 was specified by Hallale (1998). The capital cost of a continuous contact mass exchanger has been assumed in this study to be \$4245 per year per height as presented by Papalexandri, *et al*. (1994). The annual operating time used is 8600 h. The stream data are shown in Tables C2 and C3 in Appendix C.

Table 5.1 Results of multiperiod IBMS model

	Match *i,j,k*	1,1,3	1,1,4	1,2,4	1,5,5	2,5,6	3,1,4	3,5,5	4,3,1	4,4,1
$p = 1$										
A_{max}	m^2	4222	2942	2245	2143	2816	4412	1229	1510	622
A/A_{max}	%	100	100	100	100	100	100	100	100	100
F_h	kW/K	201.6	83.02	118.58	201.6	185.1	137.4	137.4	529.2	182.52
F_c	kW/K	209.4	69.12	141.6	2996.18	4931.4	69.12	1931.27	176.4	294.4
$t_{h,k}$	^{0}C	393	318.48	318.48	141.75	160	354	137.31	500	500
$t_{h,k+1}$	^{0}C	318.48	141.75	141.75	60	40	137.31	60	450	450
$t_{c,k}$	^{0}C	356	284.26	210	10	4.5	284.26	10	370	284
$t_{c,k+1}$	^{0}C	284.26	72	62	4.5	0	72	4.5	220	253
q	kW	15023	14672	20956	16479	22212	29773	10622	26460	9126
$p = 2$										
A_{max}	m^2	4222	2942	2245	2143	2816	4412	1229	1510	622
A/A_{max}	%	100	100	100	100	100	100	100	100	100
F_h	kW/K	205	82.16	122.84	205	198.8	136.4	136.4	526.2	254.96
F_c	kW/K	210.3	65.57	141	3475.65	5349.29	144.73	1873.97	175.4	318.7
$t_{h,k}$	^{0}C	406	323.81	323.81	153.93	160	362	136.11	500	500
$t_{h,k+1}$	^{0}C	323.81	153.93	153.93	60	40	136.11	60	450	450
$t_{c,k}$	^{0}C	365	284.88	210	10	4.46	284.88	10	370	290
$t_{c,k+1}$	^{0}C	284.88	72	62	4.46	0	72	4.46	220	250
q	kW	16848	13958	20868	19255	23856	30811.02	10381	26310	12748
$p = 3$										
A_{max}	m^2	4222	2826	1958	2143	2816	4412	1229	1510	622
A/A_{max}	%	100	96	87	100	100	100	100	100	100
F_h	kW/K	208.5	88.35	120.15	208.5	175.2	134.1	134.1	523.5	200.69
F_c	kW/K	211.1	72.21	140.5	3381.3	5197.9	138.89	1816.8	174.5	271.2
$t_{h,k}$	^{0}C	420	329.64	329.64	156.57	160	360	140.68	500	500
$t_{h,k+1}$	^{0}C	329.64	156.57	156.57	60	40	140.68	60	450	450
$t_{c,k}$	^{0}C	373	283.75	210	10	4.05	283.75	10	370	286
$t_{c,k+1}$	^{0}C	283.75	72	62	4.05	0	72	4.05	220	249
q	kW	18840	15289	20794	20135	21024	29410	10819	26175	10034

The following terms are used in Table 5.1:

A_{max} is the exchanger with the maximum area in the three periods

A/A_{max} is the ratio of each area to the maximum area in each period

F_h is the flowrate of hot stream through exchangers

F_c is the flowrate of cold stream through exchangers

$t_{h,k}$ is the inlet temperature of hot stream in heat exchanger

$t_{h,k+1}$ is the exit temperature of hot stream from heat exchanger

$t_{c,k}$ is the exit temperature of cold stream from heat exchanger

$t_{c,k+1}$ is the inlet temperature of cold stream in heat exchanger

q is the heat load of heat exchanger

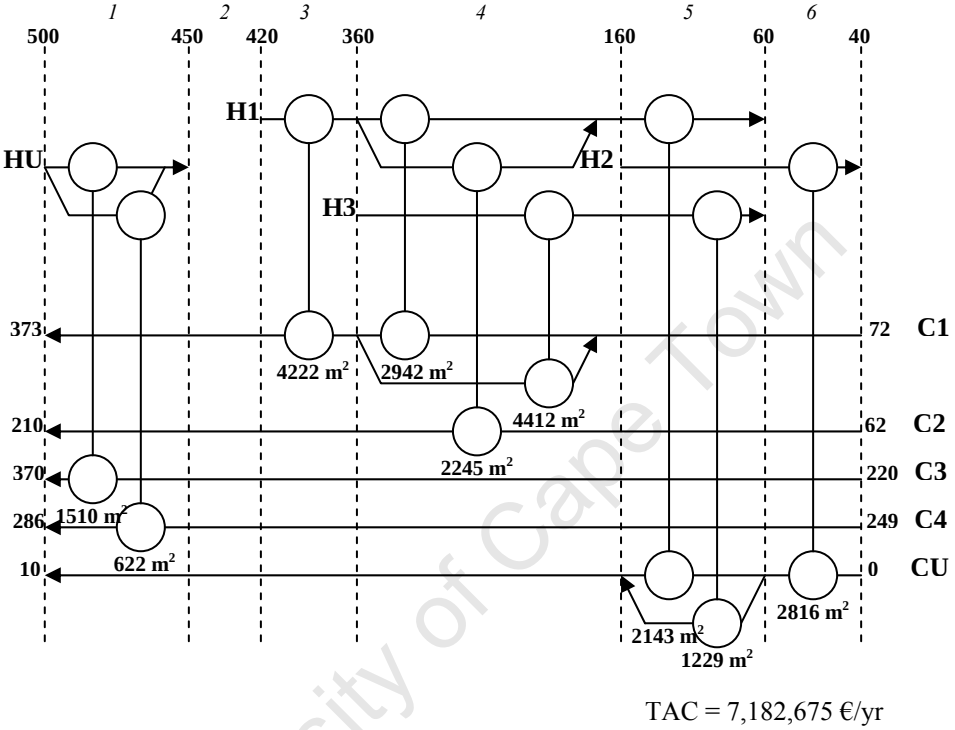


Figure 5.1: Multiperiod IBMS structure for Example 5.1.

Fraser, *et al*. (2005) used the MENS GCC to establish the best MSA (or set of MSAs) to use to accomplish the removal task. No capital cost data was presented by either El-Halwagi (1997) or Fraser, *et al*. (2005). The two sets of authors only solved the problem for an AOC scenario. The effect of the capital items was not considered in the optimisation. However the ACC can contribute significantly to the TAC of the network as it is in the case of HENS problems having multiple utilities (Shenoy, *et al*, 1998 and Isafiade and Fraser, 2007).

The minimum composition difference in the lean phase (ε_{min}) used by El-Halwagi (1997) was 0.001 for every lean stream. Fraser, *et al*. (2005) on the other hand used 0.000255 which is the optimum found through supertargeting by Hallale (1998) for the minimum composition difference in the rich phase ($\Delta y_{\min}$). Note that the supertargeting done by

Hallale (1998) only involves S_1, S_2 and S_6. Fraser, *et al*. (2005) used this value to generate the MENS GCC with R_1 and R_2 and just S_1 and S_2 as the lean streams. The Δy_{min} was further used to establish the analogous ε_{min} values for the six MSAs. In the problem statement, no target value was specified for S_4, El-Hawagi (1997) choose 0.186 while Fraser, *et al*. (2005) choose 0.170 based on the pinch composition. The reason these values are not the same is due to the difference in ε_{min} used by both sets of authors. The workers argued based on the fact that pinch technology requires that no mass should be transferred to above the pinch region. Doing this will translate to using an external MSA (which costs money) to remove mass that could be removed by a process lean stream for free.

It should be noted that not transferring mass to above the pinch could be counterproductive because process lean streams usually have smaller driving forces since they normally create the pinch. This is unlike the external lean streams which may cost more but have higher driving forces. Smaller driving forces translate to higher capital costs. For this reason preference should not be given to any lean stream in terms of its flow usage or positioning in the network. This brings to the fore one of the reasons for which pinch technology for MENS is regarded as not establishing a simultaneous trade-off among the costs for problems with multiple external MSAs. The use of a mass exchange analogue of CUP for HENS by Shenoy, *et al*. (1998) will also fail to give a guarantee of the optimal result because the CUP is also based on pinch technology.

A value which was high enough and thermodynamically feasible (0.510) has been used for the target composition of S_4 in this study. As mentioned earlier, the IBMS approach does not involve partitioning the problem at the pinch, so the process and external lean streams are allowed the same opportunity for absorbing mass from the rich streams based on thermodynamic feasibility.

The IBMS solution for this example is a network having a TAC of 608,501 \$/yr and nine units. The solution was generated in just 0.714s of CPU time. The TAC comprises of an AOC of 482,514 \$/yr and an ACC of 125,987 \$/yr. S_3 was the only external MSA used significantly (0.19 kg/s), the other MSA flows were equal to the values given as their lower bounds (0.01 kg/s) in the model. This implies that they can easily be eliminated from the set of potential external MSAs to be further considered. The best set of MSAs

presented by Fraser, *et al*. (2005) is S_6 and S_3 while El-Halwagi found only S_3 to be the best (though based on only AOC synthesis).

The AOC dominates in this problem, this can be cited as the reason for which there is no significant difference in the solutions presented by the three methods in terms of external MSA to be used. When S_4, S_5 and S_6 are eliminated from consideration in the IBMS model, a network having a TAC of 604,377 \$/yr and five units is obtained. The network is shown in Figure 5.2.

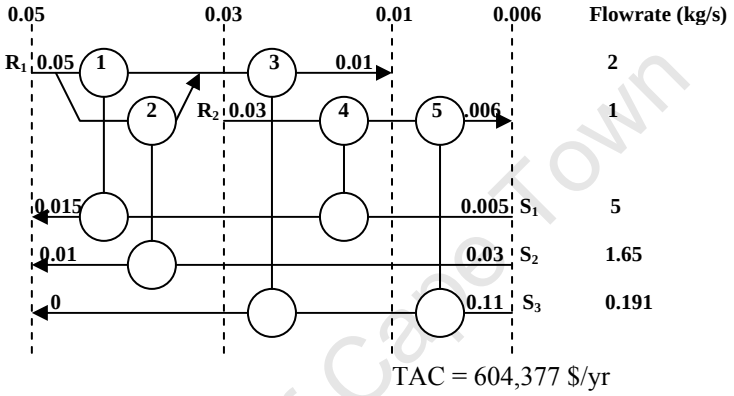


Figure 5.2. IBMS network for Example 5.2.

5.4 Reactive Mass Exchange, Non-Linear Equilibrium Problem: Example 5.3

The applicability of the IBMS model to the synthesis of MENs problems having non-linear equilibrium relations is illustrated through the use of an example. This example which was first introduced by El-Halwagi and Srinivas (1992) involves two gaseous streams (R_1 and R_2) from which H_2S has to be removed in rayon production. Available for this removal are three MSAs: caustic soda (S_1), diethanolamine (S_2) and activated carbon (S_3). Caustic soda is a process lean stream with no cost attached to its use. The stream data is shown in Tables C4 and C5 in Appendix C. The flowrates and compositions are expressed as m^3/s and $kmol/m^3$ respectively. The equilibrium relations for the lean streams as given by El-Halwagi and Srinivas (1992) are shown below:

S_1: $y = 1.945E-9\left(10^{0.529x_1}\right)$ (5.18)

S_2: $y = 7.7545E-4\left(x_2\right)^2$ (5.19)

$$S_3: \quad y = 0.015x_3 \tag{5.20}$$

Equations 5.18 and 5.19 are non-linear, convex relations in which reaction occurs while Equation 5.20 is linear. Continuous contact packed columns with 1m diameter have been assumed for the mass exchangers as done by Papalexandri, *et al*. (1994). Hallale (1998) backcalculated the overall mass transfer coefficient and got 1.70 kmol H_2S m^3/s which was assumed to be constant.

This problem has also been solved by Papalexandri, *et al*. (1994), Hallale and Fraser (2000d), Comeaux (2000) and Chen & Hung (2005a). Papalexandri, *et al*. (1994) applied their hyperstructure MINLP model and presented a network with a TAC of 11,273,500 \$/yr. According to Hallale and Fraser (2000d), the use of a lower bound on composition differences forced the use of S_3, the most expensive MSA. The network of Hallale and Fraser (2000d) which has a TAC of 28,000 \$/yr uses only S_1 at the optimum ε. Comeaux (2000) got the same network and TAC as Hallale and Fraser (2000d) while Chen and Hung (2005a) got the same network as Papalexandri, *et al*. (1994). The network of Papalexandri, *et al*. (1994) is shown in Figure 5.3 while that of Hallale and Fraser (2000d) is shown in Figure 5.4.

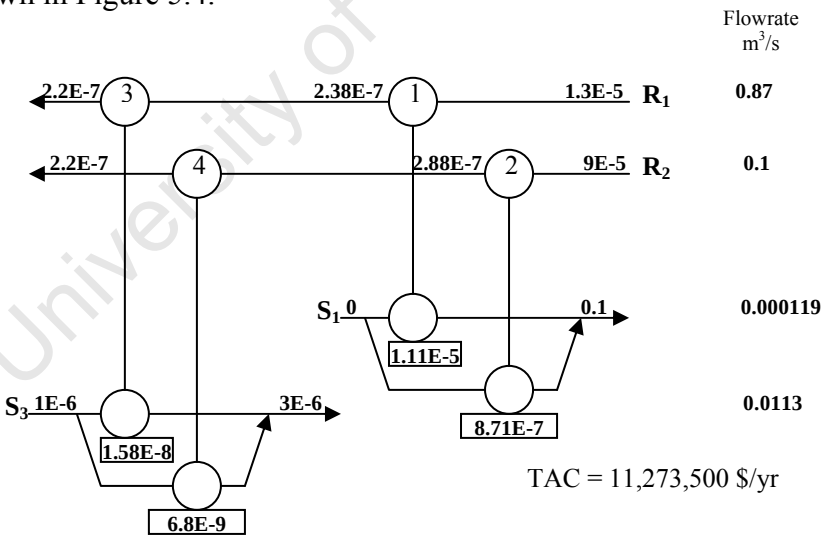


Figure 5.3. Optimum network for Example 5.3 as presented by Papalexandri, *et al*. (1994).

A rich stream IBMS gives a solution with the same TAC as that of Hallale and Fraser (2000d) and Comeaux (2000) but a different network structure without a split. This network is shown next in Figure 5.5.

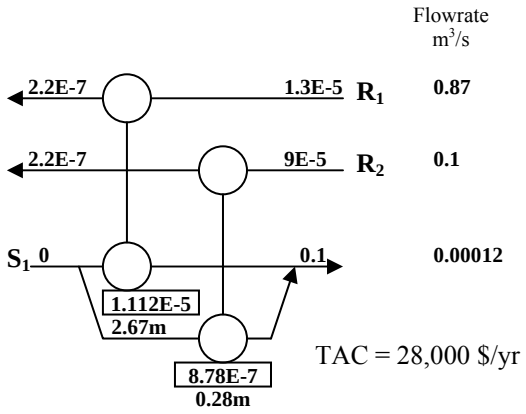


Figure 5.4. Optimum network for Example 5.3 as presented by Hallale and Fraser (2000d).

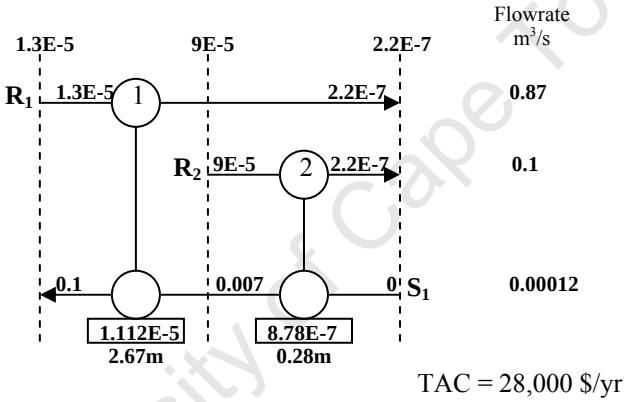


Figure 5.5. Rich stream based IBMS for Example 5.3 featuring two units.

5.5 IBMS SYNTHESIS OF COMBINED HEAT AND MASS EXCHANGE NETWORKS (CHAMENS)

This section presents the application of the HENS and MENS IBMS models generated in Chapters 3 and 4 respectively to the synthesis of combined heat and mass exchange networks. The MEN is only regarded as interacting with the HEN through lean streams whose equilibrium relations are temperature dependent. The task of selecting an optimal mass exchange temperature for a lean stream requires heating or cooling of such a stream. This implies that the lean flow, L, in Equations 4.8 and 4.10 (Chapter 4) is multiplied by its heat capacity and serves as the stream flow, F, in the hot/cold streams heat balance equations (3.7 to 3.10). The following assumptions are made:

- Every mass exchanger (with the streams passing through) operates isothermally
- Only the lean streams can assume different mass exchange temperatures
- Within the working temperature and composition ranges, the equilibrium relations are monotonic functions of the temperatures of the lean streams (El-Halwagi, 1997).

The lean substream approach of Srinivas and El-Halwagi (1994) is applied in this study to establish the optimal mass exchange temperature for lean streams. The lean substream concept requires that each lean stream be split into ND_l lean substreams. Each lean substream $S_{l(dl)}$ is a part of the lean stream l whose composition and temperature vary between a supply value of (x_l^s, T_l^s) and a target value of (x_l^t, T_l^t) with a flowrate of $L_{l(dl)}$. Each substream does not split or mix with other substreams. The optimisation task is to identify the optimal mass exchange temperature $T_{l(dl)}^*$ and flowrate $L_{l(dl)}$. The temperature of each substream lies within the working temperature range of the parent lean stream, l and the number of substreams chosen is dependent on the level of accuracy required. It should be noted that the implementation of this approach in IBMS models requires that the mass and heat exchange needs of each substream is analysed in a sequential manner.

The necessary model equations are described next.

Overall stream heat balance equations for CHAMENS

The hot and cold streams heat balance equations shown in Equations 5.21 and 5.22 represent the heating and cooling requirements of the leans streams, for other streams heating and cooling model equations, the equations presented in Chapter 3 apply.

$$\left(T_l^s - T_{l(dl)}^t\right) \cdot L_{l(dl)} = \sum_{k \in K} \sum_{j \in C} q_{l(dl)j,k} \qquad dl \in l \quad l \in S \tag{5.21}$$

$$\left(T_{l(dl)}^t - T_l^s\right) \cdot L_{l(dl)} = \sum_{k \in K} \sum_{i \in H} q_{i,l(dl),k} \qquad dl \in l \quad l \in S \tag{5.22}$$

Equation 5.21 applies to a lean substream which is being cooled from the parent stream supply temperature, T_l^s, to the lean substream mass exchange temperature, $T_{l(dl)}^t$ while

5.22 represents the same lean substream which is being heated back from its mass exchange temperature $T^t_{l(dl)}$ to its parent lean stream supply temperature, T^s_l. Note that the index *i* representing a hot stream is replaced with the indices *l* and *dl* representing a lean stream and its substream. The stream flowrate is also represented as $L_{l,dl}$, the flowrate of lean substream.

Interval heat balance

The index *i* and *j* in interval heat balance equations are also replaced with the index *dl* for both hot and cold streams.

$$\left(t_{l(dl),k} - t_{l(dl),k+1}\right) \cdot L_{l,(dl)} = \sum_{j \in C} q_{l(dl),j,k} \qquad dl \in l,\ l \in S,\ k \in K \tag{5.23}$$

$$\left(t_{l(dl),k} - t_{l(dl),k+1}\right) \cdot L_{l,(dl)} = \sum_{i \in H} q_{i,l(dl),k} \qquad dl \in l,\ l \in S,\ k \in K \tag{5.24}$$

Note that the lean substream $S_{l(dl)}$ in Equation 5.23 is a hot stream exchanging heat with a cold stream *j* while in Equation 5.24 it is a cold stream exchanging heat with a hot stream *i*.

The remaining set of IBMS equations equally has the substreams represented as hot/cold streams in the relevant equations so they will not be repeated here. However the objective function which simultaneously minimises the capital and operating costs of the mass (including regeneration) and heat exchange networks is presented.

min

$$\left\{\sum_{l \in S}(AC_{dl}) \cdot (L_{dl}) + \sum_{r \in R}\sum_{dl \in l}\sum_{b \in B} CB_{r,dl} \cdot z_{r,dl,b} + \sum_{r \in R}\sum_{dl \in l}\sum_{b \in B} ACH_{r,dl} \cdot \left[M_{r,dl,b} / K_W \left\{LMCD_{r,dl,b}\right\}\right]^{D_{r,dl}} + WT\right\}$$

$$+\left\{\sum_{v \in V}\left(AC_v\right) \cdot \left(QR_v\right) + \sum_{dl \in l}\sum_{v \in V}\sum_{b \in B} CB_{dl,v} z_{dl,v,b} + \sum_{dl \in l}\sum_{v \in V}\sum_{b \in B} ACH_{dl,v}\left[\left(Z^t_{v,b=1} - Z^s_{v,b=last}\right) \cdot VR_v \middle/ K_W \left\{LMCD_{dl,v,b}\right\}\right]^{D_{dl,v}}\right\}$$

$$+\left\{\sum_{dl \in l}\sum_{k \in K} CUC \cdot q_{l(dl),j,k} + \sum_{dl \in l}\sum_{k \in K} HUC \cdot q_{i,l(dl),k} + \sum_{i \in H}\sum_{dl \in l}\sum_{k \in K} AC_{i,l(dl)} \cdot \left[q_{i,l(dl),k} \middle/ U_{i,l(dl)} \cdot LMTD_{i,l(dl),k}\right]^{AE_{i,l(dl)}}\right\} \tag{5.25}$$

The terms in the first parenthesis in Equation 5.25 describe the minimisation of the mass exchange network involving continuous contact columns. The *WT* term is described in Equation 4.24 in Chapter 4. Model equations for stagewise columns can also be included as done in Chapter 4. Also, lean streams have been replaced by the substream, *dl*. The second parenthesis represents the minimisation of the regeneration network where the regenerable lean stream has been replaced by the substream *dl*. The third parenthesis represent the heat exchange network minimisation. The first and second terms in this parenthesis represent a substream, *dl*, exchanging heat with cold and hot utility streams respectively. The third term represents a case where the substream, *dl*, is a cold stream exchanging heat with a hot stream. The reverse equation for a hot substream can also be included.

5.5.1 Example 5.4

This example is generated in this thesis so as to convey the ability of the combined IBMS models to optimise combined heat and mass exchange networks. It should be noted that the approach presented is not exhaustive in establishing the optimal network but it demonstrates the interaction between MEN and HEN through the lean stream. The example involves the four SO_2 rich streams and one lean stream (water) presented by Hallale and Fraser (1998), however the flowrates of the rich streams for this study are different. Also no supply or target composition is specified for the lean stream because these parameters are variables to be optimised by the model since regeneration of the lean stream is involved. The stream and equipment data are shown in Tables C6 to C9 in Appendix C.

The lean stream was discretised into five substreams with the following temperatures: 284, 288, 293, 298 and 303 K. The temperature dependent equation $Y^* = (0.053T\text{-}14.5)X$ (El-Halwagi, 1997) is assumed to be applicable within the temperature range considered for mass exchange. The solutions obtained for different mass exchange temperature options are shown in Table 5.2.

Table 5.2: CHAMENS TAC for Example 5.4

Substream temperature, $T_{l,dl}$ (K)	EMCD	MEN ACC	Regeneration TAC	HEN TAC	CHAMENS TAC
303	0.0040	644 372	148 850	144 495	937 719
298	0.0025	638 737	148 850	130 216	917 804
293	0.0025	651 291	148 850	157 905	958 048
288	0.0026	640 212	148 850	201 312	990 376
284	0.0020	600 809	148 850	290 311	1 039 971

TAC in $/yr

The search approach for the optimum can only be regarded to be exhaustive within each mass exchange temperature option since there is no simultaneous optimisation across the mass exchange temperature options. The TAC for regeneration does not change since the supply and target compositions of the regenerant and the mass load to be taken up by it are fixed. The optimum EMCD for each option of mass exchange temperature does not vary significantly, except for that at 303K. The MEN ACC decreases from 303K option to 298K after which it increases at 293K and then decreases again starting from 288 K. The HEN TAC experiences a minimum at 298K mass exchange temperature, the best CHAMENS TAC is also at this temperature.

The CHAMENS TAC of operating the mass exchange at 300K and 296K were further investigated and these gave 922,353 $/yr and 921,294 $/yr respectively. This shows that 298K is the optimum temperature to use. It represents a savings in TAC of 2.1% relative to the base case (303K). The result is surprising in that it was expected that the TAC would decrease with decreasing temperature till the lowest possible value. The network of the 298K mass exchange temperature which comprises of four mass exchange units, one regeneration unit, one cooler and one heater is shown in Figure 5.6.

5.6 Conclusion

This chapter has demonstrated the applicability of the IBMS to HENS problems involving multiperiod operations and MENS problems involving multiple lean streams (process and external), non-linear equilibrium relations and combined heat and mass exchange networks. The initialisation and bound setting for each problem is very straight forward except for the combined heat and mass exchange problem where compositions (supply and target) for the regenerable lean stream had to be initialised and bounded.

The IBMS model for multiperiod heat exchange operation and that for combined heat and mass exchange networks as mentioned earlier cannot be said to be exhaustive in the search for the best solution network. Nevertheless they can readily be used to make quick assessment of designs or even to initialise the more computationally intensive hyperstructure MINLP models.

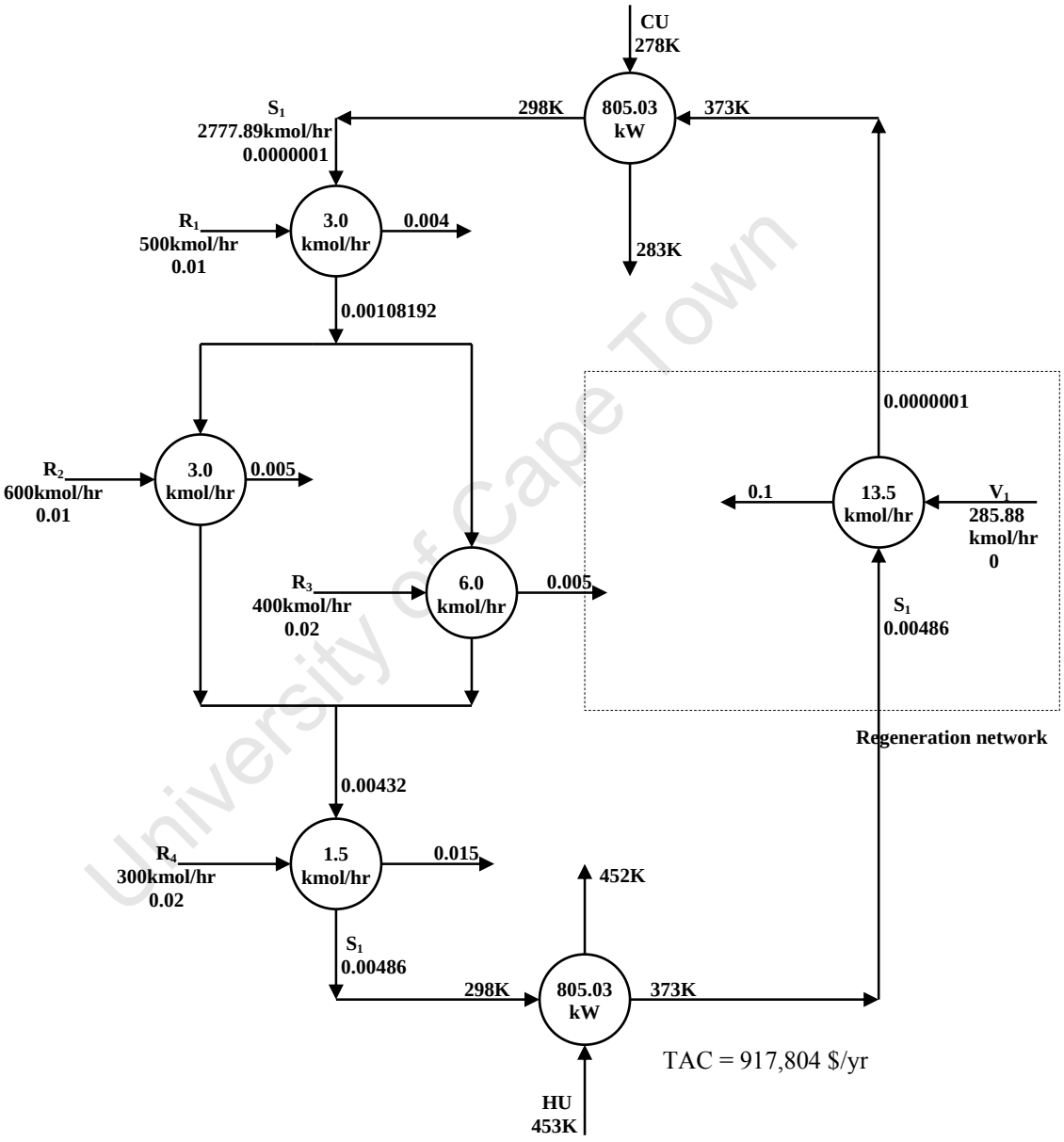


Figure 5.6. IBMS CHAMENS network for Example 5.4.

CHAPTER 6

CONCLUSIONS

6.1 Highlights

This thesis has presented new synthesis techniques for calculating the minimum total annual costs for heat and mass exchange networks. The method is based on partitioning superstructures using key variables such as temperature for heat exchange networks (HENs) and composition for mass exchange networks (MENs). The new synthesis method which is known as the interval based MINLP superstructure (IBMS) has the following characteristics and advantages over previous synthesis methods for heat and mass exchange networks.

1. The interval based superstructure is simplified since it excludes the non-linear heat (and mass) balance mixing and bypass equations, hence near minimum total cost solutions can be generated in reasonable times.

2. Partitioning the superstructure on the basis of temperature/composition helps to simplify the initialisation and bound setting for the variables. For simple heat exchange problems (including those with multiple utilities), only utility flows need to be initialised and bounded with small and big values while for simple mass exchange problems (including those with multiple lean streams), only the lean stream flows need to be initialised and bounded. More complex mass exchange networks such as those involving regeneration require the initialisation of the supply and target compositions of the regenerable lean streams as well.

3. The temperature/composition defining approach of the superstructure helps make the transfer of heat/mass within the intervals to approach a vertical profile. This implies that streams with significantly different heat transfer coefficients can be effectively handled. This is possible since the temperature/composition of streams crossing temperature/composition locations not defined by them are treated as variables to be optimised in such locations. Also, in this superstructure defining method there is a simultaneous trade-off among the costs which contribute to the total cost.

4. An exchanger minimum approach temperature/composition is imposed on the model so as to avoid the inclusion of exchangers of infinite sizes in the solutions. This implies that networks are not restricted to a fixed heat recovery approach temperature

or minimum composition difference. Hence, the optimum temperature and composition difference on each side of every exchanger is found based on economics.

5. For the IBMS for MENS, no restriction is placed on which side of the network the external lean streams need to be used as is done in the pinch approach. All lean streams (both process and external) are given equal opportunity to absorb mass from the rich streams based on economics. This allows for a proper trade-off between alternative process and external lean streams.

6. The IBMS model can handle heat and mass exchanger cost functions which are non linear and also have fixed charges. This is due to the inclusion of binary variables in the model. The presence of the binary variables in the model does not significantly increase the complexity of the model since the approach used to define the superstructure helps to reduce the search space. This IBMS also adequately calculates the minimum total costs when cost functions based on exchanger mass are used for continuous contact columns.

7. The IBMS model minimises total annual costs and at the same time generates a network design. Also restrictions or preferences can be placed on matches.

8. A key feature of the IBMS model is its ability to automatically mix split streams at equal temperatures/compositions due to the fact that every temperature/composition location in the superstructure corresponds to the supply and target of either the hot/rich or cold/lean streams. A benefit of such equal temperature/composition mixing is that near minimum solutions can be generated in single step without the need to solve an NLP suboptimisation step in order to determine split flow and temperatures. Isothermal/isocomposition mixing of streams has a disadvantage in that the search space is limited because split branches cannot go through multiple exchangers in series and problems in which the optimum involves non isothermal/isocomposition mixing are excluded from consideration. Nevertheless, for problems that are not too large, it has been demonstrated with the examples considered in this study that good solutions can still be obtained.

9. The IBMS for HENS has been successfully extended to problems having multiple hot and cold utilities, and to those involving multiple periods of operation through the use of maximum area per period method. The IBMS for mass exchanger network synthesis has been extended to problems involving regeneration, multiple lean streams (process and external), non-linear equilibrium relations and combined heat and mass exchanger networks.

The solutions of the IBMS models cannot be guaranteed to be globally optimal since the model contains non-linear and non-convex terms in the objective function and due to the fact that a gradient based solver was used. However the results obtained as mentioned earlier are comparable with those in the literature and the comparisons are shown in Tables 6.1 to 6.7.

Table 6.1. Summary of results for Example 3.1 to 3.3

Problem	SWS		NLP		IBMS	
	TAC $/yr	Units	TAC $/yr	Units	TAC $/yr	Units
3.1	235,400	6	-	-	237,800	6
3.2	576,640	7	-	-	581,942	7
3.3	151,000	9	177,400	12	168,700	10

Table 6.2. Summary of results for Example 3.4 & 3.5

Problem	CUP		IBMS	
	TAC £/yr	Units	TAC £/yr	Units
3.4	105,027	5	102,396	5
3.5	1158500	9	1150460	7

Table 6.3. Summary of results for Example 4.1

Problem	FLM		Hybrid FLM		IBMS	
	TAC $/yr	Units	TAC $/yr	Units	TAC $/yr	Units
4.1	134,000	8	134,399	10	133,323	7

Table 6.4. Summary of results for Example 4.2

Problem	Pinch		IBMS	
	TAC $/yr	Units	TAC $/yr	Units
4.2	427,061	5	446,840	4

Table 6.5. Summary of results for Example 4.3

Problem	Pinch		NLP		IBMS	
	TAC $/yr	Units	TAC $/yr	Units	TAC $/yr	Units
4.3	345,416	7	333,300	7	338,168	6

Table 6.6. Summary of results for Example 4.4

Problem	MINLP		Pinch		NLP		SWS		IBMS	
	TAC	Units	TAC	Units	TAC	Units	TAC	Units	TAC	Units
4.4	957	6	706	8	688	6	694	7	689	8

TAC * 10^{-3} $/yr

Table 6.7. Summary of results for Example 5.3

Problem	Hyper MINLP		SWS MINLP		NLP		Pinch		IBMS	
	TAC	Units	TAC	Units	TAC	Units	TAC	Units	TAC	Units
5.4	11,273,500	4	11,273,500	4	28,000	2	28,000	2	28,000	2

TAC $/yr

Table 6.8. Summary of results for Examples 5.1, 5.2 & 5.4

Problem	TAC	Units
5.1	7 182 675 €/yr	9 (2-way splits of H_1, HU, $_{C1}$ & CU)
5.2	604 377 $/yr	5 (2-way split of R_1)
5.4	917 804 $/yr	4 (MENS), 1 (Regeneration) & 2 (HENS) (2-way split of S_1)

Note that Example 5.1 cannot be compared with any network based on the reasons which have been explained in Section 5.2. Example 5.2 and 5.4 also cannot be compared with any solution because they were generated in this study so as to convey the ability of the IBMS to handle problems of their nature.

Comparison of IBMS basis

This section compares the solutions given by the different basis with which the IBMS can be generated for both HENS and MENS.

HENS

Table 6.9. Comparison of hot and cold stream IBMS basis for Example 3.1

Example 3.1: 3 hot and 3 cold streams		
IBMS basis	Hot	Cold
TAC $/yr	237,800	239,332
Number of intervals	5	5
Number of units	6	6
Type and number of splits	2-way splits of H_2 and C_1	2-way splits of H_2, C_1 and C_2

Table 6.10. Comparison of hot and cold stream IBMS basis for Example 3.2

Example 3.2: 6 hot and 2 cold streams		
IBMS basis	Hot	Cold
TAC $/yr	581,942	595,064
Number of intervals	7	3
Number of units	7	7
Type and number of splits	2-way and 3-way splits of C_1	2-way and 3-way splits of C_1

MENS

Table 6.11. Comparison of rich and lean stream IBMS basis for Example 4.1

Example 4.1: 5 rich and 3 lean streams		
IBMS basis	Rich	Lean
TAC $/yr	133,323	133,322
Number of intervals	5	4
Number of units	7	7
Type and number of splits	2-way splits of R_4 and 3-way split of S_3	2-way splits of R_4 and 3-way split of S_3

Table 6.12. Comparison of rich and lean stream IBMS basis for Example 4.2

Example 4.2: 2 rich and 2 lean streams		
IBMS basis	Rich	Lean
TAC $/yr	530,471	446,840
Number of intervals	3	3
Number of units	4	4
Type and number of splits	No split	2-way splits of S_1 and S_2

Tables 6.9 and 6.10 compares IBMS solutions generated on hot and cold stream basis for the HENS problems in Examples 3.1 and 3.2. Tables 6.11 and 6.12 compares those based on rich and lean streams for Examples 4.1 and 4.2 for MENS. For Table 6.9, no significant difference can be observed in the parameters used to compare the two bases except that three streams are split 2 ways in the cold basis unlike the hot basis where only two streams were split 2 ways. This could be explained to be due to the fact that the number of hot and cold streams is equal and none of the supply and target temperatures on the two bases coincides. For Table 6.10, the number of hot streams is more than the cold. This results in the number of intervals in the hot stream based IBMS being more than the cold basis. Nevertheless, there is still no significant difference in the other set of parameters used in the comparison.

For the MENS examples in Table 6.11, the number of rich streams is more than the lean. This only results in the number of rich basis intervals being one more than the lean while

other parameters are more or less the same. The example in Table 6.12 despite having equal numbers of rich and lean streams has significantly different solutions. The TAC of the rich basis is about 16% higher than that of the lean basis. In addition, the rich basis solution does not have any split while the lean has 2-way splits of S_1 and S_2.

It can be concluded that no generalizations can be made in terms of the best basis to use to construct the IBMS using the basic parameters such as number of streams. More detailed investigation could be done in order to see if generalizations could be made from the two IBMS bases.

6.2 Future Work

The IBMS model can be extended so as to include more options of network solutions in the following manner:

1. Non-linear heat/mass balance and mixing equations can be included in the IBMS models so that problems in which the optimum solution may be networks having non isothermal/isocomposition mixing can be adequately included in the search for the optimum. But this may require restructuring the stream existence and stream supply/target composition recognition coefficients.

2. Stream by-pass equations can also be included in the IBMS model so that configurations which involve stream split branches going through more than one exchanger in series can be considered in the search for the optimum solution network.

3. The IBMS model for MENS can be extended to solve problems involving alternative regenerants, in this scenario, the regenerants can be made to participate in all intervals defined by the rich streams. Also, more complex problems involving different process scenarios in mass exchange problems such as regeneration, multiple lean (process and external), non linear equilibrium relations, multiple components etc can be incorporated into the model. It is anticipated that problems of this nature will need good initialisation methods in order to get minimum or near minimum solutions in reasonable times.

4. The IBMS model for MENS can also be extended (as was done for HENS) to optimise multiperiod mass exchange operations through the introduction of maximum number of stages/packed height per period inequalities.

5. The non-linear heat/mass balance and mixing equations as well as the stream by-pass equations when added to the IBMS models for HENS and MENS will allow for a proper simultaneous trade-off of all the costs involved in combined heat and mass exchange network problems.

6. The IBMS models for HENS and MENS can be applied to the retrofit of existing heat and mass exchange networks through the use of constraints for reassignment of existing matches, installation of new exchangers, calculation of additional number of stages and column height etc as done by Chen and Hung (2005b).

6.3 Significance of the study

The IBMS model approach presents a new synthesis method for determining the minimum total costs for heat and mass exchange networks. A major contribution to the field of process synthesis is the superstructure partitioning approach which is based on key variables that determine the optimum driving forces for calculating areas and stages/height of heat and mass exchangers respectively. This partitioning method allows the solver to be direct the search for the optimal variables within the neighbourhood where the optimum driving forces are located. This study is the first to use the same superstructure framework for heat and mass exchanger networks synthesis and it is effective for finding near optimum solutions for a wide range of heat and mass exchange network problems.

A second major contribution of this study is the fact that for heat and mass exchange problems that are not very large, near minimum solutions can still be obtained with the IBMS model despite the automatic isothermal/isocomposition mixing of split streams. An advantage of this kind of mixing is that there is no need to include non linear heat/mass balance, mixing and bypass equations. However for bigger and more complex problems, these equations might be needed.

A third significance is that it can be used in place of the time consuming supertargeting in pinch technology method to make quick evaluations of designs or even to initialise more computationally demanding MINLP model approaches which normally include all possible flowsheets in a hyperstruture.

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APPENDIX

APPENDIX A. HEAT EXCHANGE PROBLEM DATA

This appendix presents the problem data used for examples on heat exchange networks in this thesis in Chapter 3.

Table A1: Stream and capital cost data for Example 3.1 (Shenoy, 1995)

Stream	T^s (^{0}C)	T^t (^{0}C)	F (kW ^{0}C^{-1})	h	Costs
H_1	175	45	10	0.2	-
H_2	125	65	40	0.2	-
C_1	20	155	20	0.2	-
C_2	40	112	15	0.2	-
HU_1	180	179	-	0.2	120
CU_1	15	25	-	0.2	10

h = (kW m^{-2} ^{0}C^{-1}), Capital cost = 30,000+750[Area(m^2)]$^{0.81}$ for all exchangers, Annualisation factor = 0.322, utility costs in \$ kW^{-1} yr^{-1}.

Table A2: Stream and capital cost data for Example 3.2 (Yee and Grossmann, 1990)

Stream	T^s (K)	T^t (K)	F (kW K^{-1})	Costs
H_1	500	320	6	-
H_2	480	380	4	-
H_3	460	360	6	-
H_4	380	360	20	-
H_5	380	320	12	-
C_1	290	660	18	-
HU_1	700	700	-	140
CU_1	300	320	-	10

U= 1 (kW m^{-2} K^{-1}) for all matches, Annualised cost = 1200[Area(m^2)]$^{0.6}$ for all exchangers, utility costs in \$ kW^{-1} yr^{-1}.

Table A3: Stream and capital cost data for Example 3.3 (Colberg and Morari, 1990)

Stream	T^s (K)	T^t (K)	F (kW K^{-1})	h
H_1	626	586	9.802	1.25
H_2	620	519	2.931	0.05
H_3	528	353	6.161	3.20
C_1	497	613	7.179	0.65
C_2	389	576	0.641	0.25
C_3	326	386	7.627	0.33
C_4	313	566	1.690	3.20
HU_1	650	650	-	3.50
CU_1	293	308	-	3.50

Annualised cost =8600+670[Area(m^2)]$^{0.83}$ for all exchangers (Yee and Grossmann, 1990).

Table A4: Stream and capital cost data for Example 3.4 (Shenoy, *et al*., 1998)

Stream	T^s (K)	T^t (K)	F (kW K^{-1})	h	Costs
H_1	105	25	10	0.5	-
H_2	185	35	5	0.5	-
C_3	25	185	7.5	0.5	-
HPS	210	209	-	5.0	160
MPS	160	159	-	5.0	110
LPS	130	129	-	5.0	50
CW	5	6	-	2.6	10

Annualization factor = 0.298/yr, Exchanger capital cost = 800[Area(m^2)] for all exchangers, utility costs in £ kW^{-1} yr^{-1} and h in $kW^{-1}m^{-2}\,{}^0C^{-1}$.

Table A5: Stream and capital cost data for Example 3.5 (Shenoy, *et al*., 1998)

Stream	T^s (K)	T^t (K)	F (kW $^0C^{-1}$)	h	Costs
H_1	155	85	150	0.5	-
H_2	230	40	85	0.5	-
C_1	115	210	140	0.5	-
C_2	50	180	55	0.5	-
C_3	60	175	60	0.5	-
HPS	255	254	-	0.5	70
MPS	205	204	-	0.5	50
LPS	150	149	-	0.5	20
CW	30	40	-	0.5	10
AC	40	65	-	0.5	5

Annualization factor = 0.322/yr, Exchanger capital cost =13,000 + 1000[Area(m^2)$^{0.83}$] for all exchangers, utility costs in \$ kW^{-1} yr^{-1} and h in $kW^{-1}m^{-2}.{}^0C^{-1}$.

APPENDIX B. MASS EXCHANGE PROBLEM DATA

Appendix B presents the problem data used for examples on mass exchange networks synthesis in Chapter 4.

Table B1: Rich stream data for Example 4.1 (Hallale, 1998)

Stream	G(kg/s)	Y^S	Y^t
R_1	2	0.005	0.001
R_2	4	0.005	0.0025
R_3	3.5	0.011	0.0025
R_4	1.5	0.010	0.005
R_5	0.5	0.008	0.0025

Compositions are mass fractions

Table B2: Lean stream data for Example 4.1 (Hallale, 1998)

Stream	L^c(kg/s)	X^S	X^t	m	b	Cost($/kg)
S_1	1.8	0.0017	0.0071	1.2	0	-
S_2	1.0	0.0025	0.0085	1	0	-
S_3	∞	0	0.017	0.5	0	0.001

Compositions are mass fractions

Table B3: Equipment and operating cost data for Example 4.1 (Szitkai *et al*., 2006)

Shell cost (Installed)	\$618 $M^{0.66}$ (M in kg)
Working hours	8150/yr
Annualisation factor	0.225

Table B4: Rich stream data for Example 4.2 (Hallale and Fraser, 2000a)

Stream	G(kg/s)	Y^S	Y^t
R_1	0.9	0.070	0.0003
R_2	0.1	0.051	0.0001

Compositions are mass fractions

Table B5: Lean stream data for Example 4.2 (Hallale and Fraser, 2000a)

Stream	L^c(kg/s)	X^S	X^t	m	b	Cost ($/yr)(kg/s)
S_1	2.3	0.0006	0.031	1.45	0	117,360
S_2	∞	0.0002	0.0035	0.26	0	176,040

Compositions are mass fractions

Table B6: Rich stream data for Example 4.3 (El-Halwagi, 1997)

Stream	G(kg/s)	Y^S	Y^t
R_1	2	0.050	0.010
R_2	1	0.030	0.006

Table B7: Lean stream data for Example 4.3 (El-Halwagi, 1997)

Stream	L^c(kg/s)	X^S	X^t	m	b	Cost ($/kg)
S_1	5	0.005	0.015	2.00	0	-
S_2	3	0.01	0.030	1.53	0	-
S_3	∞	0.0013	0.015	0.71	0.001	0.01

Compositions are mass fractions.

Table B8: Rich stream data for Example 4.4 (Hallale and Fraser, 2000d)

Stream	G(kg/s)	Y^S	Y^t
R_1	3.3	0.05	0.0015
R_2	0.6	0.07	0.003
R_3	1.4	0.02	0.003
R_4	0.2	0.03	0.002

Compositions are mass fractions

Table B9: Lean stream data for Example 4.4 (Hallale and Fraser, 2000d)

Stream	L^c(kg/s)	X^S	X^t	m	b	Cost ($s/kg yr)
S_1	10	0.0013	0.025	0.71	0.001	58680
S_2	10			0.13	0.001	417060
Regeneration	VR^c(kg/s)	Z^s	Z^t	m	b	Cost
V_1	10	0	0.005	1.38	-	88020

Compositions are mass fractions

APPENDIX C. EXTENDED APPLICATIONS PROBLEM DATA

Table C1: Stream and capital cost data for Example 5.1 (Verheyen and Zhang, 2006)

SOR

Stream	T^s (^{0}C)	T^t (^{0}C)	F (kW K^{-1})	Costs
H_1	393	60	201.6	-
H_2	160	40	185.1	-
H_3	354	60	137.4	-
C_1	72	356	209.4	-
C_2	62	210	141.6	-
C_3	220	370	176.4	-
C_4	253	284	294.4	-
HU_1	500	450	-	115.2
CU_1	0	10	-	1.3

Annualization factor = 0.2/yr, Exchanger capital cost = 8333.3+641.7[Area(m^2)] for all exchangers, utility costs in € kW^{-1} yr^{-1} and h = 0.2 kW^{-1}m^{-2} ^{0}C^{-1} for all streams.

MOR

Stream	T^s (^{0}C)	T^t (^{0}C)	F (kW K^{-1})	Costs
H_1	406	60	205.0	-
H_2	160	40	198.8	-
H_3	362	60	136.4	-
C_1	72	365	210.3	-
C_2	62	210	141.0	-
C_3	220	370	175.4	-
C_4	250	290	318.7	-
HU_1	500	450	-	115.2
CU_1	0	10	-	1.3

Annualization factor = 0.2/yr, Exchanger capital cost = 8333.3+641.7[Area(m^2)] for all exchangers, utility costs in € kW^{-1} yr^{-1} and h = 0.2 kW^{-1}m^{-2} ^{0}C^{-1} for all streams.

EOR

Stream	T^s (^{0}C)	T^t (^{0}C)	F (kW K^{-1})	Costs
H_1	420	60	208.5	-
H_2	160	40	175.2	-
H_3	360	60	134.1	-
C_1	72	373	211.1	-
C_2	62	210	140.5	-
C_3	220	370	174.5	-
C_4	249	286	271.2	-
HU_1	500	450	-	115.2
CU_1	0	10	-	1.3

Annualization factor = 0.2/yr, Exchanger capital cost = 8333.3+641.7[Area(m^2)] for all exchangers, utility costs in € kW^{-1} yr^{-1} and h = 0.2 kW^{-1}m^{-2} ^{0}C^{-1} for all streams.

Table C2: Rich stream data for Example 5.2 (El-Halwagi, 1997)

Stream	$G(kg/s)$	Y^S	Y^t
R_1	2	0.050	0.010
R_2	1	0.030	0.006

Table C3: Lean stream data for Example 5.2 (El-Halwagi, 1997 & Fraser, *et. al*, 2005)

Stream	$L^c(kg/s)$	X^S	X^t	m	b	Cost ($/kg)
S_1	5	0.005	0.015	2.00	0	0
S_2	3	0.01	0.03	1.53	0	0
S_3	∞	0	0.110	0.02	0	0.081
S_4	∞	0	0.510	0.09	0	0.255
S_5	∞	0	0.029	0.04	0	0.06
S_6	∞	0.0013	0.015	0.71	0.001	0.01

Note: Compositions are mass ratios.

Table C4: Rich stream data for Example 5.3 (Papalexandri, *et al*. 1994)

Stream	$G(m^3/s)$	Y^S	Y^t
R_1	0.87	1.3E-5	2.2E-7
R_2	0.1	9E-6	2.2E-7

Compositions are in $kmol/m^3$

Table C5: Lean stream data for Example 5.3 (Papalexandri, *et al*. 1994)

Stream	$L^c(m^3/s)$	X^S	X^t	m	*Cost*
S_1	0.0002	0	0.01	0.1	0
S_2	∞	2E-6	1E-3	1E-3	8.80833E8
S_3	∞	1E-6	3E-6	3E-6	9.94039E8

Compositions are in $kmol/m^3$, costs in $(\$/yr)/(m^3/s)$

Table C6: Rich stream data for Example 5.4

Stream	$G(kg/s)$	Y^S	Y^t
R_1	500	0.01	0.004
R_2	600	0.01	0.005
R_3	400	0.02	0.005
R_4	300	0.01	0.015

Table C7: Lean stream data for Example 5.4

Stream	$L^c(kmoles/hr)$	X^S	X^t	m	Cost
S_1	∞			$(0.053T\text{-}14.5)$	-
Regeneration	$VR^c(kmole/hr)$	Z^s	Z^t	m	Annual cost
V_1	∞	0	0.1	1.8	1100

Compositions in kmol/kmol, T in K and Cost in $hr/kmol yr

Table C8: Hot and cold utility stream data for Example 5.4.

Stream	T^s (K)	T^t (K)	F (kW ^{0}/ K)	h	Costs
HU1	453	452	-	0.2	120
CU1	278	283	-	0.2	30

h = (kW m^{-2} $^0K^{-1}$), utility costs = \$ kW^{-1} yr^{-1}.

Table C9: Equipment data for Example 5.4.

Shell cost (Installed)	\$618 $M^{0.66}$ (M in kg)
Heat exchanger	\$1200$A^{0.6}$ (A in m)
Annualisation factor	
MEN	0.298
HEN	0.225

APPENDIX D. GAMS code

Appendix D1. GAMS code for Example 3.5

```
$Title: HENS by hot streams interval based MINLP superstructure
*Program Name: Multiple_Utilities_Example_3.5
*Program was written by Isafiade Adeniyi

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

TABLE HOTS(JH,DATA) Hot streams data
      TIN      TOUT     H
1   155.00    85.00    0.5
2   230.00    40.00    0.5
3   255.00   254.00    0.5
4   205.00   204.00    0.5
5   150.00   149.00   0.5;

TABLE COLDS(JC,DATA) Cold streams data
      TIN      TOUT     H
1   115.00   210.00    0.5
2    50.00   180.00    0.5
3    60.00   175.00    0.5
4    30.00    40.00    0.5
5    40.00    65.00   0.5;

TABLE MHC(JH,JC) Forbidden match for hot and cold streams including utilities
     1   2   3   4   5
1    1   1   1   1   1
2    1   1   1   1   1
3    1   1   1   0   0
4    1   1   1   0   0
5    1   1   1   0   0;

SCALAR
NOI  Number of intervals in superstructure  /9/;

SET
I temperature intervals NOK +1  /1*10/;

PARAMETERS
HUC(JH)          Cost per unit of hot utility
CUC(JC)          Cost per unit of cold utility
CF               Fixed charge for units
AE               Area cost index
AC               Area cost coefficient
AF               Annualisation factor
EMAT             Exchanger minimum approach temperature
TKH(I)           Temperature at ith location
INTERVAL(I)      Existence of an interval in superstructure
H(JH,I)          Hot stream existence coefficients in interval I
H1(JH,I)         Hot stream supply and target temperature coefficients
H2(JH,I)         Hot stream supply and target temperature coefficients
H3(JH,I)         Hot stream supply and target temperature coefficients
H4(JH,I)         Hot stream supply and target temperature coefficients
H5(JH,I)         Hot stream supply and target temperature coefficients
H6(JH,I)         Hot stream supply and target temperature coefficients
```

H7(JH,I) Hot stream supply and target temperature coefficients
H8(JH,I) Hot stream supply and target temperature coefficients
H9(JH,I) Hot stream supply and target temperature coefficients
H10(JH,I) Hot stream supply and target temperature coefficients
FTB1(I) First temperature boundary in superstructure
LTB(I) Last temperature boundary in superstructure
MAXDT(JH,JC)
AREA(JH,JC,I) Area of match between JH and JC;

```
*=============================================================
AF= 0.322;   CF=13000;    AC = 1000;      AE = 0.83;

HUC('1')=0;  HUC('2')=0;  HUC('3')=70.00; HUC('4')=50.00; HUC('5')=20.00;
CUC('1')=0;  CUC('2')=0;  CUC('3')=0;     CUC('4')=10.00; CUC('5')=5.00;

TKH('1') = 255.00; TKH('2') = 254.00; TKH('3') = 230.00; TKH('4') = 205.00;
TKH('5') = 204.00; TKH('6') = 155.00; TKH('7') = 150.00; TKH('8') = 149.00;
TKH('9')= 85.00;  TKH('10') =40.00;
*=============================================================
MAXDT(JH,JC)=
MAX(0,COLDS(JC,'TIN')-HOTS(JH,'TIN'),COLDS(JC,'TIN')-HOTS(JH,'TOUT'),
COLDS(JC,'TOUT')-HOTS(JH,'TIN'),COLDS(JC,'TOUT')-HOTS(JH,'TOUT'));

INTERVAL(I)$(ORD(I) LT CARD(I)) =1;
FTB1(I)$(ORD(I) EQ 1) =1;
LTB(I)$(ORD(I) EQ CARD(I))=1;

H(JH,I)$(HOTS(JH,'TIN') GE TKH(I) AND HOTS(JH,'TOUT') LE TKH(I+1)) = 1;

H1(JH,I)$(HOTS(JH,'TIN') EQ TKH(I))=1;
H2(JH,I)$(HOTS(JH,'TOUT') EQ TKH(I))=1;
H3(JH,I)$(HOTS(JH,'TIN') EQ TKH(I))=1;
H4(JH,I)$(HOTS(JH,'TIN') EQ TKH(I))=1;
H5(JH,I)$(HOTS(JH,'TOUT') EQ TKH(I))=1;
H6(JH,I)$(HOTS(JH,'TIN') EQ TKH(I)) = 1;
H7(JH,I)$(HOTS(JH,'TIN') EQ TKH(I))=1;
H8(JH,I)$(HOTS(JH,'TOUT') EQ TKH(I)) = 1;
H9(JH,I)$(HOTS(JH,'TOUT') EQ TKH(I)) = 1;
H10(JH,I)$(HOTS(JH,'TOUT') EQ TKH(I)) = 1;
*=============================================================
```

POSITIVE VARIABLES

TH(JH,I) Temperature of hot stream JH at hot end of temperature interval I
TC(JC,I) Temperature of cold stream JC at hot end of temperature interval I
AVHT(JH) Available heat in JH
AVCD(JC) Available heat in JC
Q(JH,JC,I) Heat exchanged between JH and JC in interval I
ATHC(JH,JC,I) Approach temeperature between JH and JC in interval I
MCP1(JH) Heat capacity flowrate of JH
MCP2(JC) Heat capacity flowrate of JC;

VARIABLE

TAC Total annual cost;

BINARY VARIABLES

NHC(JH,JC,I) is 1 if a match exists between JH and JC in interval I;

EQUATIONS
AVHOT(JH)
AVCOLD(JC)
ENBALHOT(JH)

```
ENBALCOLD(JC)
INTBHOT(JH,I)
INTBCOLD(JC,I)
COLDT(JC,I)
INTH1(JH,I)
INTH2(JH,I)
INTH3(JH,I)
INTH4(JH,I)
INTH5(JH,I)
INTH6(JH,I)
INTH7(JH,I)
INTH8(JH,I)
INTH9(JH,I)
INTC(JC,I)
CSTH(JH,I)
CSTHL(JH,I)
CSTC(JC,I)
CSTCF(JC,I)
UPPERBQ(JH,JC,I)
FORBMATCH(JH,JC,I)
ATHCD1(JH,JC,I)
ATHCD2(JH,JC,I)
OBJ             Total annual cost objective function;

*=====================================================================
*Availabe heat in hot stream JH
AVHOT(JH)..AVHT(JH)=E=MCP1(JH)*(HOTS(JH,'TIN') - HOTS(JH,'TOUT'));

*Available heat in cold stream JC
AVCOLD(JC)..AVCD(JC)=E=MCP2(JC)*(COLDS(JC,'TOUT') - COLDS(JC,'TIN'));
*=====================================================================
*Overall energy balance for hot stream JH
ENBALHOT(JH)..
AVHT(JH)=E=SUM((JC,I)$(INTERVAL(I) AND (H(JH,I) EQ 1)),Q(JH,JC,I));

*Overall energy balance for cold stream JC
ENBALCOLD(JC)..
AVCD(JC)=E=SUM((JH,I)$H(JH,I),Q(JH,JC,I));
*=====================================================================
*Interval heat balance for hot stream JH
INTBHOT(JH,I)$(INTERVAL(I) AND H(JH,I))..
MCP1(JH)*(TH(JH,I)-TH(JH,I+1))=E=SUM(JC,Q(JH,JC,I));

*Interval heat balance for cold stream JC
INTBCOLD(JC,I)$INTERVAL(I)..
MCP2(JC)*(TC(JC,I)-TC(JC,I+1))=E=SUM(JH$(H(JH,I)),Q(JH,JC,I));
*=====================================================================
*Cold stream temperature at the first temperature location
COLDT(JC,I)$FTB1(I)..
COLDS(JC,'TOUT')=E=TC(JC,I);
*=====================================================================
*Assignment of superstructure interval temperatures using hot stream supply and target

INTH1(JH,I)$(H1(JH,I) AND H(JH,I))..HOTS(JH,'TIN')=E=TH(JH,I);
INTH2(JH,I)$(H2(JH,I) AND H(JH,I))..HOTS(JH,'TOUT')=E=TH(JH,I);
INTH3(JH,I)$(H3(JH,I) AND H(JH,I) )..HOTS(JH,'TIN')=E=TH(JH,I);
INTH4(JH,I)$(H4(JH,I)  AND H(JH,I))..HOTS(JH,'TIN')=E=TH(JH,I);
INTH5(JH,I)$(H5(JH,I) AND H(JH,I))..HOTS(JH,'TOUT')=E=TH(JH,I);
INTH6(JH,I)$(H6(JH,I) AND H(JH,I))..HOTS(JH,'TIN')=E=TH(JH,I);
INTH7(JH,I)$(H7(JH,I) AND H(JH,I))..HOTS(JH,'TIN')=E=TH(JH,I);
```

```
INTH8(JH,I)$(H8(JH,I) AND H(JH,I))..HOTS(JH,'TOUT')=E=TH(JH,I);
INTH9(JH,I)$(H9(JH,I) AND H(JH,I))..HOTS(JH,'TOUT')=E=TH(JH,I);

*Asssignment of cold stream temperatures at the last temperature location
INTC(JC,I)$LTB(I)..COLDS(JC,'TIN')=E=TC(JC,I);
*=====================================================================
*Feasibility of hot stream temperatures
CSTH(JH,I)$(INTERVAL(I) AND H(JH,I))..TH(JH,I)=G=TH(JH,I+1);

CSTHL(JH,I)$(LTB(I) AND H10(JH,I))..TH(JH,I)=E=HOTS(JH,'TOUT');

*Feasibility of cold stream temperatures
CSTC(JC,I)$(INTERVAL(I))..TC(JC,I)=G=TC(JC,I+1);

CSTCF(JC,I)$FTB1(I)..COLDS(JC,'TOUT')=E=TC(JC,I);
*=====================================================================
*Logical constraint
UPPERBQ(JH,JC,I)$(INTERVAL(I)) ..
  Q(JH,JC,I)-MIN(AVHT(JH),AVCD(JC))*NHC(JH,JC,I)=L=0;
*=====================================================================
*Approach tempratures
ATHCD1(JH,JC,I)$(INTERVAL(I) AND H(JH,I))..
ATHC(JH,JC,I)=L=TH(JH,I) - TC(JC,I)+MAXDT(JH,JC)*(1 - NHC(JH,JC,I)) ;

ATHCD2(JH,JC,I)$(INTERVAL(I))..
ATHC(JH,JC,I+1)=L=TH(JH,I+1)-TC(JC,I+1)+MAXDT(JH,JC)*(1 - NHC(JH,JC,I)) ;
*=====================================================================
*Forbidden matches
FORBMATCH(JH,JC,I)$(MHC(JH,JC) EQ 0)..
 Q(JH,JC,I) =E=0;
*=====================================================================
*Objective function
 OBJ..
  TAC=E=
AF*((CF*(SUM((JH,JC,I)$(INTERVAL(I)),NHC(JH,JC,I))))+
AC*SUM((JH,JC,I)$(INTERVAL(I)),(Q(JH,JC,I)*(1/HOTS(JH,'H')+1/COLDS(JC,'H'))/
((((1e-6)**3+(ATHC(JH,JC,I)*ATHC(JH,JC,I+1))*((ATHC(JH,JC,I)
+ATHC(JH,JC,I+1))*0.5))**0.3333)+1E-6)+1E-6)**AE))

+ SUM((JH,JC,I),Q(JH,JC,I)*HUC(JH))+SUM((JH,JC,I),Q(JH,JC,I)*CUC(JC));
*=====================================================================

MODEL MULTIPLEUTIL_EXAMPLE_3_5 /ALL/;

*Upper/lower bounds and initialisation

MCP1.L('1')=150.00;  MCP1.LO('1')=150.00;  MCP1.UP('1')=150.00;
MCP1.L('2')=85.00;  MCP1.LO('2')=85.00;  MCP1.UP('2')=85.00;
MCP1.L('3')=1;  MCP1.LO('3')=1;  MCP1.UP('3')=10000;
MCP1.L('4')=1;  MCP1.LO('4')=1;  MCP1.UP('4')=10000;
MCP1.L('5')=1;  MCP1.LO('5')=1;  MCP1.UP('5')=10000;
MCP2.L('1')=140;  MCP2.LO('1')=140;  MCP2.UP('1')=140;
MCP2.L('2')=55;  MCP2.LO('2')=55;  MCP2.UP('2')=55;
MCP2.L('3')=60;  MCP2.LO('3')=60;  MCP2.UP('3')=60;
MCP2.L('4')=1;  MCP2.LO('4')=1;  MCP2.UP('4')=10000;
MCP2.L('5')=1;  MCP2.LO('5')=1;  MCP2.UP('5')=10000;

EMAT=9.1;  ATHC.LO(JH,JC,I)=EMAT;  ATHC.UP(JH,JC,I)=1000;
```

```
OPTION LIMROW =50;
SOLVE MULTIPLEUTIL_EXAMPLE_3_5 USING MINLP MINIMIZING TAC;

*Calculating areas for units in superstructure

AREA(JH,JC,I)$(INTERVAL(I) AND H(JH,I) )=
Q.L(JH,JC,I)*(1/HOTS(JH,'H')+1/COLDS(JC,'H'))/
(((1e-6)**3+(ATHC.L(JH,JC,I)*ATHC.L(JH,JC,I+1))*((ATHC.L(JH,JC,I)
+ATHC.L(JH,JC,I+1))*0.5))**0.3333)+1E-6;

DISPLAY AREA;
```

Appendix D2. GAMS code for Example 4.1

```
$Title: MENS by rich streams interval based MINLP superstructure
*Program Name: MENS_Example_4.1
*Program was written by Isafiade Adeniyi

SETS
 I       Rich streams /1*5/
 J       Process and external lean streams /1*3/
 DATA      /YIN,YOUT,G/;


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


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


SCALAR
NOK              Number of intervals in superstructure  /5/;

SET
K composition intervals NOB +1  /1*6/;

PARAMETERS
AF               Annualisatin factor
ACH              Annual cost per height for continuous contact columns
D                Area cost exponent for mass exchangers
KW               Lumped mass transfer coefficient
AC(J)            Annual operating cost per unit of lean stream
EMCD             Exchanger minimum composition difference
TKH(K)           Composition at ith location
AVRICH(I)        Available mass in rich stream I
INTERVAL(K)      Intervals in superstructure
R(I,K)           Rich stream existence coefficients in interval K
R1(I,K)          Rich stream supply and target composition coefficients
```

R2(I,K)
R3(I,K)
R4(I,K)
R5(I,K)
R6(I,K)
C(J,K)
FCB1(K) First composition boundary in superstructure
LCB(K) Last composition boundary in superstructure
MAXDC(I,J) Upper bound for composition difference
W
HEIGHT(I,J,K) Height of exchanger between streams I and J in interval K;
*===

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

TKH('1') = 0.01100;  TKH('2') = 0.01000;  TKH('3') = 0.00800;
TKH('4') = 0.00500;  TKH('5') = 0.00250;  TKH('6') = 0.00100;

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

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

INTERVAL(K)$(ORD(K) LT CARD(K)) =1;
FCB1(K)$(ORD(K) EQ 1) =1;
LCB(K)$(ORD(K) EQ CARD(K))=1;

R(I,K)$(RICH(I,'YIN') GE TKH(K) AND RICH(I,'YOUT') LE TKH(K+1)) = 1;

R1(I,K)$(RICH(I,'YIN') EQ TKH(K))=1;
R2(I,K)$(RICH(I,'YIN') EQ TKH(K))= 1;
R3(I,K)$(RICH(I,'YIN') EQ TKH(K))=1;
R4(I,K)$(RICH(I,'YIN') EQ TKH(K))=1;
R5(I,K)$(RICH(I,'YOUT') EQ TKH(K))=1;
R6(I,K)$(RICH(I,'YOUT') EQ TKH(K))=1;
```

*===

POSITIVE VARIABLES

CR(I,K) Composition of rich stream I at rich end of composition interval K
CL(J,K) Composition of lean stream J at rich end of composition interval K
AVLEAN(J) Available mass in lean stream J
M(I,J,K) Mass exchanged between rich stream I and lean stream J in interval K
L(J) Flowrate of lean stream J
DCRC(I,J,K) Approach composition between I and J in rich end of K
NHC(I,J,K) Relaxed binary variable
PNHC(I,J,K) Positive tolerance
SNHC(I,J,K) Negative tolerance;

VARIABLE

TAC total annual cost;

BINARY VARIABLES

NNHC(I,J,K) is 1 if a match exists between I and J in interval K;

EQUATIONS

MABALR(I)
MABALL(J)
MBRST(I,K)
MBLST(J,K)
AVLEAN1(J)
FIRSTCOMP(J,K)

```
CINR1(I,K)
CINR2(I,K)
CINR3(I,K)
CINR4(I,K)
CINR5(I,K)
CINR6(I,K)
CINL(J,K)
CONSCR(I,K)
CONSCRL(I,K)
CONSCL(J,K)
CONSCLF(J,K)
BOUNDM(I,J,K)
DTREMN1(I,J,K)
DTREMN2(I,J,K)
DTLEMN1(I,J,K)
DTLEMN2(I,J,K)
N1(I,J,K)
P(I,J,K)
S(I,J,K)
OBJ                Total annual cost objective function;
*=============================================================
*Availabe mass in lean stream J
AVLEAN1(J)..AVLEAN(J)=E=L(J)*(LEAN(J,'YOUT') - LEAN(J,'YIN'));
*=============================================================
*Overall mass balance for rich stream I
MABALR(I)..
((RICH(I,'YIN')-RICH(I,'YOUT'))*RICH(I,'G'))
=E=SUM((J,K)$(INTERVAL(K) AND (R(I,K) EQ 1)),M(I,J,K));

*Overall mass balance for rich stream J
MABALL(J)..AVLEAN(J)=E=SUM((I,K)$R(I,K),M(I,J,K));
*=============================================================
*Interval mass balance for rich stream I
MBRST(I,K)$(INTERVAL(K) AND R(I,K))..
RICH(I,'G')*(CR(I,K)-CR(I,K+1))=E=SUM(J,M(I,J,K));

*Interval mass balance for lean stream J
MBLST(J,K)$INTERVAL(K)..
L(J)*(CL(J,K)-CL(J,K+1))=E=SUM(I$(R(I,K)),M(I,J,K));
*=============================================================
*Lean stream composition at the first composition location
FIRSTCOMP(J,K)$FCB1(K)..LEAN(J,'YOUT')=E=CL(J,K);
*=============================================================
*Assignment of superstructure interval compositions using rich stream
*supply and target compositions
CINR1(I,K)$(R1(I,K) AND R(I,K))..RICH(I,'YIN')=E=CR(I,K);
CINR2(I,K)$(R2(I,K) AND R(I,K))..RICH(I,'YIN')=E=CR(I,K);
CINR3(I,K)$(R3(I,K) AND R(I,K))..RICH(I,'YIN')=E=CR(I,K);
CINR4(I,K)$(R4(I,K) AND R(I,K))..RICH(I,'YIN')=E=CR(I,K);
CINR5(I,K)$(R5(I,K) AND R(I,K))..RICH(I,'YOUT')=E=CR(I,K);
CINR6(I,K)$(R6(I,K) AND R(I,K))..RICH(I,'YOUT')=E=CR(I,K);

*Asssignment of lean stream composition at the last composition location
CINL(J,K)$LCB(K)..LEAN(J,'YIN')=E=CL(J,K);
*=============================================================
*Feasibility of rich stream compositions
CONSCR(I,K)$(INTERVAL(K) AND R(I,K))..CR(I,K)=G=CR(I,K+1);
CONSCRL(I,K)$(LCB(K) AND R6(I,K))..CR(I,K)=E=RICH(I,'YOUT');

*Feasibility of lean stream compositions
```

```
CONSCL(J,K)$INTERVAL(K)..CL(J,K)=G=CL(J,K+1);
CONSCLF(J,K)$FCB1(K)..LEAN(J,'YOUT')=E=CL(J,K);
*=========================================================
*Logical constraint
BOUNDM(I,J,K)$(INTERVAL(K))..
M(I,J,K)-MIN(AVRICH(I),AVLEAN(J))*NHC(I,J,K)=L=0;
*=========================================================
*Approach compositions
DTREMN1(I,J,K)$(INTERVAL(K))..
DCRC(I,J,K)=L=CR(I,K) - CL(J,K)+MAXDC(I,J)*(1 - NHC(I,J,K)) ;
DTREMN2(I,J,K)$(INTERVAL(K))..
DCRC(I,J,K)=G=CR(I,K) - CL(J,K)-MAXDC(I,J)*(1 - NHC(I,J,K));
DTLEMN1(I,J,K)$(INTERVAL(K))..
DCRC(I,J,K+1)=L=CR(I,K+1)-CL(J,K+1)+MAXDC(I,J)*(1 - NHC(I,J,K)) ;
DTLEMN2(I,J,K)$(INTERVAL(K)) ..
DCRC(I,J,K+1)=G=CR(I,K+1)-CL(J,K+1)-MAXDC(I,J)*(1 - NHC(I,J,K)) ;
*=========================================================
P(I,J,K)$(INTERVAL(K) AND R(I,K))..PNHC(I,J,K)=E=.000000001;
S(I,J,K)$(INTERVAL(K) AND R(I,K))..SNHC(I,J,K)=E=.000000001;

N1(I,J,K)$(INTERVAL(K) AND R(I,K))..
NHC(I,J,K)=E=NNHC(I,J,K)+(PNHC(I,J,K)-SNHC(I,J,K));
*=========================================================
*Objective function
 OBJ..
TAC =E=(AF*(SUM((I,J,K)$(INTERVAL(K)),NHC(I,J,K))
+ACH*SUM((I,J,K)$(INTERVAL(K)),(M(I,J,K)*(1/KW)/((((1e-6)**3+
(DCRC(I,J,K)*DCRC(I,J,K+1))*((DCRC(I,J,K)+
DCRC(I,J,K+1))*0.5))**0.3333)+1E-6)+1E-6)**D)))

+SUM((J),L(J)*AC(J)) + W*(SUM((I,J,K),PNHC(I,J,K)+SNHC(I,J,K)));
*=========================================================
MODEL MENS_EXAMPLE_4_1 /ALL/;

*Upper/lower bounds and initialisation

L.L('1')=1;  L.LO('1')=1;  L.UP('1')=1.5;
L.L('2')=.1;  L.LO('2')=.1;  L.UP('2')=1;
L.L('3')=1;  L.LO('3')=1;  L.UP('3')=6;

EMCD =.000000000046;
DCRC.LO(I,J,K)=EMCD;  DCRC.UP(I,J,K)=1;

SOLVE MENS_EXAMPLE_4_1 USING MINLP MINIMIZING TAC;

*Calculating areas for units in superstructure

HEIGHT(I,J,K)$(INTERVAL(K) AND R(I,K))=(M.L(I,J,K)*(1/KW)/((((1e-6)**3+
(DCRC.L(I,J,K)*DCRC.L(I,J,K+1))*((DCRC.L(I,J,K)+
DCRC.L(I,J,K+1))*0.5))**0.3333)+1E-6)+1E-6);

DISPLAY  AVRICH,HEIGHT;  OPTION CL:5:1:1;
DISPLAY CL.L;  OPTION CR:5;  DISPLAY CR.L;
OPTION M:6;  DISPLAY M.L;  OPTION L:5;  DISPLAY L.L;
```

Appendix D3. GAMS code for Example 5.1

```
$Title: MULTIPERIODHENS by hot streams interval based MINLP superstructure
```

*Program Name: Multiple_Utilities_Example_3.5
*Program was written by Isafiade Adeniyi

SETS
JH Hot streams and utilities /1*4/
JC Cold streams and utilities /1*5/
P Number of periods /1*3/
DATA /TIN,TOUT,MCP,H/;

TABLE HOTS(JH,P,DATA) Hot streams data

	TIN	TOUT	H
1.1	393	60	0.2
1.2	406	60	0.2
1.3	420	60	0.2
2.1	160	40	0.2
2.2	160	40	0.2
2.3	160	40	0.2
3.1	354	60	0.2
3.2	362	60	0.2
3.3	360	60	0.2
4.1	500	450	0.2
4.2	500	450	0.2
4.3	500	450	0.2;

TABLE COLDS(JC,P,DATA) Cold streams data

	TIN	TOUT	H
1.1	72	356	0.2
1.2	72	365	0.2
1.3	72	373	0.2
2.1	62	210	0.2
2.2	62	210	0.2
2.3	62	210	0.2
3.1	220	370	0.2
3.2	220	370	0.2
3.3	220	370	0.2
4.1	253	284	0.2
4.2	250	290	0.2
4.3	249	286	0.2
5.1	0	10	0.2
5.2	0	10	0.2
5.3	0	10	0.2;

TABLE MHC(JH,JC) Forbidden match for hot and cold streams including utilities

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

SCALAR
NOI Number of intervals in superstructure /6/;

SET
I temperature intervals NOK +1 /1*7/;

PARAMETERS
HUC(JH) Cost per unit of hot utility
CUC(JC) Cost per unit of cold utility

CF Fixed charge for units
AE Area cost index
AC Area cost coefficient
AF Annualisation factor
EMAT Exchanger minimum approach temperature
NOP Number of periods
DOP(P) Duration of period P
TKH(P,I) Temperature at pth period and ith location
INTERVAL(P,I) Existence of an interval in superstructure
H(JH,P,I) Hot stream existence coefficients in period P and interval I
H1(JH,P,I) Hot stream supply and target temperature coefficients at pth period and ith interval
H2(JH,P,I)
H3(JH,P,I)
H4(JH,P,I)
H5(JH,P,I)
H6(JH,P,I)
H7(JH,P,I)
FTB1(P,I) First temperature boundary in superstructure and period P
LTB(P,I) Last temperature boundary in superstructure and period P
MAXDT(JH,JC,P) Upper bound for temperature difference in period P
HOTUTILCOST(JH,JC,P,I) Hot utility cost in period P and interval I
COLDUTILCOST(JH,JC,P,I) Cold utility cost in period P and interval I
TOTUTILCOST(JH,JC,P,I) Total utility cost in period P and interval I
AOCCOST
AREA(JH,JC,P,I) area of exchanger between JH and JC in period P and interval I;

```
*=====================================================================
AF   = 0.2;  CF =8333.3;  AC = 641.7;  AE = 1;  NOP=3;  DOP('1')=1;
DOP('2')=1;  DOP('3')=1;  HUC('4')=115.2;  CUC('5')=1.3;

TKH('1','1') = 500;  TKH('2','1') = 500;  TKH('3','1') = 500;
TKH('1','2') = 450;  TKH('2','2') = 450;  TKH('3','2') = 450;
TKH('1','3') = 393;  TKH('2','3') = 406;  TKH('3','3') = 420;
TKH('1','4') = 354;  TKH('2','4') = 362;  TKH('3','4') = 360;
TKH('1','5') = 160;  TKH('2','5') = 160;  TKH('3','5') = 160;
TKH('1','6') = 60;   TKH('2','6') = 60;   TKH('3','6') = 60;
TKH('1','7') = 40;   TKH('2','7') = 40;   TKH('3','7') = 40;

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

INTERVAL(P,I)$(ORD(I) LT CARD(I)) =1;
FTB1(P,I)$(ORD(I) EQ 1) =1;
LTB(P,I)$(ORD(I) EQ CARD(I))=1;

H(JH,P,I)$(HOTS(JH,P,'TIN') GE TKH(P,I) AND HOTS(JH,P,'TOUT') LE TKH(P,I+1)) = 1;

H1(JH,P,I)$(HOTS(JH,P,'TIN') EQ TKH(P,I))=1;
H2(JH,P,I)$(HOTS(JH,P,'TOUT') EQ TKH(P,I))=1;
H3(JH,P,I)$(HOTS(JH,P,'TIN') EQ TKH(P,I))=1;
H4(JH,P,I)$(HOTS(JH,P,'TIN') EQ TKH(P,I))=1;
H5(JH,P,I)$(HOTS(JH,P,'TIN') EQ TKH(P,I))=1;
H6(JH,P,I)$(HOTS(JH,P,'TOUT') EQ TKH(P,I)) = 1;
H7(JH,P,I)$(HOTS(JH,P,'TOUT') EQ TKH(P,I)) = 1;
*=====================================================================
```

POSITIVE VARIABLES

TH(JH,P,I) Temperature of JH in P and hot end of temperature interval I
TC(JC,P,I) Temperature of JC in P and hot end of temperature interval I
AVHT(JH,P) Available heat in JH in period P
AVCD(JC,P) Available heat in JC in period P

Q(JH,JC,P,I) Heat exchanged between JH and JC in period P and interval I
ATHC(JH,JC,P,I)Approach temeperature between JH and JC in P and interval I
MCP1(JH,P) Heat capacity flowrate of JH in period P
MCP2(JC,P) Heat capacity flowrate of JC in period P
AX(JH,JC,I) Maximum area between JH and JC in interval I;

VARIABLE
TAC Total annual cost;

BINARY VARIABLES
NHC(JH,JC,I) is 1 if a match exists between JH and JC in interval I;

EQUATIONS
AVHOT(JH,P)
AVCOLD(JC,P)
ENBALHOT(JH,P)
ENBALCOLD(JC,P)
INTBHOT(JH,P,I)
INTBCOLD(JC,P,I)
COLDT(JC,P,I)
INTH1(JH,P,I)
INTH2(JH,P,I)
INTH3(JH,P,I)
INTH4(JH,P,I)
INTH5(JH,P,I)
INTH6(JH,P,I)
INTC(JC,P,I)
CSTH(JH,P,I)
CSTHL(JH,P,I)
CSTC(JC,P,I)
CSTCF(JC,P,I)
UPPERBQ(JH,JC,P,I)
FORBMATCH(JH,JC,P,I)
ATHCD1(JH,JC,P,I)
ATHCD2(JH,JC,P,I)
AX1(JH,JC,P,I)
OBJ Total annual cost objective function;

```
*=====================================================================
*Availabe heat in hot stream JH in period P
AVHOT(JH,P)..AVHT(JH,P)=E=MCP1(JH,P)*(HOTS(JH,P,'TIN') - HOTS(JH,P,'TOUT'));

*Available heat in cold stream JC in period P
AVCOLD(JC,P)..AVCD(JC,P)=E=MCP2(JC,P)*(COLDS(JC,P,'TOUT') - COLDS(JC,P,'TIN'));
*=====================================================================
Overall energy balance for hot stream JH and period P
ENBALHOT(JH,P)..
  AVHT(JH,P) =E=SUM((JC,I)$(INTERVAL(P,I) AND (H(JH,P,I) EQ 1)),Q(JH,JC,P,I));

Overall energy balance for cold stream JC and period P
ENBALCOLD(JC,P)..
  AVCD(JC,P)=E=SUM((JH,I)$H(JH,P,I),Q(JH,JC,P,I));
*=====================================================================
*Interval energy balance for hot stream JH and period P
INTBHOT(JH,P,I)$(INTERVAL(P,I) AND H(JH,P,I))..
MCP1(JH,P)*(TH(JH,P,I)-TH(JH,P,I+1))=E=SUM(JC,Q(JH,JC,P,I));

*Interval energy balance for cold stream JC and period P
INTBCOLD(JC,P,I)$INTERVAL(P,I)..
MCP2(JC,P)*(TC(JC,P,I)-TC(JC,P,I+1))=E=SUM(JH$(H(JH,P,I)),Q(JH,JC,P,I));
*=====================================================================
```

```
*Cold stream temperature in period P and at the first temperature location
COLDT(JC,P,I)$FTB1(P,I)..COLDS(JC,P,'TOUT')=E=TC(JC,P,I);
*=====================================================================
*Assignment of superstructure interval temperatures using hot stream
*supply and target

INTH1(JH,P,I)$(H1(JH,P,I) AND H(JH,P,I))..HOTS(JH,P,'TIN')=E=TH(JH,P,I);
INTH2(JH,P,I)$(H2(JH,P,I) AND H(JH,P,I))..HOTS(JH,P,'TOUT')=E=TH(JH,P,I);
INTH3(JH,P,I)$(H3(JH,P,I) AND H(JH,P,I))..HOTS(JH,P,'TIN')=E=TH(JH,P,I);
INTH4(JH,P,I)$(H4(JH,P,I) AND H(JH,P,I))..HOTS(JH,P,'TIN')=E=TH(JH,P,I);
INTH5(JH,P,I)$(H5(JH,P,I) AND H(JH,P,I))..HOTS(JH,P,'TIN')=E=TH(JH,P,I);
INTH6(JH,P,I)$(H6(JH,P,I)AND H(JH,P,I))..HOTS(JH,P,'TOUT')=E=TH(JH,P,I);
*Asssignment of cold stream temperatures at the last temperature location
INTC(JC,P,I)$LTB(P,I)..COLDS(JC,P,'TIN')=E=TC(JC,P,I);
*=====================================================================
*Feasibility of hot stream temperatures
CSTH(JH,P,I)$(INTERVAL(P,I) AND H(JH,P,I))..TH(JH,P,I)=G=TH(JH,P,I+1);
CSTHL(JH,P,I)$(LTB(P,I) AND H7(JH,P,I))..TH(JH,P,I)=E=HOTS(JH,P,'TOUT');
*Feasibility of cold stream temperatures
CSTC(JC,P,I)$(INTERVAL(P,I))..TC(JC,P,I)=G=TC(JC,P,I+1);
CSTCF(JC,P,I)$FTB1(P,I)..COLDS(JC,P,'TOUT')=E=TC(JC,P,I);
*=====================================================================
*Logical constraint
UPPERBQ(JH,JC,P,I)$(INTERVAL(P,I)) ..
Q(JH,JC,P,I)-MIN(AVHT(JH,P),AVCD(JC,P))*NHC(JH,JC,I)=L=0;
*=====================================================================
*Approach temperatures
ATHCD1(JH,JC,P,I)$INTERVAL(P,I)..
ATHC(JH,JC,P,I)=L=TH(JH,P,I) - TC(JC,P,I)+MAXDT(JH,JC,P)*(1 - NHC(JH,JC,I));

ATHCD2(JH,JC,P,I)$INTERVAL(P,I)..
ATHC(JH,JC,P,I+1)=L=TH(JH,P,I+1)-TC(JC,P,I+1)+MAXDT(JH,JC,P)*(1 - NHC(JH,JC,I));
*=====================================================================
*Forbidden matches
FORBMATCH(JH,JC,P,I)$(MHC(JH,JC) EQ 0)..Q(JH,JC,P,I) =E=0;
*=====================================================================
*Maximum area per period
AX1(JH,JC,P,I)$(INTERVAL(P,I) AND  H(JH,P,I))..
AX(JH,JC,I)=G=Q(JH,JC,P,I)*(1/HOTS(JH,P,'H')+1/COLDS(JC,P,'H'))/(((1e-6)**3+
(ATHC(JH,JC,P,I)*ATHC(JH,JC,P,I+1))*((ATHC(JH,JC,P,I)+
ATHC(JH,JC,P,I+1))*0.5))**0.3333)+1E-6;
*=====================================================================
*Objective function
OBJ..
TAC=E= AF*(CF*(SUM((JH,JC,I),NHC(JH,JC,I))))+
AF*(AC*(SUM((JH,JC,I),(AX(JH,JC,I)))))
+ SUM((P),(DOP(P)/NOP)*SUM((JH,JC,I),Q(JH,JC,P,I)*HUC(JH)))
+SUM((P),(DOP(P)/NOP)*SUM((JH,JC,I),Q(JH,JC,P,I)*CUC(JC)));
*=====================================================================
MODEL AUTIL /ALL/;

*Upper/lower bounds and initialisation
*INTERVAL 1

MCP1.L('1','1')=201.6;  MCP1.LO('1','1')=201.6;  MCP1.UP('1','1')=201.6;
MCP1.L('1','2')=205;  MCP1.LO('1','2')=205;  MCP1.UP('1','2')=205;
MCP1.L('1','3')=208.5;  MCP1.LO('1','3')=208.5;  MCP1.UP('1','3')=208.5;
MCP1.L('2','1')=185.1;  MCP1.LO('2','1')=185.1;  MCP1.UP('2','1')=185.1;
MCP1.L('2','2')=198.8;  MCP1.LO('2','2')=198.8;  MCP1.UP('2','2')=198.8;
MCP1.L('2','3')=175.2;  MCP1.LO('2','3')=175.2;  MCP1.UP('2','3')=175.2;
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MCP1.L('3','1')=137.4;  MCP1.LO('3','1')=137.4;  MCP1.UP('3','1')=137.4;
MCP1.L('3','2')=136.4;  MCP1.LO('3','2')=136.4;  MCP1.UP('3','2')=136.4;
MCP1.L('3','3')=134.1;  MCP1.LO('3','3')=134.1;  MCP1.UP('3','3')=134.1;
MCP1.L('4','1')=1;  MCP1.LO('4','1')=1;  MCP1.UP('4','1')=1000000;
MCP1.L('4','2')=1;  MCP1.LO('4','2')=1;  MCP1.UP('4','2')=1000000;
MCP1.L('4','3')=1;  MCP1.LO('4','3')=1;  MCP1.UP('4','3')=1000000;
MCP2.L('1','1')=209.4;  MCP2.LO('1','1')=209.4;  MCP2.UP('1','1')=209.4;
MCP2.L('1','2')=210.3;  MCP2.LO('1','2')=210.3;  MCP2.UP('1','2')=210.3;
MCP2.L('1','3')=211.1;  MCP2.LO('1','3')=211.1;  MCP2.UP('1','3')=211.1;
MCP2.L('2','1')=141.6;  MCP2.LO('2','1')=141.6;  MCP2.UP('2','1')=141.6;
MCP2.L('2','2')=141;  MCP2.LO('2','2')=141;  MCP2.UP('2','2')=141;
MCP2.L('2','3')=140.5;  MCP2.LO('2','3')=140.5;  MCP2.UP('2','3')=140.5;
MCP2.L('3','1')=176.4;  MCP2.LO('3','1')=176.4;  MCP2.UP('3','1')=176.4;
MCP2.L('3','2')=175.4;  MCP2.LO('3','2')=175.4;  MCP2.UP('3','2')=175.4;
MCP2.L('3','3')=174.5;  MCP2.LO('3','3')=174.5;  MCP2.UP('3','3')=174.5;
MCP2.L('4','1')=294.4;  MCP2.LO('4','1')=294.4;  MCP2.UP('4','1')=294.4;
MCP2.L('4','2')=318.7;  MCP2.LO('4','2')=318.7;  MCP2.UP('4','2')=318.7;
MCP2.L('4','3')=271.2;  MCP2.LO('4','3')=271.2;  MCP2.UP('4','3')=271.2;
MCP2.L('5','1')=1;  MCP2.LO('5','1')=1;  MCP2.UP('5','1')=100000;
MCP2.L('5','2')=1;  MCP2.LO('5','2')=1;  MCP2.UP('5','2')=100000;
MCP2.L('5','3')=1;  MCP2.LO('5','3')=1;  MCP2.UP('5','3')=100000;

EMAT =0.26;  ATHC.LO(JH,JC,P,I)=EMAT;  ATHC.UP(JH,JC,P,I)=1000;
*Resetting some GAMS options

OPTION ITERLIM = 1000000000;
OPTION LIMROW =50;
OPTION DOMLIM =100000000;
SOLVE AUTIL USING MINLP MINIMIZING TAC;

*Calculating areas for units in superstructure

AREA(JH,JC,P,I)$(INTERVAL(P,I) AND H(JH,P,I))=
Q.L(JH,JC,P,I)*(1/HOTS(JH,P,'H')+1/COLDS(JC,P,'H'))/(((1e-6)**3+
(ATHC.L(JH,JC,P,I)*ATHC.L(JH,JC,P,I+1))*((ATHC.L(JH,JC,P,I)+
ATHC.L(JH,JC,P,I+1))*0.5))**0.3333)+1E-6;

AOCCOST=SUM((P),(DOP(P)/NOP)*SUM((JH,JC,I),Q.L(JH,JC,P,I)*HUC(JH)))+
SUM((P),(DOP(P)/NOP)*SUM((JH,JC,I),Q.L(JH,JC,P,I)*CUC(JC)));

DISPLAY AREA,AOCCOST;
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