

OPTIMIZATION OF MASS EXCHANGE NETWORK BY MINLP

A DISSERTATION

on

OPTIMIZATION OF MASS EXCHANGE NETWORK

*Submitted in partial fulfilment of the
requirements for the award of the degree*

of

MASTER OF TECHNOLOGY

in

CHEMICAL ENGINEERING

(With specialization in **Industrial safety and Hazards Management**)

by

PRAMOD KUMAR SINGH



**DEPARTMENT OF CHEMICAL ENGINEERING
INDIAN INSTITUTE OF TECHNOLOGY ROORKEE,
ROORKEE -247667 (INDIA)**

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CANDIDATE'S DECLARATION

I, hereby, declare that the work which is being presented in the dissertation entitled “**Optimization of Mass Exchange Network**”, in partial fulfilment of the requirements for the award of the degree of Master of Technology in Chemical Engineering with specialization in **Industrial Safety and Hazards Management**, submitted in the Department of Chemical Engineering, Indian Institute of Technology - Roorkee, Roorkee, is an authentic record of my own work carried out during the period from May 2013 to June 2014, under the guidance of **Dr. Shabina Khanam**, Assistant Professor, Department of Chemical Engineering, Indian Institute of Technology, Roorkee.

The matter embodied in the dissertation has not been submitted for the award of any other degree.

Date: 25th June ,2014

Place: Roorkee

Pramod Kumar Singh

CERTIFICATE

This is to certify that above statements made by the candidate is correct to the best of my knowledge.

Dr. Shabina Khanam

Assistant professor

Department of Chemical Engineering

Indian Institute of Technology Roorkee

Roorkee, India

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When it comes to acknowledging the support and guidance of others in your personal or academic development, it is not an easy task. At the same time there are people without whom it is not possible to imagine the journey as well as the end of the work.

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NOMENCLATURE

A	Absorption Factor, dimensionless
U_{\min}	Minimum number of units
G	Mass flow rate of rich streams, kmol/hr
G_m	Mass flow rate of rich stream ,kg/hr
K	composition interval number, dimensionless
N_R	Total number of rich streams, dimensionless
N_S	Total number of Lean streams, dimensionless
b	constant in equilibrium relation , dimensionless
L	Lean stream flow rate , kmol/hr
ΔT	minimum temperature difference,
X	lean stream composition
Y	Rich stream composition
Greek letters	
ε	Minimum composition difference
subscript	
i	gas stream number
k	composition interval number
max	limiting value
superscript	
in	inlet composition
out	outlet composition
s	supply composition
t	target composition

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CHAPTER 1

INTRODUCTION

Mass Exchange Network (MEN) is a systematic generation of mass exchangers to transfer certain components from rich stream(s) to lean stream(s). It can be counter-current direct current mass transfer operation which utilizes a number of MSAs. The use of MEN has been growing steadily for diverse applications like feed separation, product separation, product finishing and recovery of valuable materials. Recently MEN has been widely used in waste minimisation.

Some very popular examples where MENs are extensively deployed includes removal of copper from Ammoniacal etching solution and a rinse water stream, removal of hydrogen disulphide from two rich streams: coke oven gas and tail gas from Claus unit, removal/recovery of phenols from waste streams of coal conversion plant, carbon dioxide removal in a formaldehyde plant.

Broadly MENs can be used in two ways. First type include design of a new plant which is in design stage and second using it retrofit an existing plant for the purpose of improving its efficiency. These problems are intensive and require a rigorous and specialised approach for its solution.

The synthesis of MEN networks can be broadly classified into two categories. In the first category design targets are achieved first and then a feasible MEN structure is drawn meeting all the criteria defined. The most prominent among this approach is pinch method where prior knowledge of structure is not required. The second method first draws all possible structure and then applies various mathematical tools to arrive at most optimum mass exchange networks.

Pinch is a thermodynamic and heuristic based method which does not require prior knowledge of networks. The concept of pinch based design was given El.- Halwagy et al in 1989. The design starts at the pinch division which is also the most constrained part and moves away from it.

Pinch technology was first introduced by Linhoff and Hindmarsh in 1983 to design heat exchange network. One of the great advantage of Pinch that is its independence of priori knowledge of structure was unleashed by El-Halwagy and Manousothekis (1989) for the

synthesis of mass exchange networks. They further presented an automated synthesis procedure in 1989b using linear programming. Their work was further improved by Hallale and Frasser by introducing the concept of super targeting which was again inspired from the success of this approach in design of Heat Exchange Networks.

On the other hand MINLP/MILP is a method based on structure of the network and mathematical formulation of the network. Papalexandri et al (1994) suggested formulation and solution of a mixed integer linear programming to optimise the solution of the network. It also gives the concept of hyper structure. However MINLP approach found difficulty in solving kremser equation. Szitkai et al further suggested a solution for MINLP approach for kremser equation. since they formulated piping system as well as mass exchange network as variables, the number of variables becomes very large.

Lee and Park extended the work of Friedler et al (1994) to suggest another method of design based on process graph theory. This method applies two step method. In the first step method all feasible structures are evaluated using combinational aspect of P-Graph theory so that only feasible structures are generated. In the second step feasible structures determined by are solved through MINLP. The significance of the P-Graph approach lies in fact that it generates only feasible structures unlike MINLP.

The problems of local optimum and a vast network of structures generated by earlier structures remained an area of concern. This problem was attempted by Garrard and Fragga through the application of Genetic Algorithm. Genetic algorithm approach given by Garrard and Fragga finds better results than other works on Genetic algorithm. Genetic algorithm is based on the biological principle of natural selection. The fundamental idea of GA is to place the parameter to be optimised of a problem within a chromosome which consist of gene. Each gene is mapped with certain parameter and further populations are generated by Crossover and Mutation. A fitness based selection is applied within the members to select the best.

Another landmark development in the field of Mass Exchange Network was design of exchangers which can accommodate the minimum utility concern for both mass and heat exchanger. The assumption of mass transfer being only an isothermal process was discarded. The concept of Input Variable, Output Variable and I-O relation was used to determine optimum utility consumption for both cold/hot utility as well as MSA.

CHAPTER 2

LITERATURE REVIEW

2.1 PINCH TECHNOLOGY

Pinch technology is primarily a methodology of minimising energy consumption in different processes by calculating minimum energy consumption and then achieving them by varying process operating conditions, energy supply methods and heat recovery systems.

The success of pinch technology in predicting the optimum design of Heat Exchange Networks (HENS) provided the impetus to search for similar application in different mass transfer operations. The search for an analogous method in mass transfer processes was met with analogous design of Mass Exchange Networks (MENS).

2.1.1 Analogy between MENS and HENS:

HENS	MENS
1.driving force ; minimum temperature difference between hot streams and cold streams	1.driving force ;Minimum composition difference between Rich streams and Lean streams
2.Transfer of heat energy from hot streams to cold streams	2.Transfer of desired component from Rich streams to Lean streams
3.Working capital calculated in terms of hot and cold utility	3.Working capital calculated in terms of Mass separating agents
4.Capital Cost Targeting is done by Area Targeting	4.Capital Cost Targeting is done in terms of Height targeting or Number of Trays Targeting
5.Driving Force Plot	5.Y-X plot
6.As driving force increases working capital while fixed cost of exchanger decreases	6.As driving Force increases MSA cost increases and capital cost decreases

2.1.2 A Typical MEN problem

“Given a set of multi-component feed streams of known composition . We have to design a series of systematic steps which produces product of desired component with minimum venture cost”

By “ MEN synthesis It means a systematic arrangement of Mass Exchanger to achieve desired objective taking into account Thermodynamic constraints. A Mass Exchange operation may consist of absorption, drying, distillation, humidification or all of these. The list of industries which can employ the concept of MENS is huge . However unlike HENS where only temperature difference is the sole parameter . The case of MENS becomes complex due to their dependence on composition difference between various streams as well as role played by solute –solvent interaction.

Problem Statement

Given a set of Rich streams $R = \{i\} i=1 \text{ to } N_R$, a set of lean streams $S = \{j\} j=N_S + 1, N_S + N_E$. It was required to synthesise a network of mass exchanger to preferentially dissolve $P = \{p\} p=1 \text{ to } N_P$

Of some component from Rich streams to Lean streams.

Each Rich streams has a mass flow rate G_i and has to be brought from a supply concentration $Y_i^s = \{y_{p,i}^s \mid p \in P\}$ to a target concentration $Y_i^t = \{y_{p,i}^t \mid p \in P\}$. Each lean stream has a supply of $X_j^s = \{x_j^s \mid p \in P\}$ and a target supply of $X_j^t = \{x_j^t \mid p \in P\}$. This should not exceed some constrained value

$$x_{p,j}^t \leq x_{p,j}^c \quad \forall p \in P$$

The flow rate of each lean stream phase is bounded by the following constraints

$$L_j \leq L_j^c$$

2.1.3 Assumptions made

1. Mass flow rate of each streams remain unchanged throughout the exchanger

2. Recycling within the exchanger is prohibited.

3. The equilibrium relation between any rich stream and lean stream is governed by the following equation

$$y_p = m_{p,j}x_{p,j} + b_{p,j} \quad j = 1, 2, \dots, N_S + N_E \text{ and } p \in P \quad (2)$$

Where $m_{p,j}$ and $b_{p,j}$ are constants

The first assumption is satisfied when transferrable component is in a very small quantity.

Even if the component to be transferred is in large quantity we can use mole fraction of the rich component based on transferrable component free basis.

The second assumption excludes the possibility of recycling which can be taken care of by mixed integer linear programming.

The third assumption directs us that equilibrium relation to be linear. However this is not always so. This problem can be taken care of taking smaller intervals so that for all practical purposes the equilibrium relation is linear.

2.1.4 DESIGN PROCEDURE

2.1.4.1 Minimum cost of MSA

The minimum cost of MSA is determined by the consideration of thermodynamic constraints. The objective during MEN synthesis would be on minimizing the cost of MSA when we use a single MSA. In many industries the cost of MSA has crucial role in determining overall annualised cost of the plant. The increase in solvent flow rate also increases the cost of regeneration where recycling is being done. So in most cases minimizing MSA cost forms essential part of MEN synthesis.

2.1.4.2 Minimum number of mass exchanger units

The purpose of calculating and then minimising total number of units aims at minimising total fixed cost of the exchanger. In addition we also wish to minimise additional separators, piping, maintenance and instrumentation cost which are indirectly related to number of units. The minimum number of units is calculated by the given formulae

$U = N_R + N_S + N_E - N_i$ Where N_i is the number of sub-problems into which original problems may be divided

2.1.4.3 Composition interval temperature (CIT)

CIT is a tool developed to analyse the transfer of a component from one level to another. It incorporates thermodynamic constraints into the synthesis of MEN. Using the concept of composition interval we introduce the concept of minimum

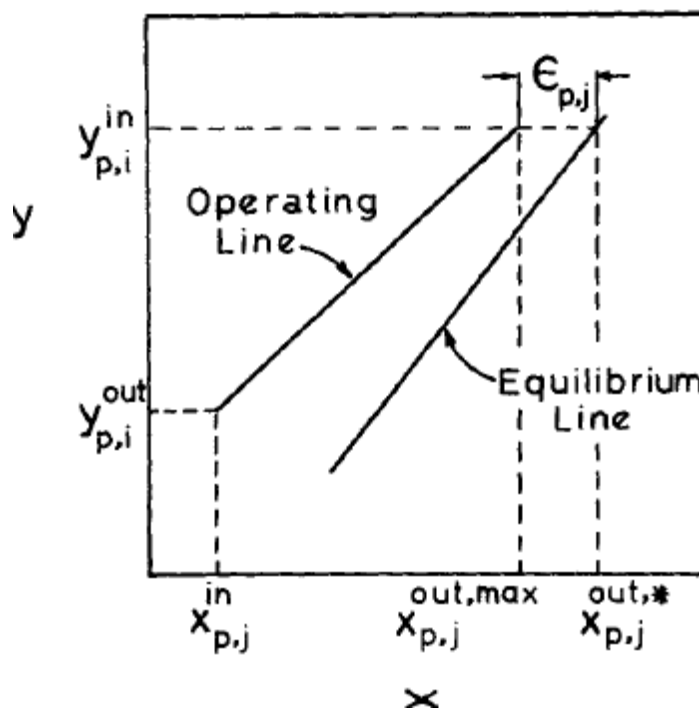


FIG 2.1 OPERATING LINE AND EQUILIBRIUM LINE

The equation of operating line is obtained by the mass balance between rich stream and lean stream which may be represented as follows

$$G_i(y_{p,i}^{in} - y_{p,i}^{out}) = L_j(x_{p,j}^{out} - x_{p,j}^{in})$$

The slope of operating line is given by solvent flow rate to the rich stream flow rate. The equilibrium relation between rich and lean streams is experimentally determined. Although the equilibrium relation is simple when only a single component is transferred, it becomes complex when multiple components are transferred.

$\epsilon_{p,j}$ is called minimum composition difference. It acts as driving force between operating line and equilibrium line. Increasing it increases operating cost but decreases capital cost and vice-versa.

2.1.4.4 Concept of pinch

Pinch forms an important part of MEN synthesis. Pinch is the point across which there is no transfer of materials from rich stream to lean stream or in other words it requires infinite driving force for mass transfer to occur through pinch. Naturally pinch is the most constrained area of MEN design synthesis. All design starts from pinch and moves away from it. At pinch minimum composition difference between operating and equilibrium lines vanishes to zero.

The concept of pinch is graphically represented in the following figure,

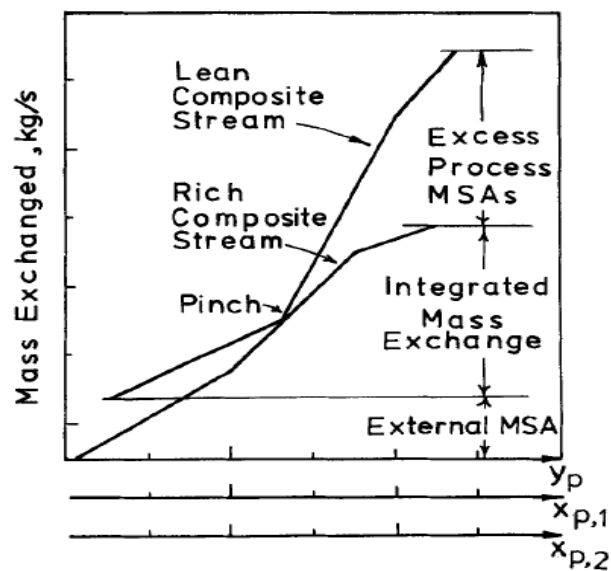


FIG 2.2 MASS TRANSFER COMPOSITE CURVES

From the figure it is clear that Pinch divides the problem into two distinct regions. One above the pinch and one below the pinch. In other words, now we have one rich end and one lean end.

Any stream or a part of a stream which has a composition higher than that at the pinch is called the rich end, and one that has a lower composition than the pinch is called the lean end.

2.1.5 PINCH FEASIBILITY CRITERIA.

1. above pinch Number of rich streams should be less than or equal to number of streams immediately below the pinch .If this condition is not satisfied stream splitting is required

$$N_{ra} \leq N_{la}$$

Where N_{ra} = Number of rich streams above the pinch

N_{la} = Number of lean streams above the pinch

2. Below the pinch number of rich streams or part of streams should be greater than number lean streams or part of stream

$$N_{lb} \leq N_{rb}$$

N_{lb} = number of lean streams below the pinch

N_{rb} = number of rich streams above the pinch

2.1.6 OPERATING LINE vs equilibrium line'

1. For rich end phase the following inequality must hold. It means the slope of operating line must be larger than equilibrium line

$$\frac{L_j}{m_{p,j}} \geq G_i$$

2. For lean end phase the following inequality must hold

$$\frac{L_j}{m_{p,j}} \leq G_i$$

2.1.7 Improvement of preliminary design

Owing to the existence of pinch the problem can be sub -divided into two distinct sub problems. One above pinch and the other below the pinch. As a result it is found that number of

utility becomes one greater than that calculated in first step. Therefore minimum utility network will involve one more unit than target number of units

2.2 Genetic Algorithm

Genetic algorithm is a stochastic optimization method based on biological principle of natural selection. The basic idea of GA is to place the parameters of the problem to be optimised within a chromosome (or individual) which consists of genes. Each parameter is coded to a gene in the chromosome. Parameters may be real numbers, integers, or even complex data structures such as trees or graphs. These parameters in most cases will have bound, however they may be selected from a set of discrete values and the gene is described by an *allele set*.

A genetic algorithm takes a population of chromosomes and generates new populations using a variety of operators including *crossover* and *mutation*. Members on which to operate are chosen from the population using a *fitness* based selection method. Wang et al was first to propose GA for synthesis of HEN.

The **fitness** measure of a population member is a measure of usefulness of the particular solution encoded by the chromosome is. In optimization, the **fitness** is quite often the value of the objective function for the given parameters or it may be the solution to an Linear Programming or Non Linear Programming that is generated from the chromosome.

A genetic algorithm terminates when a user specified criterion is met. The first step in using genetic algorithms for a new type of problem is to define a suitable encoding. The encoding of chromosomes must be able to represent a diverse and rich solution space and it is crucial that subsets of the chromosomes describe appropriate building blocks for solutions.

The work of Wang et al has been extended for the design of MEN due to its similarity with MEN to define the structure of MEN. However this comes with demerits of earlier problems. In fact encoding simultaneously the structure and operating conditions of the structure is a difficult task. Michalewicz in 1994 proposed encoding degree of freedom as free variables along with structure to take care of high constraints.

Goldberg in 1989 introduced the concept of penalty function for handling constraints which was further enhanced by Richardson et al (1989). The concept of level was introduced to encode the structure of mass exchanger. The number of levels is a user defined parameter.

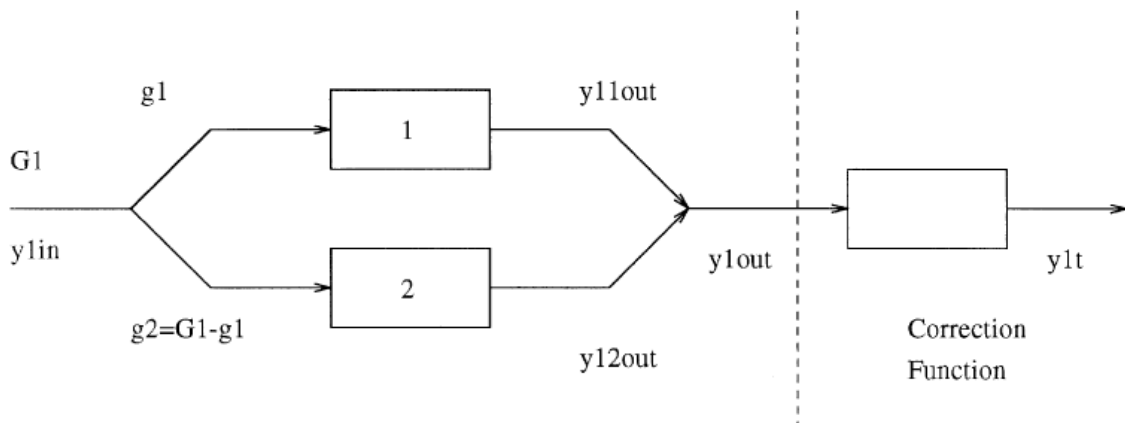


FIG 2.3 Network super structure without bypasses and with correction function

The length of chromosome is important factor for defining the actual make-up of the chromosome. It is done by finding the possible matches between rich streams and lean streams

2.2.1 Advantages of Genetic Algorithm

1. It has been made possible by encoding to simultaneously determine both the structure and actual mass exchange networks. It is further observed that the nonlinear and non convex problems are solved consistently and satisfactorily
2. It is also noted that the infeasible networks which appear initially disappear gradually as especially genetic operators especially replacement policy are applied .It allows only for fit members to exist in the end.
3. Method of genetic algorithm can be applied not only for linear problems but also for nonlinear problems.
4. Multiple solutions are available at the end and
5. They are suitable for use on parallel computers
6. They perform a global search are less likely to be trapped in local optimum

2.3 MILP/MINLP

Papalexandri et al proposed a hyper structure design for MEN design contrary to earlier methods of decomposition of network structure. The synthesis task of MEN is then reduced to formulation of mixed integer linear programming which optimizes working and capital cost simultaneously.

Szitkai et al have recommended MINLP approach for both continuous and discontinuous Kremser equations. Kremser equation assumes linear phase equilibrium relations.

2.3.1 Formulation of Kremser equations

Kremser equations give the required number of equilibrium stages for linear phase equilibrium relations for any mass transfer operation.

MINLP or any mathematical method involves three steps of design .The first step involves development of a super structure .The second steps involves formulation of mathematical program and the last step is finding the solution of the mathematical model. The superstructure of Papalexandri et al contains all imaginable structure without taking into care thermodynamic feasibility of the network. The mathematical program developed now using binary variables. However due to mathematical difficulty thermodynamic constraints are applied to eliminate infeasible network.

Universal optimality of the solution is achieved when both the objective function and the feasibility region of the MINLP are convex. However MINLP problems contain non -linear equality constraints (phase equilibria, mass balance), non -convex equations (Kremser equation) and non -convex function in the objective function like cost function. Although non convexity can be handled by MINLP solver(GAMS/DICOPT++) global optimal solution is elusive

Kremser equation is given by

$$\text{If } A \neq 1 \quad \text{then} \quad N_{A \neq 1} = \frac{\ln \left(\left(1 - \frac{1}{A} \right) \left(\frac{y_i^{in} - m_j x_j^{in} - b_j}{y_i^{out} - m_j x_j^{in} - b_j} \right) + \frac{1}{A} \right)}{\ln(A)}$$

Where

$$A = \frac{L_j}{m_j G_i}$$

If $A=1$ then
$$N_{A=1} = \frac{y_i^{in} - y_i^{out}}{y_i^{out} - m_j x_j^{in} - b_j}$$

A= absorption factor

2.3.2 Advantages of MINLP method

1. It does not require iterative approach of pinch based design methods.
2. Non-convex relations, non-convex equations are easily handled by this method.
3. Capital and operating cost can be optimized for a large number of networks.

2.4 State -Space Approach

This approach was first elaborated by Bagajewickz et al. This method is helpful in eliminating the drawbacks of MINLP methods.

This method was first introduced in the design of energy efficient distillation network by Bagajewicz and Manousiouthekis in 1990-1992. Roxenby and Manousiouthekis, in 1994, applied this method for non-isothermal separation networks. They traduced for the first time an approach which can solve the problem of minimum utility consumption for simultaneous exchange of heat and mass transfer.

The pinch technology fails for simultaneous exchange of mass and heat as it requires priori knowledge of inlet and outlet temperature, inlet and outlet composition and knowledge of stream population. The trade -off between mass separating agents and heating-cooling utility requires knowledge of temperature at which mass transfer takes place.

Roxenby and Manousiouthekis,in 1994 studied the case of non- isothermal heat exchange networks. Srinivas and El.Halwagy further simplified the network by some assumption like non-isothermal mass exchange, zero heat transfer in mass exchangers, equilibrium values

having linear relationship with temperature. Papalexandri and Pistikopolous have recommended the extension of superstructure representation. These hyper-structure represents the special case of State space approach.

State space approach works on a set of variables which characterizes the behaviour of the system. These variables are further classified into Input and output variables. The relation between these two is called Input-Output relation (I-O relations). The set over which Input-Output variables assume their values are called input-output spaces

Any set of variables whose knowledge along with the knowledge of input and I-O relations determines the set of outputs is called a set of state variables. The set over which they assume values are called state spaces and the relation between state knowledge are referred to as input-state-output relations.

The state-space approach is helpful in calculating the total annualised cost of problems with simultaneous exchange of mass and heat. It happens in two steps. In the first step the utility cost and mass separating agent cost is calculated on the basis of minimum temperature difference or minimum composition difference. In the second step minimum number of fixed utility is calculated on the basis of that calculated in step 1.

The analysis and synthesis of chemical process networks requires developing Input-space-Output relations. These are complex systems whose relations are based on basic principles of mass and heat transfer. The minimum utility consumption. There are two operators used to represent heat and mass exchange network; a distribution network where stream mixing and splitting occurs and a process operator where heat or mass transfer takes place.

2.5 Process-Graph Theory

Lee and Park, in 1996 proposed the process graph theory for optimal synthesis of mass exchange network. This approach has been able to mitigate the limitations of both pinch based design on one hand and MINLP method on the other.

2.5.1 Assumptions made

1. Mass flow rate of each stream is constant throughout the network
2. The equilibrium relation between phases is independent of presence of solute in other solvent
3. Only counter-current mass exchangers are considered
4. Mass exchange between rich-rich and lean-lean streams is neglected

Uniform temperature and pressure is assumed throughout the exchangers to facilitate the use of single equilibrium relation throughout the exchanger

2.5.2 Design procedure

The design procedure in process graph theory consists of two main steps

1. Evaluation of all feasible structure

A material set of process graph theory is obtained from information about rich and lean streams. Operating unit set is obtained from information of mass exchange units. The union of material set and operating set is gives maximal structure which generates all possible networks structure.

2. Determination of operating conditions

A non- linear programming is formulated for each network structure generated step. The optimization of the above structures gives the operating conditions of the structure. This method which utilizes the concept of P –Graph theory and non -linear programming formulation - to find the optimal mass exchange network . The proposed two step procedure determines network structure as well as operating conditions. The reduction in optimization problem is due to the generation only feasible structure in step 1 of design. The significance of this method lies in its efficient use of combinatorial problem as well as simplification of optimisation problem.

2.5.3 Disadvantages of the P-Graph theory

1. It requires a good ,feasible , starting guess.
2. In some cases dramatic increase in space size is observed as the size of the solution expands
3. Need for simplification of non- linear programming to guarantee global optimality or alternatively need for a differential function for a non-linear programming solver

CHAPTER 3

Motivation for the current project;

The design of MEN was studied by various methods. Although Pinch design is easy , it does not takes into many complexities of the MEN. For example it calculates minimum cost utility for a fixed composition difference for a particular network only. To improve the shortcomings of pinch design various mathematical approach like P-Graph theory , State -Space approach and MINLP was studied. It was found that most of these methods were cumbersome andnot easy to apply. On the other hand MINLP approach by mathematical formulation and thermodynamic constraints was able to give an improve the limitations of earlier methods. In light of the above our objective has been defined as follows

OBJECTIVE

1. To identify the problem in the Mass exchange network
2. To define objective function and formulate mathematical problem of the MEN
3. To solve the Mathematical Problem using MINLP solver software GAMS
4. To calculate the cost of the MEN obtained by above method

CHAPTER-4

PROBLEM STATEMENT

IN this problem some problems of mass exchange network are formulated which will be targeted and designed by MINLP approach

4.1– A. The sulphur dioxide is removed from a set of four gas streams (1 to 4) using freshwater as a mass separating agent. \

4.1.1 INPUT DATA

The stream is shown in the **Table 4.1** below

TABLE 4.1 Stream data for water minimisation problem

GAS STREAM	G	Ys	Y ^t
1	50	.01	0.004
2	60	0.01	0.005
3	40	0.02	0.005
4	30	0.02	0.005

Y_s supplied mole ratio

Y_t targeted mole ratio

the minimum composition difference for this problem is taken to be 5×10^{-6}

4.1.2 Expected output

To design a mass exchange network for this problem and the mass equipment used in the MEN

4.2 Water minimisation with water sources

The problem 3.1 is again solved using two water sources ; freshwater and wash water streams .

4.2.1 INPUT DATA

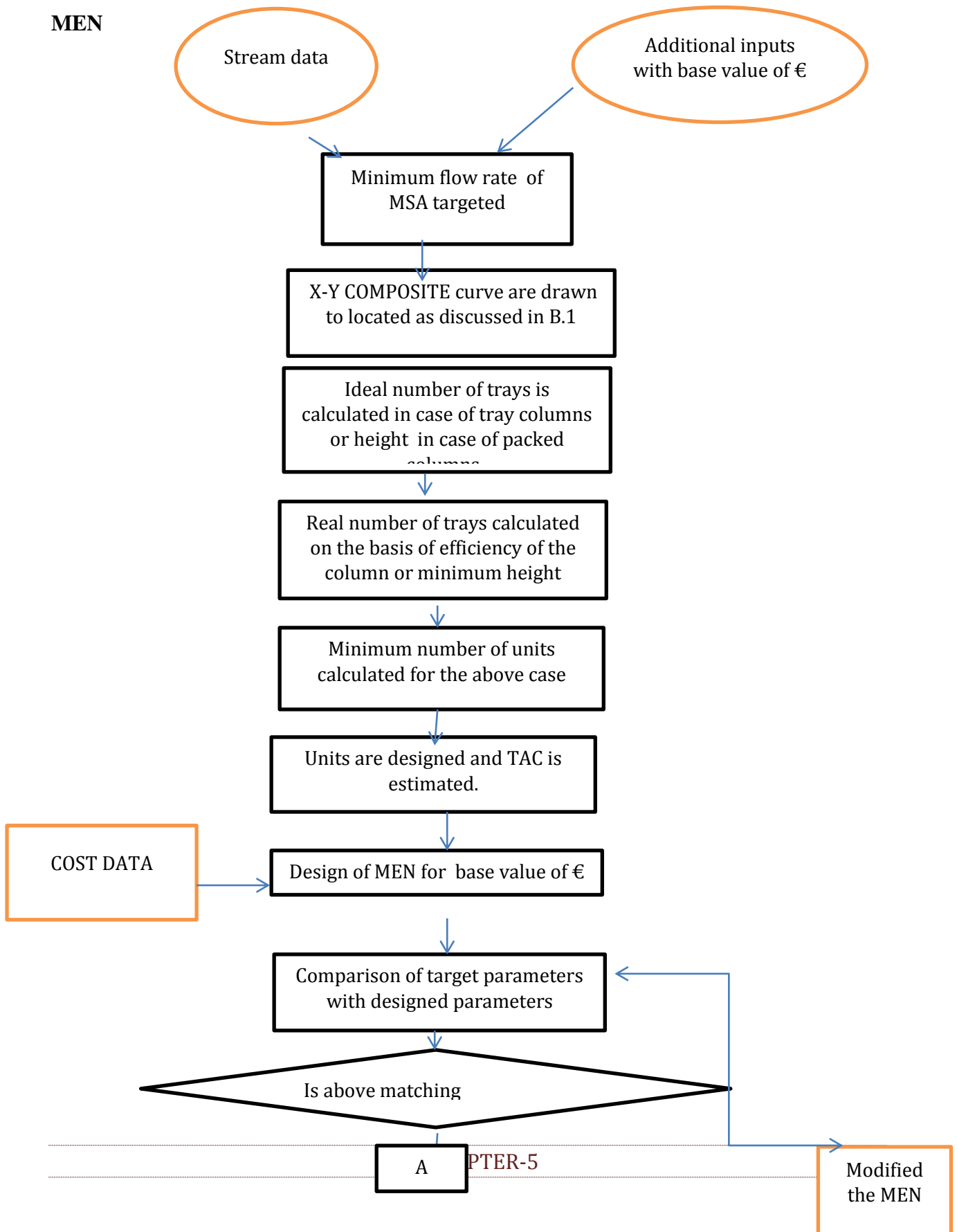
The stream data for this problem is same as in previous problem 3.1 . The flow rate and supply composition of wastewater are 1500kmol/hr and .0003 , which are fixed . The minimum composition difference is taken as 5×10^{-4}

4.2.2 EXPECTED OUTPUT

To design a MEN for multiple water sources and equipment used in this

4.1.2 FLOWCHART OF DIFFERENT STEPS REQUIRED DURING TARGETING AND DESIGN OF

MEN



This chapter is devoted to explain the methodology adopted for targeting minimum Mass exchanger network operating cost as well as total annual cost .MINLP method which is a mathematical method has been proposed for solving the problems

5.1 METHOD OF MINLP

Here the stepwise methodology for MINLP method is discussed in detail. In the present work four mass exchanger problems are targeted and designed by MINLP method. These problems were discussed in detail in chapter -3. The details of the problems are further separately discussed in Appendix-A. Although different problems require different approach ,yet there is some similarity in the way they are approached. This is discussed below.

5.1.1 Algorithm

5.1.1.1 Input Data for Mass exchange network

5.1.1.2 Stream data

The stream information is in the form of supply composition, target composition as well as mass flow rate of each stream

5.1.1.3 Additional inputs

In solving the program by MINLP method , we require several other inputs as well. They are unit cost of Mass exchanger ,equilibrium relation between rich streams and lean streams, minimum composition difference between equilibrium line and operating line. Unit cost of single plates are also given .Some of the data's need to be initialized for arriving at coherent solution.

5.1.1.4 Targeting base case

The base case simply refers to the initial value of minimum composition difference assigned to the problem

Following steps are followed in general for all problems of Mass exchange network by MINLP method

Step 1: The minimum operating flow rate for desired duty is targeted .This is operating cost of the problem.

Step 2: The X-Y composite curves for all streams in the process is drawn and the point of pinch is identified at minimum composition difference .

Step3: The number of ideal trays are calculated in this case from program results itself.The fixed cost may be in the form packed column depending upon the choice of equipment used.The number of trays are calculated by Kremser equation

Step 4: The real number of trays are calculated by dividing the ideal number of trays calculated in step 3 by an efficiency term(E) .

Step 5: Minimum number of units is targeted for the above situation

Step 6: Mass exchange network is designed for the above situation and Total Capitalised 1 Cost(TCC) is calculated.

Step 7: Now total annual cost is targeted.

5.1.1.5 Design of the base case

The design of mass exchange network is done considering feasibility criteria.

5.1.1.6 Matching designed parameters with targeted parameters

It is not always possible to get the same value for different parameters of mass exchange network for both targeted design and actual design. The difference in parameters leads to increment of TAC(Total Annual Cost). As increment is un economical , to arrive at optimum design retrofit may be considered.

5.1.1.7 Targeting optimum value of €

The steps of 4.1.1.2 are repeated over a wide range of € and graph between total annual cost VS Minimum composition difference is drawn. The value of € for which Total Annual Cost is minimum is said to be optimum value of minimum composition difference.

5.1.1.8 Targeting for minimum value of €

The value of minimum composition difference calculated in 4.1.1.5 is called optimum value of minimum composition difference . Based on this value Mass exchange network is retargeted.

5.1.1.9 Design for optimum value of €

Design of MEN for optimum value of minimum composition difference is done as described in 4.1.1.3.

5.1.1.10 Conformity between targeted parameters and designed parameters at optimum value of €.

The redesign of the actual design is recommended only when there is large difference between actual design and targeted design .in such cases modification may be done.

5.1.1.11 Comparison of results of MEN at base value of € and targeted value of €.

The comparison between TAC (Total annual cost) value at base value and optimum value gives an idea of savings in the actual mass exchanger design.

5.1.1.12 Selection Criteria for Mass exchange network

When more than one MEN is available for same value of minimum mass exchange network ,The engineer applies his experience is selecting the most appropriate network which suits the needs of the industry.

CHAPTER-6

RESULTS AND DISCUSSIONS

This Chapter deals with important results obtained by solving four mass exchange network (MEN) problems (problem 3.1 to 3.2). The detailed problem description and cost data for these problems are given in Table 3.1, Table 3.2, Table 3.3, Table A.1, Table A.2 and Table A.3. The description of the problems is shown in Appendix A. The MENs were developed by MINLP approach described in Chapter 4. The MINLP approach is capable of solving non-linear equations like Kremser equation which is solved by software GAMS. The modified network enhances the mass exchange between exchangers and reduces the utility requirement, which in present case is Mass Separating Agents. The optimum network is one which gives minimum annual cost.

The solution of mass exchange network consists of mainly four steps described in Chapter --- 5 namely the targeting phase, the design phase (design of MEN), the modification phase and then the optimum design phase. A step wise algorithm was developed for the above task. A program in Algebraic solver GAMS .The details of the algebraic .The details of the results obtained by this program are discussed in this chapter.

6.1 SALIENT FEATURES OF PROBLEM 3.1

In this problem SO₂ is absorbed in fresh water (mass separating agent) from four rich streams .The stream data and cost data are given in Table 3.1 and Table A.1, respectively.

The base minimum composition is taken as $5 * 10^{-6}$ kmol SO₂/kmol Water. With this base value of minimum composition difference the computer program show the following results in terms of targets.

1. The minimum flow rate of fresh water stream = 1590kmol/hr
2. Total number of trays target for all absorption columns =140
3. Total minimum number of units target = 5
4. Total capital cost target of the network =Rs 27399600

The details of the total capital cost targeting is given in the Table B-5 OF Appendix B .During cost targeting the sizing of the absorption column of the network is done . For convenience the data of Table B-5 is reproduced in Table 5.1

TABLE6.1. Capital Cost Targeting of Network

Gas Streams	Number of Mass Transfer units	Diameter (m)	Number of trays	Height(m)	Capital Cost (Rs)
1	1	0.64	23	14	4873236
2	1	0.7	23	14	5509639
3	1	0.58	24	15	4712752
4	1	0.58	51	28.5	8888122
5	1	0.5	19	12.5	3641691

6.1.1 Development of MEN

Two MENS are developed, one for minimum flow rate of mass exchange network and the other for minimum total annual cost based on the targeted values shown in Table 5.1

6.1.1.1 Design of Network for minimum flow rate of mass separating agents

For above case, When the flow rate of fresh water stream is minimum (equal to 1400 kmol/hr), the pinch point composition $X_{pinch}=0.000503$ and $Y_{pinch}=0.01$ and minimum composition is equal to 5×10^{-6} .

The detailed design of the network is shown in Figure 5.1 and henceforth will be referred to as Network-2 (where is network-1?). The MEN in Fig. 5.1 has following features:

1. Total number of trays required for all absorption =187 (71 trays are below the pinch and 116trays are above the pinch)
2. Total minimum number of units (absorption columns) required=5 (3 below the pinch and 2 above the pinch)

3. Total actual capital Cost of the network = Rs 34757251

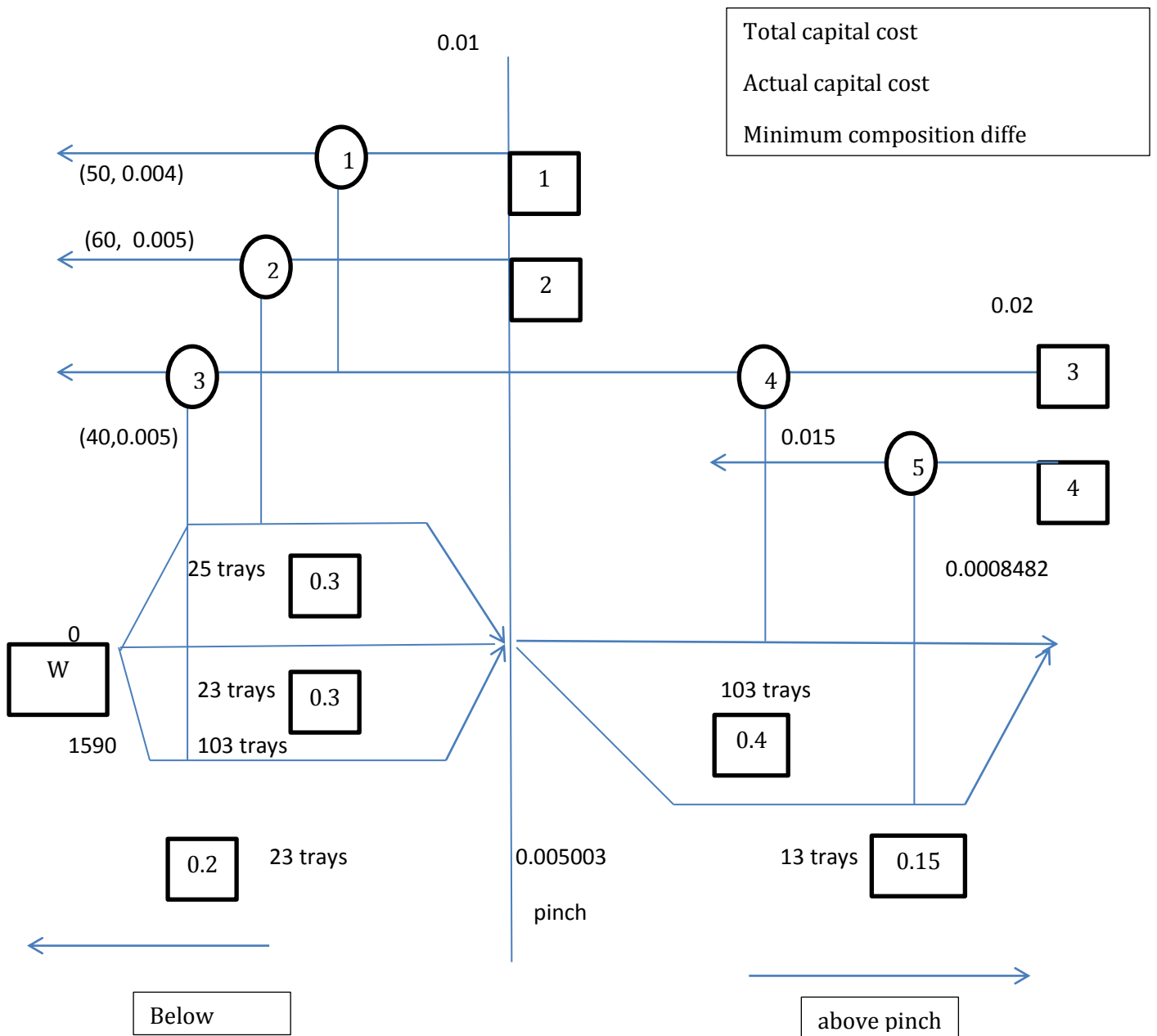


Fig 5.1 The complete network design for the base case (NETWORK -1)

In network-1, it is observed that below the pinch number of targeted trays and actual trays are same but above the pinch the number of trays is 101 which is more than 70 targeted. This increase in total number of trays leads to increase in total capital cost. This requires our design to be improved further. It is done by adding an extra mass exchanger to the network as shown in fig 5.2. By adopting this provision the mass transfer load of rich stream number 3 is being shared between absorption column 4 and 5 out of which unit number 5 is new addition. Previously, unit number 4 used to take the entire load of stream number 3 above the

pinch. The MEN (Network-1) is redesigned and shown in fig 5.2 (henceforth it will be called Network-2), Which has following salient features:

1. Total number of trays required for all absorption columns =141(71 trays are below the pinch and 70 above the pinch).
2. Total number of units required=6 (3 units below the pinch and 3 units above the pinch)
3. Total Actual capital cost of the network=Rs29043827

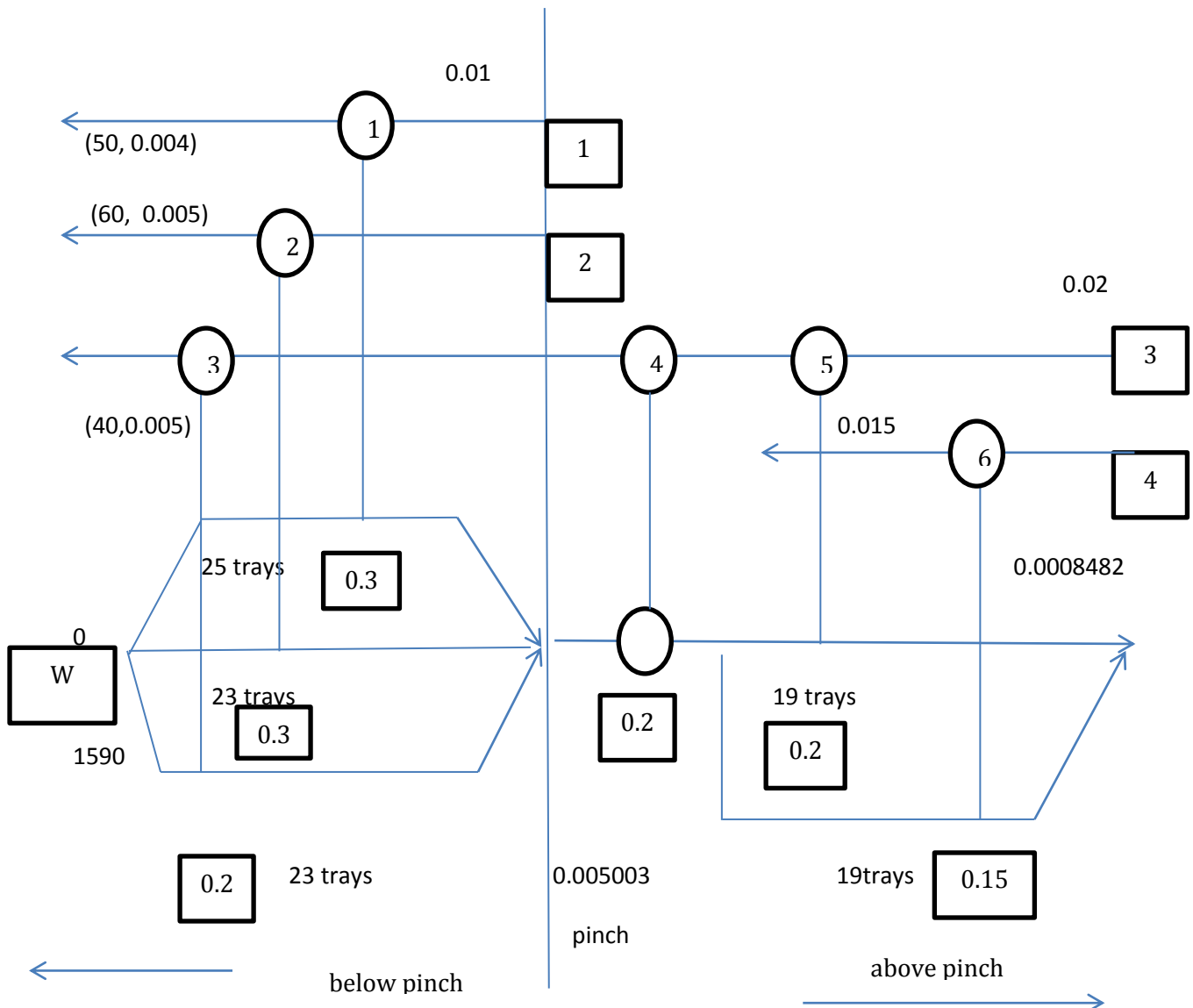


Figure5.2 Improved MEN Design for base case(Network-2)

In the new improved design (Network-2) using the base case detailed in section 5.1 , the number of trays required 142 which is almost the same as targeted but this is achieved by placing unit 6 in place of unit 5 in the network design. This network has actual capital cost 6% more than the targeted design. Hence it is observed that an optimally designed network

does not guarantee minimum number of units as well. Network -2 is acceptable for minimum flow rate of mass separating agents .

6.1.1.2 Design of network for minimum total annual cost

In the design of MEN the minimum composition difference is very important parameter. As the value of minimum composition difference is increased the cost of utility increases where as the capital cost of the network decreases due to increase in the driving force for mass transfer between operating conditions and equilibrium conditions. Thus, there is always a compromise between operating cost and capital cost. This directs us to find an optimum value of minimum composition difference so that total annual cost is minimum. The total annual cost is sum of annualized capital cost and annual operating cost. For the present case the value of minimum composition difference was varied between 5×10^{-6} kmol SO₂/kmol Water and 1×10^{-4} kmol/SO₂. It is observed from the graph (where?) that the total annual cost increases for values less than 5×10^{-6} kmol SO₂/kmol Water and for values more than 1×10^{-4} kmol/SO₂.

From the graph it is observed that total annual cost is minimum for a value of minimum composition difference of 5×10^{-6} kmol SO₂/kmol Water.

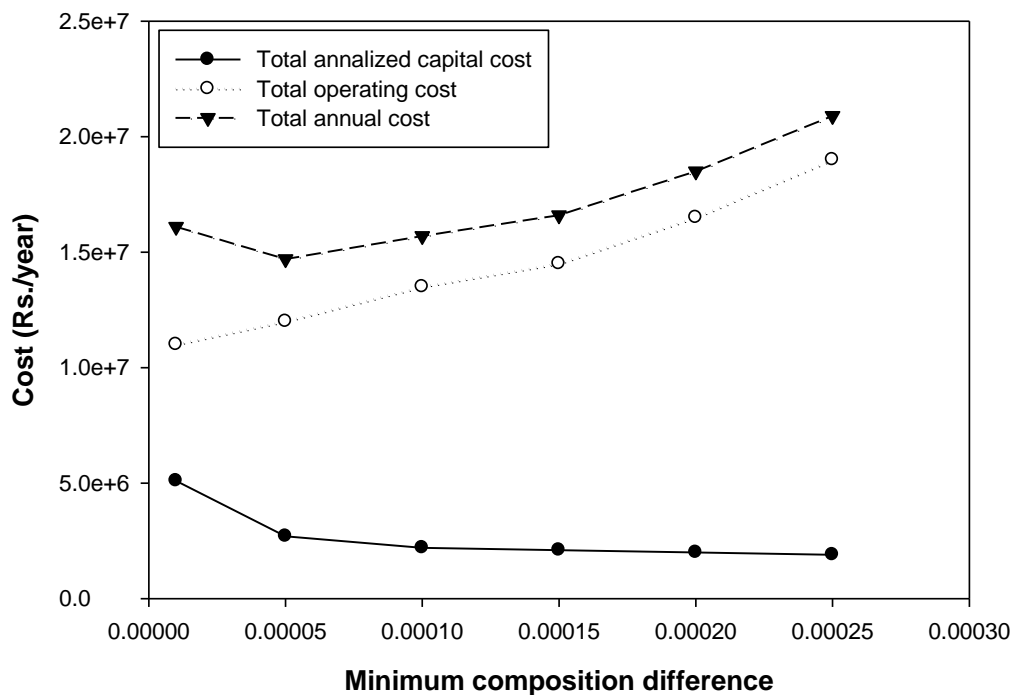


Figure 5.3

The following values of different parameters are obtained:

1. The flow rate of fresh water = 1700kmol/hr
2. Total number of trays target for minimum columns=61
3. Total minimum number of units =5
4. Total annual cost target of the network=Rs 15355127/year

At this minimum value of € The MEN is redesigned and is shown in figure 5.4 which has following characteristics

1. The flow rate of fresh water = 1700kmol/hr
2. Total number of trays target for minimum columns=61
3. Total minimum number of units =5
4. Total annual cost target of the network=Rs 14355197

0.01

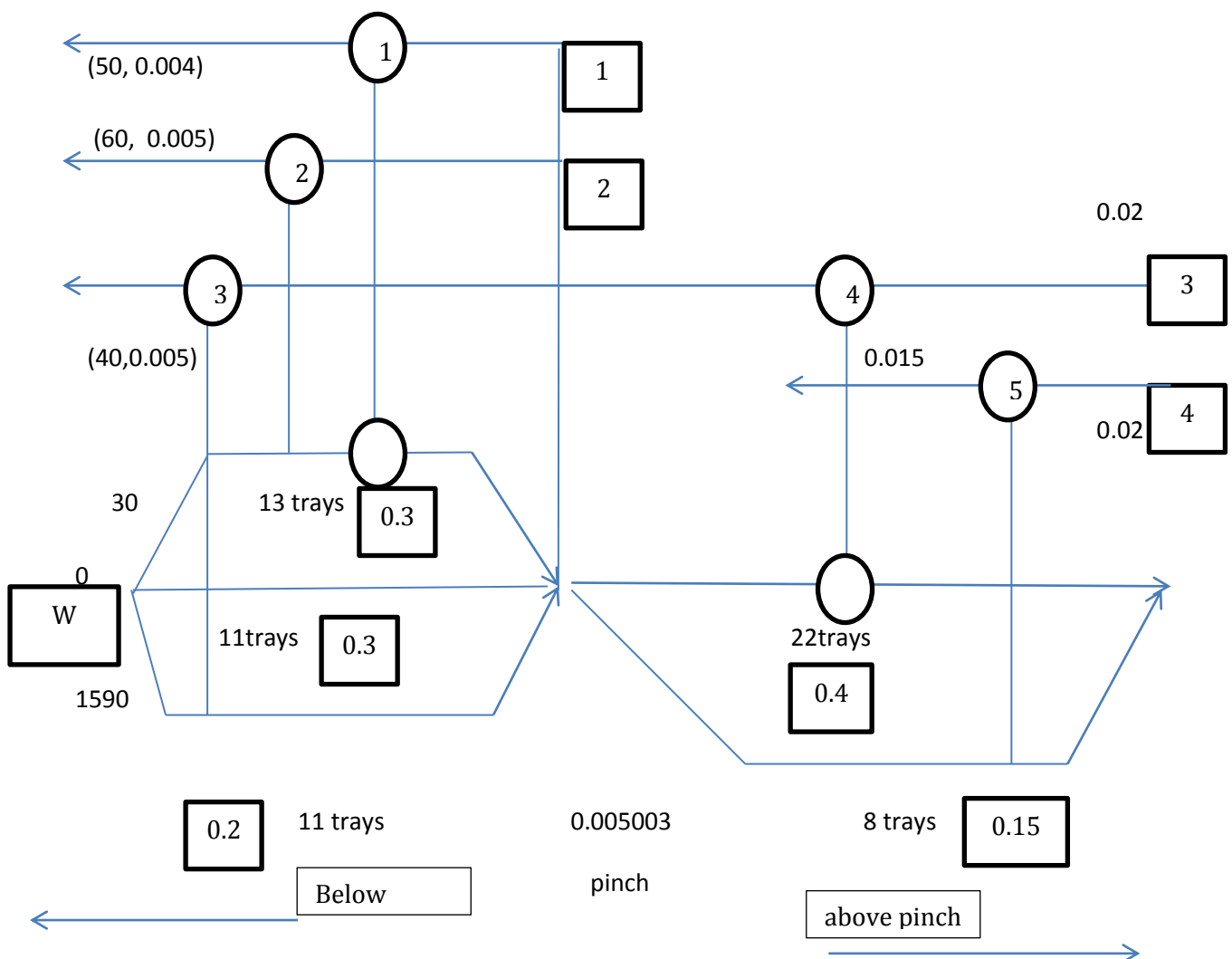


Fig 5.4 The complete network design for the base case (NETWORK -3)

At this minimum value of composition difference MEN is redesigned which has following features

1. The MSA flow rate = 1700 kmol/hr
2. Total number of trays required for absorption= 65
3. Total number of units=5
4. Total annual cost of the network= Rs 144722578/year

Now network -3 satisfies the targeted value with 5 number of units with 65 number of trays while network -2 gives satisfactory answer with 6 number of units.

6.1.2 Selection of Final Network

Hence the selection of final network will be between network 2 and network -3. A comparative results for both the network is presented for convenience to decide on the best network selection

Table 6.2 Comparative results for network -2 and Network-3

	Number of trays target	Actual number of trays	Number of units target	Actual number of units target	Target TAC (Rs/year)	Actual TAC (Rs/year)	% difference in actual and target
Network-2	140	141	5	6	15884418	16165059	1.7
Network-3	64	65	5	5	14355197	14472578	0.82

From the above table it can be concluded that for same value of minimum composition difference the Network-3 is more economical and has minimum TAC between the two.

For the other problems the final MEN is designed for optimum composition difference.

6.2 SALIENT RESULTS OF PROBLEM 3.2

In this problem SO₂ is absorbed in two freshwater streams(mass separating agents). One is freshwater and other one is wastewater stream. The stream data and cost data are given in Table 3.1 and Table A.1 .Tray type absorption columns are used as mass transfer equipment. The Whole problem is described in Appendix A .. The flow rate and supply composition of wastewater are fixed as 1500kmol/hr and 0.0003 respectively .

The base minimum composition between operating line and equilibrium composite curve is taken as

5×10^{-6} kmol SO₂/kmol Water. With this value of minimum composition difference , the GAMS program gives the following results in terms of targets

1. The minimum flow rate of freshwater stream = 984 kmol/hr
2. Total number of trays target for all absorption columns = 138
3. Total minimum number of units targets= 7
4. Total annual cost target of the network= Rs 22191309/year

The details of the capital cost targeting are described below

Table 6 .3 Capital Cost Targeting of the network

Gas streams	Number of mass transfer units	Absorption Columns			Capital Cost (Rs)
		Diameter (m)	Number of Trays	Height(m)	

Below the pinch

1	2	0.64	18	12	40306628
1		0.64	18	12	4030628
2	1	0.7	36	21	7420361
3	1	0.58	36	21	6581571

Above the pinch

3	2	0.58	24	15	4712752
3		0.58	6	6	1845169
4	1	0.5	4	5	1406469

6.2.1 DEVELOPMENT OF MEN

As discussed in section 5.1 that the minimum total annual cost comes out to be minimum for minimum composition difference. Hence in this problem MEN design for this problem will be done for the same value of minimum composition difference.

As minimum composition difference is a very sensitive parameter. Total annual cost, Total capitalized cost and operating cost are calculated from the Program And B for a range of values. Further a graphical representation is done for the data obtained for the above parameters. The optimum value of minimum composition was found to be 5×10^{-6} kmol SO_2/kmol Water.

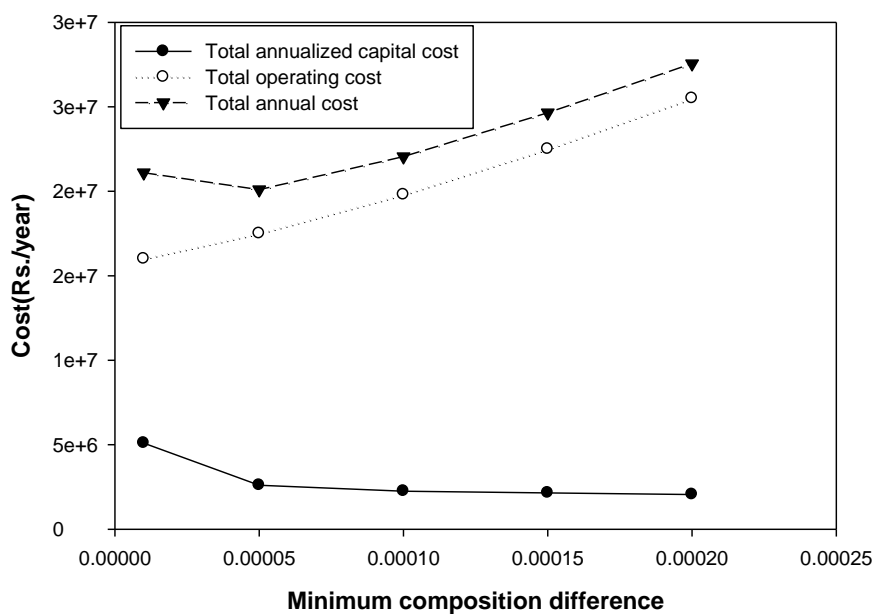


Fig 5.5

The salient results of this network was found to be as follows

1. Total flow rate of freshwater stream =1228 kmol/hr
2. Total number of trays required for all absorption columns=62
3. Total number of units =7
4. Total actual annual cost of the network = Rs 21223530/year

It is observed that the required number of units in Network is 62 while the targeted number of trays is 58 but the number of units required is same as the targeted value of 7. The difference between actual number of trays and targeted number of trays is mere 0.68%. Hence for final selection Network will be chosen.

CONCLUSIONS AND RECOMMENDATIONS

7.1 CONCLUSIONS

1. It can be safely concluded that the TAC of Mass Exchange Network design for optimum value of minimum composition is less than the targeted value of TAC for base value of minimum composition difference when utility (Mass Separating agents) is minimum.
2. It can also be safely concluded that analysis of MEN design using MINLP improves the operation of MEN during the target stage itself without going into details. Here the insight of engineer is not required.
3. The design having minimum number of units may not give minimum total annual cost .In fact design having number of units more than bare minimum is able to give minimum total annual cost most of the time.
4. In many cases the TAC vs€ may be flat in the region of optima.This arises due to shape of plots between capital cost vs€ or for plots between operating cost vs €. Therefore depending upon the cases a unimodel TAC vs € is not uncommon.

7.2 RECOMMENDATIONS

- 1.The computer program developed for solving the two problems should further be developed to solve problems of harmful gases recovery from effluent gases from the industry.
- 2.The program was developed assuming linear equilibrium relation between two phases for solute or material to be transferred. The attempt should be made to extend this approach to solve problems containing non-linear equilibrium relation between two phases.
3. Other optimization techniques like Super targeting , MILP , NLP , Process –Graph theory , State Space Approach can be used for arriving at different values of optimization variable and compare them.

APPENDIX –A

PROBLEM DESCRIPTIONS

PROBLEMS TO BE SOLVED

A-1 Removal of SO₂ from a mixture of four process gases is done by using freshwater as Mass Separating Agent to absorb SO₂. Each gases mainly consists of air containing traces of solute to be removed. Each of these gases are insoluble in water .This is necessary condition for separation to be effective. The composition of SO₂in four gases is expressed in mole ratio represented by; **Y**. Each stream has a supply composition as well as target composition which is denoted by Y_s AND Y_t respectively. The gas flow rate G is expressed on sulphur dioxide free basis. The schematic diagram of absorption tower is shown in Figure A.1 .These flow rated remain fixed as SO₂ is absorbed .The gas streams are all at room temperatures and Gas is supplied at this temperature

The aim of MEN design is to find minimum mass separating agents required for desired separation and hence give minimum capital cost .The mass exchange units in this problem are absorption columns.

The stream data is give in Chapter -3

The equilibrium relation between rich and lean stream is given by following equation

$$Y^* = mX + b$$

Wherem = slope of equilibrium line =26.1 and b (intercept of equilibrium line) = -0.00326

X is the composition (molar ratio) of SO₂ in water.

Cost data for this problem is taken from Coulson et al.(1993) and is shown in the Table A.1

Table A.1 . Cost Data for water minimization problem

Water cost	Rs 42.272/ton
Operating cost	8600h/year
Column capital cost	
Shell	Rs 422720*H ^{0.95} *D ^{0.6}
trays	Rs 20079e ^{0.8D} per tray
Capital annualization factor	0.2

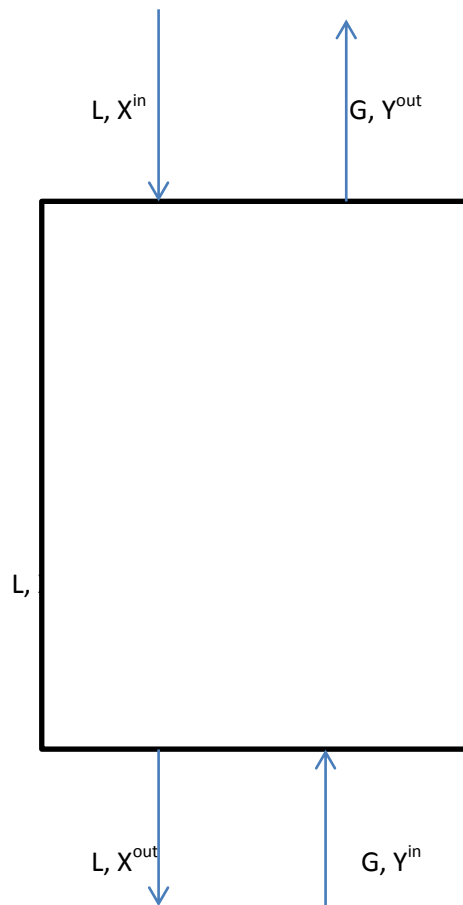


Fig.A.1 The schematic Diagram of absorption column

A-2 Description of Problem 3.2

The above problem is repeated with multiple water sources. The stream data and cost data are same for this problem. There are two mass separating agents in this case; one is freshwater stream and other is wastewater stream source. The wastewater having flow rate of 1500 kmol/hr , is going to a treatment plant having SO₂ Concentration of 0.003. The use of wastewater is an economical decision to reduce the usage of freshwater stream for separation process. The wastewater stream is available free of cost. The presence of other contaminant does not affect equilibrium solubility relation between rich stream and lean stream. This is one of the assumptions of the problem. Minimum composition difference is $5 * 10^{-6}$ kmol SO₂/ kmol water

B.1 Computer programs for solving the above problems

sets i Rich streams /1*4/
 j lean streams /1/ ;

Scalar nok number of stages in superstructure / 4/;

Set k composition locations nok + 1 /1*4/
 st(k) stages
 first(k) first composition location
 last(k) last composition location ;
 st(k) = yes\$(ord(k) lt card(k)) ;
 first(k) = yes\$(ord(k) eq 1) ;
 last(k) = yes\$(ord(k) eq card(k)) ;

Binary Variables

z(i,j,k) ;
 parameters
 GR(i) MASS flowrate of RICH stream ,
 YIN(i) supply composition of rich stream,
 YOUT(i) target composition of rich stream ,
 XIN(j) supply composition of lean stream,
 XOUT(j) target composition. of lean stream,
 eGR(i) total mass content of P in Rich Stream,
 eGL(j) Total mass content of P in Lean Phase,

A Absorption factor for mass exchange network
 MSACOST cost of mass separating agents ,
 unitc fixed cost for exchangers,
 GLcost(j) unit cost for individual Lean streams,
 gamma(i,j) upper bound of driving force,
 NUMcoeff plate cost coefficient for exchangers,
 aexp cost exponent for exchangers,
 NL total number of plates by kremser equation ,
 eampp minimum compoition approach ,
 E efficiency of plates;

Positive variables

YR(i,k) Composition of rich stream i as it enters stage k
 XL(j,k) composition of lean stream j as it leaves stage k
 M(i,j,k) mass exchanged between i and j in stage k
 em(i,j,k) composition approach between i and j at location k
 KY(i,j) overall mass transfer coeffiecient between i and j streams ,

$b(i, j)$ slope in equilibrium relation
 $c(i, j)$ constant in equilibrium relation
 $W(i, j)$ constraint for mass transfer
 $dy(i, j, k)$ driving force between rich and lean stream at stage k
 $numplate1(i, j, k)$ number of plates calculated by kremser equation for $A <> 1$
 $numplate2(i, j, k)$ number of plates calculated by kremser equation for $A = 1$
 $N(i, j, k)$ number of plates calculated by kremser equation for both the condition in k stage
 $teN(i)$ total number of plates from all superstructure

$GL(j)$ mass flow rate of MSA

Variable cost total annual cost ;

Equations

$ER(i, k)$ mass exchanged by rich stream i in stage k for p component
 $eqteR(i)$ total mass exchanged by rich stream i for p component
 $eL(j, k)$ mass exchanged by rich stream j in stage k for p component
 $monYR(i, k)$ monotonicity of yR
 $monXL(j, k)$ monotonicity of XL
 $monYRL(i, k)$ monotonicity of YR $k = last$
 $monXLF(j, k)$ monotonicity of tc for $k = 1$
 $YINR(i, k)$ supply composition of rich streams in stage k
 $XINL(j, k)$ supply composition of rich streams in stage k
 $logM(i, j, k)$ logical constraints on M
 $logemR(i, j, k)$ logical constraints on em at the Rich end
 $logemL(i, j, k)$ logical constraints on em at the Lean end
 $eqNUM1(i, j, k)$ number of plates calculated by kremser equation for $A <> 1$ in k stage
 $eqNUM2(i, j, k)$ number of plates calculated by kremser equation for $A = 1$ in k stage
 $eqN(i, j, k)$ number of stages calculated by kremser equation for both condition
 $eqteN(i)$ total number of stages
 $eqGL(j)$ mass flow rate of MSA calculation

obj objective function ;

$$eqteR(i).. (YIN(i)-YOUT(i))*GR(i) =e= \sum((j,st),M(i,j,st));$$

$$eqGL(j)..GL(j)=e= \sum(i,(YIN(i)-YOUT(i))*GR(i))/(XOUT(j)-XIN(j));$$

$$eL(j,k)\$st(k).. GL(j)*(XL(j,k) - XL(j,k+1)) =e= \sum(i,M(i,j,k)) ;$$

$$ER(i,k)\$st(k).. GR(i)*(YR(i,k) - YR(i,k+1)) =e= \sum(j, M(i,j,k)) ;$$

$$YINR(i,k)\$first(k).. YIN(i) =e= YR(i,k) ;$$

$$XINL(j,k)\$last(k).. XIN(j) =e= XL(j,k) ;$$

$$monYR(i,k)\$st(k).. YR(i,k) =g= YR(i,k+1) ;$$

$$monXL(j,k)\$st(k).. XL(j,k) =g= XL(j,k+1) ;$$

monYRL(i,k)\$last(k).. YR(i,k) =g= Yout(i) ;
monXLF(j,k)\$first(k)..Xout(j) =g= XL(j,k) ;

logM(i,j,k)\$st(k)..M(i,j,k) - (W(i,j)*z(i,j,k)) =l= 0 ;

logemR(i,j,k)\$st(k)..dy(i,j,k) =l= YR(i,k) - b(i,j)*XL(j,k)-c(i,j) +
gamma(i,j)*(1 - z(i,j,k)) ;

logemL(i,j,k)\$st(k)..dy(i,j,k+1) =l= YR(i,k+1)-b(i,j)*XL(j,k+1)-c(i,j) +
gamma(i,j)*(1 - z(i,j,k)) ;

eqNum1(i,j,k).. numplate1(i,j,k) =e= log(1-.45)*(YR(i,k)-b(i,j)*XL(j,k)-c(i,j))/(YR(i,k)-b(i,j)*XL(j,k+1)) + .83/.079;

eqNUM2(i,j,k).. numplate2(i,j,k) =e= (YR(i,k)-YR(i,k+1))/(YR(i,k)-b(i,j)*XL(j,k+1)-c(i,j));
eqN(i,j,k).. N(i,j,k)=e= numplate1(i,j,k)*(A(i,j)=1)+numplate2(i,j,k)*(A(i,j)<>1);
eqteN(i)..teN(i)=e=(sum((j,st),N(i,j,st))/E);

obj.. cost=e= unitc*(sum((i,j,st),z(i,j,st))) +
NUMcoeff*(sum((i,j,k),(M(i,j,k)*KY(i,j)))/(((dy(i,j,k)*dy(i,j,k+1)*(dy(i,j,k)) + dy(i,j,k+1))/2+ 1e-6)**0.33333)*(1e-6)**aexp))+ sum (j,GL(j)*GLcost(j));

* process streams

* RICH STREAMS

YIN('1')=.01; YOUT('1')=.004; GR('1')=50;
YIN('2')=.01; YOUT('2')=.005; GR('2')=60;
YIN('3')=.02; YOUT('3')=.005; GR('3')=40 ;
YIN('4')=.02; YOUT('4')=.015 ; GR('4')=30 ;

* LEAN STREAMS

XIN('1')=.03; XOUT('1')=.04;

A(i,j)= 1.4;

* costs and coefficients

GLcost('1')= 450;

*

unitc =6500; NUMCoeff=400; aexp =1;

eampp = .008;

* bounds

```
dY.lo(i,j,k) = eampp ;
dY.lo(i,j,k+1) = eampp ;
YR.up(i,k) = YIN(i) ;
YR.lo(i,k) = YOUT(i) ;
XL.up(j,k) = XOUT(j) ;
XL.lo(j,k) = XIN(j) ;
E=.8;
* Ky(i,j)=1;
b.lo(i,j)=3;
teN.lo(i)=1;
```

* initialization

```
YR.l(i,k) = YIN(i) ;
XL.l(j,k) = XIN(j) ;

eGR(i) = GR(i)*(YIN(i) - YOUT(i)) ;

gamma(i,j) = max(XIN(j) - YIN(i), XIN(j) - YOUT(i),
                XOUT(j) - YIN(i), XOUT(j) - YOUT(i)) ;

dY.l(i,j,k) = YIN(i) - XIN(j) ;
```

Model super/all/ ;

```
Option optcr = 0 ;
Option limrow = 0 ;
Option limcol = 0 ;
Option solprint = off ;
Option sysout = off ;
Option iterlim = 100000 ;
Option reslim = 10000 ;
```

Solve super using RMINLP minimizing cost ;

* total number of plates by kremser equations

NL(i)= sum((j,k),N.l(i,j,k))/1;

display NL;

*MSA FLOW RATE

GL.l(j)= sum(i,(YIN(i)-YOUT(i))*GR(i))/(XOUT(j)-XIN(j)) ;

display GL.l;

* utility costs

MSAcost = sum(j,GL.l(j)*GLcost(j)) ;

display MSAcost ;

REFERENCE

1. El.Halwagy,M.M and Manoussiouthekis,V ,”Synthesis of mass exchange networks”
AIChE J ,35 No.8, pp 1233-1244, August 1989
2. .Hallae, N and Fraser, D,M ,” Supertargeting for mass exchange networks, part1:
Targeting and Design technique”, Trans Ichme , 78 , pp 202-207, partA , March 2003.
3. Hallale , N and Fraser , D.m ., “ Supertargeting for mass exchange networks, part 2:
applications” , Trans IchmE , 78 , pp208-216, partA, March 2000
4. Hallale , N and Frase , D.M ,” Capital cost targets for mass exchange networks, A special
case : Water minimisation “, chem Engg . Sci , 53, No. 2 293-313, 1998
5. Lee ,Seungkon and Park Sunwon , “ Synthesis of mass exchange network using Process-
Graph theory “, Computers Chem Engg Vol .20 S uppl, S 201-S 205, 1996
6. Szitkaki et al. “ Comparision of Mathematical Programming and pinch based technique
for mass exchange network synthesis
7. Garrard , Anthony and Fragga , Eric S (1998) “ Mass exchange Network Synthesis using
Genetic Algorithm”, Computer Chem Engg Vol 22, pp- 1837-1850
8. Thunyawart Jutamart et al Simulation of Mass exchange Network using modified Genetic
Algorithm “ , Korean J.Chem, 28(2), 332-341(2011)
9. Chen ,Chenng Liang ,Hung Ping –Sung , “Retrofit of Mass Exchange Networks with
Superstructure based MINLP Formulation”, Ind. Eng.Chem , 44, pp 7189-7199(2005)
10. Stephanopoulos ,G ,A.W Westerberg, ,” Studies of Process Synthesis , II: Evolutionary
Synthesis of Optimal Process Flowsheets” , Chem .Engg. Sci. ,31,195(1976)
11. SZItkai, Z, et al” Solution of MEN synthesis Problems using MINLP:Formulations of the
Kremser Equation “
12. Papalexandri K.P et al, (1994),” Mass Exchange Network for Waste minimisation “ Trans
I ChemE, Vol72 , Part A , p279-293.

