ENERGY MANAGEMENT IN DISTILLATION

A DISSERTATION

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By

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CANDIDATE'S DECLARATION

I hereby certify that the work which is being presented in the dissertation entitled **"ENERGY MANAGEMENT IN DISTILLATION"** in partial fulfilment of the requirement for the award of the Degree of Master of Engineering, submitted in the Department of Chemical Engineering, University of Roorkee, Roorkee is an authentic record of my own work carried out during the period from July 1999 to March 2000 under the supervision of **Dr. T. N. S. Mathur**.

The matter embodied in this thesis has not been submitted by me for the award of any other degree.

Date : 31st **March 2000**
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ABSTRACT

As the distillation columns call for energy consumption and huge capital outlays, the energy management in distillation has become a need of the hour. Energy management involves the reduction of energy consumption and identification of the regions where energy can be better utilized.

This thesis brings out a theoretical investigation on energy management in distillation by the use of heat pump with conventional distillation column. The use of heat pump for energy management has been described by replacing coolant with an evaporating refrigerant at low pressure and by replacing steam heating of a reboiler with a condensing refrigerant at a high pressure. Heat pump assisted distillation columns reduce the requirement of hot utilities and cold utilities which will bring down the total costs involved in the process. But, at the same time, employing new equipments like compressor, heat exchangers etc. which require additional capital costs, pose a challenge to the economic efficiency of the process. Thus, the dissertation work includes the determination of hot and cold utilities by Ponchon Savarit method (a graphical method) and by simulation of distillation column.

Economic analysis of the heat pump assisted distillation configuration has been done. Due to reduction in requirement of utilities in the heat pump assisted distillation configuration, saving in the total costs has been shown compared to the conventional distillation column.

CONTENTS

Page No.

LIST OF FIGURES

LIST OF TABLES

D Variation of Annual Fixed Costs for Heat Pump Assisted Distillation Column with ΔT_r

NOMENCLATURE

A_c	Surface area of condenser, m^2
A_{comp}	Surface area of compressor, m^2
A_{ji}	Absorption factor; defined by Eq. 4.5
A_R	Surface area of reboiler, m^2
B^o, B^1	Functions in generalized second-virial-coefficient correlation
c	Total number of components
C_C, $C_{C,A}$	Fixed cost and annual fixed cost of condenser respectively, Rs.
C_{Comp}, $C_{Comp,A}$	Fixed cost and annual fixed cost of compressor respectively, Rs.
$C_{L,i}$	Heat capacity of component i in liquid state, kJ/kmole K
$C_{L,mix}$	Heat capacity of the mixture in liquid state, kJ/kmole K
C_p	Heat capacity at constant pressure, kJ/kmole K
$\langle C_p \rangle_H$	Mean heat capacity for enthalpy calculations, kJ/kmole K
$\langle C_p \rangle_S$	Mean heat capacity for entropy calculations, kJ/kmole K
C_R, $C_{R,A}$	Fixed cost and annual fixed cost of reboiler, Rs.
d_i	Flow rate of component in the distillate, kmole/hr
D	Total flow rate of distillate, kmole/hr
F	Total flow rate of feed, kmole/hr
H_{Lj}	$= \sum_{i=1}^{c} H_{Lji} x_{ji}$, for an ideal solution; evaluated at the temperature T_j, pressure and composition of the liquid leaving the jth plate, kJ/kmole
H_{Gj}	$= \sum_{i=1}^{c} H_{Gji} y_{ji}$, for an ideal solution; evaluated at the temperature T_j, pressure and composition of the vapour leaving the jth plate, kJ/kmol
H_D	Enthalpy of distillate, kJ/kmole

H_F, H	Enthalpy of feed, regardless of state, kJ/kmole
H_w, H_{LW}	Enthalpy of residue, kJ/kmole
$H_G(x_j)_k$	$= \sum_{i=1}^{C} H_{Gki}\, x_{ji}$, for an ideal solution; evaluated at the temperature and pressure of the vapour leaving the kth stage and at the composition of the vapour leaving the jth stage.
$H_L(y_j)_k$	$= \sum_{i=1}^{C} H_{Lki}\, y_{ji}$, for an ideal solution; evaluated at the temperature and pressure of the liquid leaving the kth stage and at the composition of the liquid leaving the jth stage.
H^R	Residual enthalpy, kJ/kmol
$(H^R)^0$,$(H^R)^1$	Functions in generalised residual enthalpy correlation
ΔH_s	Heat of solution, kJ/kmole
ΔH	Enthalpy change, kJ/kmole
K_{ji}	Equilibrium vapourisation constant, evaluated at the temperature and pressure of the liquid leaving the jth stage
l_{ji}	Flow rate at which component i in the liquid phase leaves the jth mass transfer section, kmole/hr
l_{oi}	Flow rate of component i in the liquid reflux; kmole/hr
l_{fi}, v_{fi}	Flow rate of component i in the liquid and vapour parts, respectively, of a partially vapoured feed, kmol/hr. For the bubble point liquid and subcooled feeds, $v_{Fi} = FX_i$ and $l_{Fi} = 0$
L_j	Total flow rate of which liquid leaves the jth stage, kmole/hr
m	Mass flow rate, kg/sec
M	Molecular weight, kg/mole
N	Total number of stage
P_A	Vapour pressure of component A, atm
P_B	Vapour pressure of component B, atm

P	Total pressure, atm
P_c	Critical pressure, bar
P_r	Reduced pressure, bar
P_o	Reference pressure, bar
Q_c	Condenser duty, kW
Q_L	Heat losses
Q_R	Reboiler duty, kW
Q'	Heat removed in the condenser and the permanently removed distillate, per mole of distillate, kJ/kmole
Q''	Net flow of heat outward at the bottom, per mole of residue, kJ/kmole
R	Universal gas constant
R_{ex}	External reflux ratio
$R_{ex,min}$	Minimum reflux ratio
S^R	Residual entropy
$(S^R)^o$, $(S^R)^1$	Functions in generalised residual entropy correlation
S_{ji}	$K_{ji}V_j/L_j$, stripping factor for component i, evaluated at the conditions of the liquid leaving the j^{th} stage.
ΔT_r	Temperature gradient across the reboiler. °C
T	Absolute temperature, K
T_1	Temperature of heat pump – reboiler, K
T_2	Temperature of compressed (saturated or superheated) vapour, K
T_3	Temperature of heat pump – condenser, K
T_A, T_B	Boiling point temperatures of pure A and B respectively
T_c	Critical temperature, K
T_b	Bubble point temperature, K
T_{c1}	Dew point of overhead vapours coming from condenser, K
T_{c2}	Bubble point of overhead condensed vapours, sent as reflux to top plate, K
T_d	Dew point temperature, K

T_o	Reference temperature, K
T_r	Reduced temperature, K
T_{r1}	Dew point of residue product
T_{r2}	Bubble point of residue product
T_s	Temperature of steam
v_{ji}	Flow rateat which component i in the vapour phase leaves the j^{th} stage, kmole/hr
V_j	Total flow rate of vapour leaving the j^{th} stage, kmole/hr
w	Flow rate of component i in the residue (or bottom), kmole/hr
W	Total flow rate of the residue, kmole/hr
W_s	Compressor work
x_{ji}, x	Mole fraction of component i in the liquid leaving the j^{th} stage
x_i	Abscissa of the point of intersection of the operating lines for a binary mixture
x_A, x_B	Mole fraction of component A and B respectively in the liquid mixture
x_{wi}	Mole fraction of component i in the residue
X_F,X_i	Total mole fraction of component i in the feed (regardless of state)
X_D, $X_{D,i}$	Total mole fraction of component i in the distillate (regardless of state)
y_{ji}, y	Mole fraction of component i (or more volatile component) in the vapour leaving plate j.
y_A, y_B	Mole fraction of component A and B respectively in vapour mixture
y_j	Ordinate of the point of intersection of operating lines for a binary mixture
Z	Compressibility factor

Greek Symbols

α_{ji}	Relative volatility, $\alpha_{ji} = K_{ji} / K_{jb}$
θ	A multiplier defined by Eq. 4.13
ω	Acentric factor
λ_A, λ_B	Heat of vaporization of pure component A and B respectively at dew point
β'	Fraction of the bottom product sent as reflux in the stripping section
ρ_w	Density of water
θ_i	Inlet temperature difference of hot fluid and cold fluid
θ_o	Outlet temperature difference of hot fluid and cold fluid
ζ	Feed vector

Subscripts

av	Average
A	Component A
B	Component B
ben	Benzene
ca	Calculated value
co	Corrected value
f	Variables associated with partially vaporized feed
F	Feed plate
i	Component number
j	Plate number; j= 0 for the accumulator; j = 1 for top plate; j = F for feed plate; j = N for bottom plate and j = N+1 for reboiler
N	Total number of plates or stages
ref	Refrigerant
tol	Toluene

Mathematical Symbols

$\sum_{i=1}^{C} x_i$	Sum over all values x_i, i = 1, 2, ….., C or ($1 \le i \le C$)
$\{x_y\}$	Set of all values x_j belonging to the particular set under consideration

CHAPTER - 1

INTRODUCTION

Chemical Process Industries (CPI) are reasonably intelligent users of energy. Mass and energy-balances are the backbones of chemical engineering and the efficient use of energy and energy management are well established concepts which have always been practised up to a certain extent. However, following the escalating energy crisis and subsequent large increase in oil prices, the importance of efficient use of energy has greatly enhanced. There is a long term need to improve further the efficiency of energy utilization within a chemical process industry.

Chemical process industries employ a variety of separation processes such as absorption, crystallization, distillation, evaporation, extraction etc. in order to separate a binary or multicomponent mixture into its components. Of all these separation processes, distillation is the most widely used technique and is well known for its high energy consumption. Estimates indicate that 30-60% of the total energy demand by chemical industries is used to run distillation equipment only [15]. Therefore, it is essential that distillation process be analyzed for identifying various places of energy losses and suitable energy management measures be taken.

Various techniques by which energy consumption in distillation can be reduced, are : reduction of temperature-gradient in the reboiler and the condenser to permit use of low temperature steam and heat recovery at higher temperatures respectively; recovery of heat by side stream-withdrawal; tray-retrofit; heat pump; splitting of column; feed optimization; minimizing pressure drop inside the column;

adequate insulation etc. Use of these techniques depend upon the process conditions and the individual systems. Bulk of the literature available on this subject is based on actual plant observations wherein ways are suggested to reduce the energy consumption in CPI. Therefore, there is a need to further explore these energy management techniques so that they can have much broader applicability than indicated in literature, so far.

Heat pumping is one of the promising and potential techniques for energy management in distillation. Heat pump is used to upgrade thermal energy by recovering heat from a relatively low temperature and delivering it at a higher temperature. Their use in CPI, has been limited, primarily due to the high capital cost of the equipment, the higher temperatures that are typically encountered in industrial processes, and some of the complexities associated with their use. However, several factors are expected to change the present situation :

- the critical need to save energy (application of heat pumps is usually associated with process integration);
- the progress that has been made recently in designing and constructing heat pumps, which has led to improved reliability and efficiency, and
- the launching of demonstration and promotional programs for heat pump applications.

Besides the reduction of energy consumption, heat pump systems can be considered in grass-root or retrofitting design because they are easy to introduce and the plant operation is simple [2].

Keeping in view the above facts, it was proposed to investigate the applicability of heat pump in distillation with the following objectives :

(1) To determine the requirement of cold and hot utilities in the conventional distillation column for a particular system and to show the reduction in requirement of utilities with the help of heat pump.

(2) To recommend the suitability of using heat pump as a method of energy management and thereby obtain the feasible and economic range of temperature gradient across the reboiler in heat pump assisted distillation column.

CHAPTER - 2

LITERATURE REVIEW

Null [4, 12] conducted a study to develop guidelines for conditions under which heat pumps can be economical in distillation process design. He summarised his findings as mentioned below.

Heat pumps have extensive applicability to distillation wherever direct refrigeration or chilled water are required for condensation. The heat pump configuration is most advantageous when the fractionation system has a low temperature difference across the column. The heat pump system requires a certain balance of thermal loads to minimize the use of external heat on refrigeration sources. The thermal balance of the system is particularly sensitive to the thermal conditions of the feed and products. He compared the economics of conventional distillation column to the heat pump assisted distillation configurations (heat pump with external refrigerant, heat pump with compression of overhead vapour, heat pump with reboiler liquid flashing).

Kenney [5] discussed the two projects by which Exxon Chemical had achieved significant reduction in the energy demand of two separation processes. The first was the application of the multiple effect principles. The principle was : Use the energy discarded from one step of the separation to drive a second, generally lower pressure, separation step. In grass root installations, this principle was applied liberally since economics were favourable and the designer had control over the many other factors which might influence his decision. Basically, the project involved raising the pressure on a xylene splitter tower so that the overhead could be used to reboil an adjacent debenzenizer. The potential fuel savings were in the order of 55-60 million Btu/hr. The return on this project was high enough to make all the trouble well worthwhile on an energy saving basis alone.

The second project was the addition of a major heat pump, or vapour recompression distillation system, to a light ends tower. The principle of the system involved the use of a compressor to recycle the latent heat in the vapour from the top of the tower at conditions suitable for during the reboiler at the bottom of the tower. By doing this, energy input to the tower was reduced to between 10 and 15% of the gross energy normally consumed in the reboiler. The key variables in analyzing heat pump installations on distillation towers included pressure difference between the top and bottom of the tower, the absolute pressure level of the tower (which affects both the relative volatility and the compressor ratio) the log mean temperature difference for the reboiler versus the horse power required to provide it, and the size of the duty involved. It was shown that for a tower of 50-100 million Btu/hr range, economics could be very attractive if the temperature difference between the top and bottom of the tower was below 10-16°C.

One of the energy saving methods in distillation is the use of intermediate condensers and reboilers. This method allows some heat to be introduced into the column at lower temperatures than the bottom reboiler and some of the heat to be removed at higher temperatures than the overhead condenser. The economic feasibility of such an application depends on the investment for additional equipment necessary for the modified operation and on the extent the thermal efficiency of the process can be increased with limited number of additional condensers and reboilers. Kayihan [6] described the optimum use of the heat exchanger equipment such that the thermodynamic efficiency was maximized by appropriate choice of location and load for a given number of those intermediate elements.

An objective function was defined in terms of the net work consumption of the column with any specified number of condensers and reboilers. Constraining conditions were set such that the total heat load and separation remained the same as the conventional case with only one reboiler and condenser. The resulting non-linear problem could be solved numerically for specific cases. The solution gave the best locations and the loads for interstage heat removal and/or addition. The results showed that the intermediate condenser (reboiler) significantly changed the thermodynamic efficiency when the feed concentration was low (high) and that the dominant contribution was due to the first additional condenser (reboiler) where the subsequent ones had decreasing effects.

Bannon and Marple [7] illustrated the improvement in heat recovery with two-stage condensation of column overhead and properly designed circulatory reflux systems. He summarized his findings as mentioned below :

For a column having a boiling range top product and an overhead temperature high enough to be useful, heat recovery can be considerably increased by condensing the overhead in two stages. The first stage produces reflux and the second stage condensate/non condensibles form the column top product. The heat from reflux condensation is available for use at significantly higher temperature level than would otherwise be the case. If such two-stage top condensation is added to a column previously set-up with single-stage condensation, the entire first stage of the condenser will deliver its heat at a temperature above the previous column top temperature.

Circulating reflux systems are commonly used in side product columns to generate intermediate reflux. The temperature level and thus the value of the heat removed from these systems can be increased by using multiple systems and high circulating rates.

Townsend and Linnhoff [10] described site combined heat and power, on plant generation, heat pumps and refrigeration system. He explained the concept of "appropriate heat engine" and heat pump placement in process networks based on a fundamental new insight. "Appropriate" placement took advantage of integration opportunities with the remainder of the process and yielded marginal efficiencies far greater than that would have been achieved through stand alone heat engines. In this study, criteria for heat engine and heat pump placement in chemical process networks were derived, based on the "temperature interval" (T.I.) analysis of the heat exchanger network problem. Using these criteria, the author gave a method for identifying the best outline design for any combined system of chemical process, heat engines and heat pumps. The method eliminated inferior alternatives early, and positively led on to the most appropriate solutions.

Colmenares and Seider [11] presented a non-linear programming strategy for integration of heat engines and heat pumps with chemical processes. The strategy utilized the temperature interval method and showed how to use negative heat deficits to obtain lower cost designs. Two important situations were presented in which the resulting designs were less costly when the heat engines and heat pumps were integrated with temperature intervals having negative heat deficits. Their conclusions can be summarised as :

1. When multiple hot utilities are available, the optimal integration of heat engines above the pinch temperature often involves driving the heat engine with heat from a temperature interval having a negative hot deficit. This violates the initial guidelines of Townsend and Linnhoff [10] and is successful when a low-cost hot utility can replace high priced fuel to drive a heat engine.

2. Below the refrigeration temperature , the optimal integration of heat pumps often involves delivering the heat of condensation to temperature intervals with negative cold deficits. This also violates the initial guidelines of Townsend and Linnhoff [9], but adopts the quantitative recommendations laid by them and is successful when the cost of compression to condense the working fluid with cooling water exceeds the added cost of cooling water due to heat transfer to the process below the refrigeration temperature.

Glinos and Malone [13] discussed the application of thermodynamic principles to the synthesis of distillation sequences. The thermodynamic analysis had an advantage when heat integration of the distillation system was planned or to further discriminate among configurations having comparable economic performance. Network consumption was taken as objective function because of its two properties. The properties are :

(1) It is approximately constant with respect to temperature and pressure changes; it is also independent of the number of effects when multieffect distillation is employed.

(2) It is directly proportional to a lower bound on the minimum energy requirement of an extensively heat integrated separation trains.

The method was used to evaluate the optimality regions for the two alternative simple sequences for a ternary mixture (direct and indirect) and the results agreed well with the commonly used heuristics.

Swaney [14] developed an extended transportation array representation for the design of process heat recovery networks incorporating heat engines and heat pumps. The formulation automatically accounted for the relocation of pinches in the integrated system. The optimal heat flow pattern was determined based on simple economic criteria. Simplified models of heat engines and heat pumps systems were developed that permitted integration options to be identified on the basis of heat flows without requiring specific cycle designs. The solution array identified design alternatives and provided a decision framework to guide in selecting the final design topology.

Meili [15] described the fundamental of heat pumps and their use in distillation. Two configurations of heat pump assisted distillation were explained along with their advantages, disadvantages and their application criteria. The three typical distillation columns with heat pumps (those separating ethylbenzene-styrene; propane-propylene and isopropanol-water) described in this study showed that heat pumps could yield significant ranges on energy costs in distillation.

Humphrey and Seibert [16] discussed the thermodynamic efficiency of a separator which could have profound impact on the overall cost of a process. The energy saving technologies suggested by him included the recovery of energy lost at the reboiler through the condenser. In this heat recovery approach, energy expended in one distillation column was reused in the same or a different unit.

Chou [17] explained the advantages of subcooled distillate in distillation to reduce the costs. According to his findings, the temperature of distillate condensate depends on certain factors like pressure drop between the tower and drum, weather conditions, fouling factor, and safety factor incorporated in design process, and distillate vapour flow rate. He suggested that using two cooling media, such as cooling water and a refrigerant or a cooling water and air might be more economical in addition to the size consideration.

Ziegler and Riesch [18] compared the absorption systems to conventional compression system and summarised their findings as mentioned below :

Absorption systems have large potential for energy saving especially when they are operated from cogeneration systems or by waste heat. Compression-absorption systems allow the use of well-known compression technology, but are more flexible with regard to temperature range of application. So, temperature as high as 150°C, for example, can be reached with moderate pressure of 20 bars or below if NH_3/H_2O is worked with the experimental results and data from the existing plant. Ziegler showed that well designed compression machinery can be superior to absorption system. Absorption machines are operated by heat, therefore their use is considered where waste heat from cogeneration plants including engines, is available.

Fonyo and Mizsey [19] scrutinized the influence of relevant parameters on the economics of distillation plants involving distinct heat pump cycles and compared the results to conventional and integrated schemes. On the basis of the COP, energy costs and efficiencies, simple expressions were proposed for preliminary economic analysis and design of heat pump assisted distillation. The influence of heat pump type, purity requirement, column pressure drop, feed rate, energy cost, relative volatility etc. on the energetic aspects and economic range of application was presented. A design strategy for selecting the most economical distillation system, considering different types of heat pump structures (vapour recompressor, bottom flash, closed cycle, absorption cycle), was proposed, based on pinch technology, primary energy rate, energy cost factor and estimated payback time of excess capital. The strategy was demonstrated by industrial case studies.

Ognisty [20] employed thermodynamic analysis as a tool for identifying opportunities for improvement in distillation column design. He used lost work profiles in terms of pressure-drop and heat transfer and mass transfer-mixing effects. The goal of reducing the lost work was to lower the utility consumption as close as practical to the thermodynamic minimum.

Annakou and Mizsey [21] investigated a propylene propane splitter associated by a heat pump of the vapour recompresson type by rigorous methods. They scrutinized two schemes, a single compressor scheme and a double compressor scheme in parallel arrangement and compared to the conventional stand alone column. The investigation included parametric study and operability assessment. The system studied consisted of a distillation column designed to separate a mixture of propylene and propane. The column had 180 trays and a high reflux ratio. The overhead vapour was split into two parts : one going to the heat pump compressor and then used to reboil the bottoms in the reboiler condenser, the other part fed to the second compressor. In the second compressor, the steam was lifted up to high enough pressure so that the cooling water could be used to condense it. The distillate product was withdrawn and rest was sent to a flash tank. Results of the investigation showed that both the schemes (a single compressor scheme and a double compressor scheme) had lower annual total cost than the conventional stand alone column by about 37%.

Offers, Dussel and Stichlmair [22] presented a novel method for the calculation of minimum reflux. This method needs the knowledge of the phase equilibrium at the feed concentration only. With this data, the characteristic direction of internal concentration profile was deduced and a further step led to the direct calculation of the minimum reflux without any iteration. This method was used for rough estimations and for calculating a starting value for rigorous column simulations.

Gelegenis and Koumoutsos [23] explained the application of heat pumps in chemical process industries, their selection and applicability criteria. They also discussed how the selection of the working fluid and equipments (compressor, drives and heat exchanger) was to be made.

Taprap and Ishida [24] adopted the graphical construction called an energy utilization diagram (EUD) for analysis of energy transformation and energy losses in distillation columns. They decomposed the overall energy loss on one plate of a column into six kinds of energy losses and represented the losses graphically. Two of them were caused by mixing and cooling in the vapour phase and the other two by mixing and heating in the liquid phase. To display the remaining two yielded by condensation and evaporation of each component, the concept of the individual energy level was applied. The relationship between the individual energy level and the x-y diagram was presented as well as the effects of the reflux ratio and the feed location on the EUD for the whole column. The methodology was illustrated for the separation of n-hexane and n-octane.

Agrawal, Fidkowski and Xu [25] introduced the distillation systems composed of a prefractionator and a main column. The columns were operated at different pressures, but the temperatures of the utilities were the same as for a single column performing the same separation. The energy integration of the columns was realized by condensing a vapour overhead from the prefractionator in an intermediate reboiler located in the stripping section of the main column or by boiling a bottoms liquid from the prefractionator in an intermediate condenser placed in the rectifying section of the main column. Analysis was performed to determine feasible regions of operational parameters and to minimize vapour flows. A detailed simulation example of the benzene-toluene separation showed that for certain feed compositions, it was possible to reduce energy requirements of a conventional binary distillation column by almost one third using this new distillation column.

Bausa, Watzdorf and Marquardt [26] presented a new general method for calculating the minimum energy demand for distillation columns applicable to all types of splits and mixtures in both simple and complex columns. This method stemmed from a geometric analysis of the plate to plate profiles and used all pinch points of both column sections. No a priori choice of relevant solution branches of the pinch equation was required. The computational effort was low since no rigorous plate to plate calculation were necessary.

Agrawal and Herron [28] identified optimal thermodynamic feed conditions for distillation of ideal binary mixture through thermodynamic efficiency analysis of distillation column. Due to simplifying assumptions, temperatures did not appear explicitly in the final thermodynamic efficiency equations. These equations were found to be functions of only feed compositions, the thermodynamic state of the feed, and the relative volatility of the more volatile component A with respect to component B. According to their findings, for most binary mixtures, two feeds with same composition, but one saturated vapour and the other saturated liquid, can improve a distillation column's efficiency substantially. They found that the maximum benefit was obtained for a 50-50 mixture. They stressed that two feed case was less efficient than the single two phase feed case when the relative volatilities exceeded certain calculable values.

Fonyo and Benko [30] analysed the various heat pump assisted process configurations for two industrial case studies using a design strategy based on preliminary screening, rigorous steady state simulation and economic evaluation. The influence of heat pump type, heat load, column temperature difference, utility cost, exchanger minimum approach temperature (EMAT) on the energetic aspects and economic range of application were examined. Certain well designed heat pump options showed better economic figures than the base case separation system which used only steam and cooling water. The results of the study conducted by Fonyo and Benko showed that larger heat load and smaller process temperature difference provided shorter payback time for heat pumping.

Meili [31] compared the conventional steam heated recycle column against several heat pump assisted systems (systems using vapour ejector, system using direct vapour recompression and systems using an auxiliary circuit) in terms of savings in money and payback time.

CHAPTER - 3

THEORETICAL INVESTIGATION

As described in Chapter 2, various energy saving measures can be used to reduce the consumption of utilities in an existing distillation column. Heat pumping is one of the potential techniques that can be incorporated in the conventional design without major investments and without much difficulties. Heat pumping affects directly the quantum of energy in terms of the steam in reboiler and cooling water in condenser, thus reducing the total costs involved, considerably. This chapter brings out theoretical investigation regarding the determination of the following :

(1) Bubble points and Dew points for binary mixture at different compositions.

(2) Enthalpies of mixture in liquid state and gaseous state at different compositions

(3) Heat loads for conventional distillation column by Ponchon Savarit method.

(4) Number of stages in conventional distillation column

(5) Compressor work required in heat pump assisted distillation column, with the help of Lee and Kesler generalised correlations and virial coefficients.

3.1 DETERMINATION OF BUBBLE POINT AND DEW POINT

When a state of equilibrium exists between a vapour and liquid phase composed of two components A and B, the system is described by the following set of independent equations

Equilibrium relationships $$\begin{cases} Py_A = P_A x_A \\ Py_B = P_B x_A \\ y_A + y_B = 1 \\ x_A + x_B = 1 \end{cases} \tag{3.1}$$

where it is understood that Raoult's law is obeyed since P_A and P_B depend on T alone, Eq. (3.1) consists of four equations in six unknowns. Thus, to obtain a solution to this set of equations, two variables must be fixed. For the determination of bubble point, the total pressure P is fixed, a solution is obtained for each of several temperatures lying between the temperatures at which the separate vapour pressures, P_A and P_B are equal to the total pressure P. Addition of the first two expressions of Eq. (3.1) followed by rearrangement of the result so obtained yields

$$P = P_A x_A + P_B x_B$$

or $$\frac{P_A x_A + P_B x_B}{P} = 1 \tag{3.2}$$

Elimination of x_B by use of the fourth expression of Eq. (3.1) followed by rearrangement of the result so obtained yields

$$x_A = \frac{P - P_B}{P_A - P_B} \tag{3.3}$$

From the definition of a mole fraction ($0 \le x_A \le 1$), Eq. (3.3) has a meaningful solution at a given P for any T lying between the boiling point temperatures T_A and T_B of pure A and pure B, respectively. After x_A has been computed by the use of Eq. (3.3), at the specified P and T, the corresponding value of y_A which is in equilibrium with the value of x_A so obtained is computed by the use of first expression of Eq. (3.1)

$$\begin{aligned} y_A &= \left(\frac{P_A}{P}\right) x_A \\ y_B &= \left(\frac{P_B}{P}\right) x_B \end{aligned} \tag{3.4}$$

Eq. (3.4) in combination with fourth expression of Eq. (3.1) gives

$$P\left(\frac{y_A}{P_A} + \frac{y_B}{P_B}\right) = 1 \tag{3.5}$$

An algorithm developed for the calculation of bubble points and dew points for different compositions of the binary mixture, is given below :

Algorithm :

(1) Assume a temperature for a particular composition of binary mixture

(2) For that temperature calculate the vapour pressures (P_A, P_B) of each component by using Antoine equation given in the Appendix-B.

(3) For the assumed temperature, if the Eq. (3.2) and (3.5) are satisfied within the prescribed tolerances, the bubble point and dew point respectively, has been achieved. Otherwise, follow step 4.

(4) For the bubble point if $\frac{P_A x_A + P_B x_B}{P} < 1$, then increase the assumed temperature by the step-size chosen judiciously and repeat steps 1 through 3, otherwise, if, $\frac{P_A x_A + P_B x_B}{P} > 1$, then decrease the assumed temperature by the step-size and repeat steps 1 through 3.

For the dew point, if $P\left(\frac{y_A}{P_A} + \frac{y_B}{P_B}\right) > 1$, then increase the assumed temperature by the step-size and repeat steps 1 through 3, otherwise, if, $P\left(\frac{y_A}{P_A} + \frac{y_B}{P_B}\right) < 1$, then decrease the assumed temperature by the step-size and repeat steps 1 through 3.

3.2 ENTHALPY OF MIXTURE

Liquid solution enthalpies include both sensible heat and the heat of mixing of the components

$$H_L = C_{L,mix}\,(T_b - T_o) + \Delta H_s \tag{3.6}$$

ΔH_s is the heat of solution at T_o and the prevailing concentration referred to the pure liquid components. For saturated liquids, T_b is the bubble point corresponding to the liquid concentration at the prevailing pressure. For an ideal solution, such as benzene-toluene solution, heat of solution is zero and the heat capacity is the weighted average of those for the pure components.

For present purposes, saturated vapour enthalpies can be calculated adequately by assuming that the unmixed liquids are heated separately as liquids to the gas temperature, T_d (the dew point), each vaporized at this temperature, and the vapours mixed.

$$H_G = y_A\left[C_{L,A}(T_d - T_o) + \lambda_A\right] + (1-y)\left[C_{L,B}(T_d - T_o) + \lambda_B\right] \tag{3.7}$$

3.3 OVERALL MATERIAL BALANCE AND ENTHALPY BALANCE

Total material balance for envelope I, Fig. 3.1 gives

$$V_1 = D + L_0$$

$$= D + RD = D(R+1) \tag{3.8}$$

Enthalpy balance for envelope 1 gives

$$Q_c = D\left[(R+1)H_{G1} - RH_{L0} - H_D\right] \tag{3.9}$$

which provides the heat load of the condenser.

The reboiler heat is then obtained by a complete enthalpy balance about the entire apparatus, envelope II

$$Q_R = DH_D + WH_W + Q_c + Q_L - FH_F \tag{3.10}$$

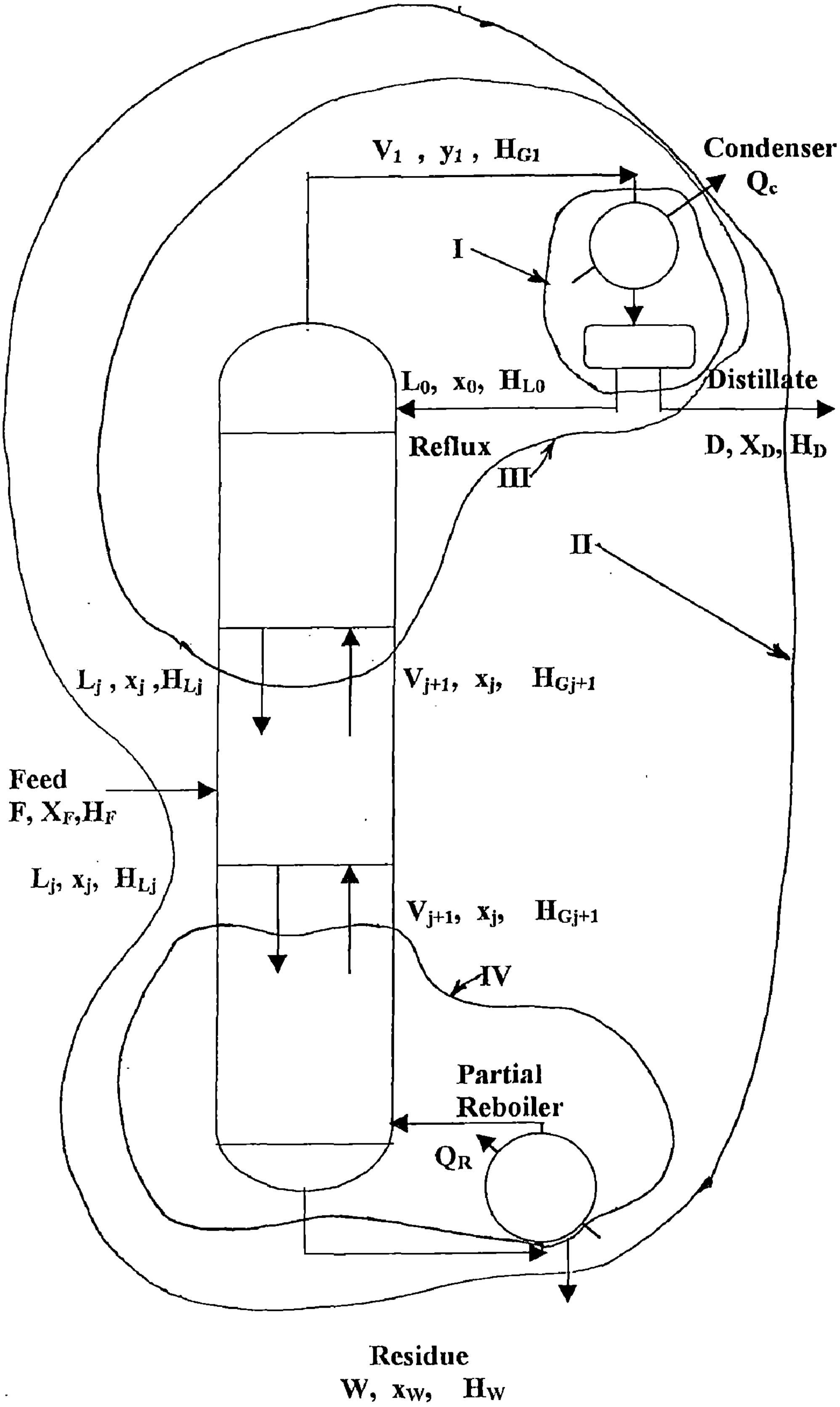

Fig 3.1 Material and Enthalpy Balance of a Distillation Column

Heat economy is frequently obtained by heat exchange between the residue product, which issues from the column at its bubble point, and feed for purposes of preheating the feed. Eq. (3.10) still applies provided any such exchanger is included inside envelope II.

There two graphical methods to develop the relationship between number of trays (stages), liquid/vapour ratios, and product compositions are :

(1) Ponchon Savarit method

(2) McCabe and Thiele method

The first of these, the method of Ponchon and Savarit is rigorous and can handle all situations but it requires detailed enthalpy data for its applications.

3.4 DETERMINATION OF HEAT LOADS BY PONCHON AND SAVARIT METHOD

The heat loads (i.e. condenser duty and reboiler duty) for a distillation column are determined by applying enthalpy balance equations for each tray, in enriching section and stripping section separately.

3.4.1 Enthalpy Balance in Enriching Section

Consider the enriching section through tray j envelope III, Fig. 3.1 . Tray j is any tray in this section. An enthalpy balance, envelope III with heat loss negligible is

$$V_{j+1} H_{G_{j+1}} = L_j H_{Lj} + Q_c + DH_D \tag{3.11}$$

Let Q' be the heat removed in the condenser and the permanently removed distillate, per mole of distillate. Then

$$Q' = \frac{Q_c + DH_D}{D} = \frac{Q_c}{D} + H_D \tag{3.12}$$

and $$V_{j+1} H_{G_{j+1}} - L_j H_{Lj} = DQ' \tag{3.13}$$

The internal reflux ratio in the enriching section can be calculated as

$$\frac{L_j}{V_{j+1}} = \frac{x_D - y_{j+1}}{x_D - x_j} = \frac{Q' - H_{G_{j+1}}}{Q' - H_{Lj}} \tag{3.14}$$

Δ_D represents a fictitious stream, in amount equal to the net flow outward (in this case D) and of properties (Q', X_D) such that

$$V_{j+1} - L_j = \Delta_D \tag{3.15}$$

The ratio of molar flowrate of liquid stream at any stage, j in enriching section and that of the distillate is defined as

$$\frac{L_j}{D} = \frac{Q' - H_{G_{j+1}}}{H_{G_{j+1}} - H_{Lj}} = \frac{x_D - y_{j+1}}{y_{j+1} - x_j} \tag{3.16}$$

Applying this to the top tray provides the external reflux ratio, which is usually the one specified

$$R_{ex} = \frac{L_o}{D} = \frac{Q'' - H_{G1}}{H_{G1} - H_{L0}} = \frac{\text{line } \Delta_D V_1}{\text{line} V_1 L_o} = \frac{\text{line} \Delta_D V_1}{\text{line } V_1 D} \tag{3.17}$$

For a given reflux ratio, the line length ratio of Eq. (3.17) can be used to locate Δ_D vertically on fig. C.1, given in the Appendix -C and the ordinate Q' can then be used to compute the condenser heat load.

3.4.2 Enthalpy Balance in Stripping Section

Consider the envelope IV in Fig. 3.1, where, j is any tray in the stripping section. An enthalpy balance for envelope IV is

$$L_j H_{Lj} + Q_R = V_{j+1} H_{G_{j+1}} + W H_W \tag{3.18}$$

Q" is defined as the net flow of heat outward at the bottom, per mole of residue

$$Q'' = \frac{W H_W - Q_R}{W} = H_W - \frac{Q_R}{W} \tag{3.19}$$

and $$L_j H_{Lj} - V_{j+1} H_{G_{j+1}} = W Q'' \tag{3.20}$$

Thus Δ_W is a fictitious stream, in amount equal to the net flow outward (in this case W), of properties (Q", x_W), such that

$$L_j - V_{j+1} = \Delta_W \tag{3.21}$$

The ratio of molar flow rate of liquid stream at any stage, j , in the stripping section and that of residue is defined as

$$\frac{L_j}{W} = \frac{H_{G_{j+1}} - Q''}{H_{G_{j+1}} - H_{Lj}} = \frac{y_{j+1} - x_w}{y_{j+1} - x_j} \tag{3.22}$$

3.4.3 Enthalpy Balance in the Complete Distillation Column

Eq. (3.10) is a complete enthalpy balance for envelope I, Fig 3.1. If in the absence of heat losses ($Q_L = 0$), the definition of Q' and Q" are substituted into Eq. (3.10), it becomes

$$FH_F = DQ' + WQ'' \tag{3.23}$$

The ratio of molar flow rate of distillate to that of residue is defined as

$$\frac{D}{W} = \frac{x_F - x_W}{x_D - x_F} = \frac{H_F - Q''}{Q' - H_F} \tag{3.24}$$

This is the equation if a straight line on the H-xy diagram through (Q', x_D) at Δ_D, (H_F, x_F) at F, and (Q", x_w) at Δ_W as plotted in Fig. C.1.

In other words,

$$F = \Delta_D + \Delta_W \tag{3.25}$$

The location of F, representing the feed is decided by its thermodynamic state. F may be on the saturated-liquid or vapour curve; between them; above the saturated vapour curve or below the saturated liquid curve. In any event, the two Δ points and F must lie on a single straight line.

After locating F and the concentration abscissas x_D and x_W corresponding to the products on the H-xy diagram, Δ_D is located vertically on the line $x = x_D$ by the computation of Q' or by the line length ratio of Eq. (3.17) using the specified reflux ratio R. The line $\Delta_D F$ extended to $x = x_W$ locates Δ_W, where ordinate can be used to compute Q_R.

3.5 DETERMINATION OF NUMBER OF STAGES IN CONVENTIONAL DISTILLATION COLUMN

The enriching stages can be located on the H-xy diagram alone by alternating construction lines to Δ_D (Q', x_D) and tie lines, each tie line representing an ideal tray. Similarly, stripping stages can thus be determined entirely on the H-xy diagram by alternating construction lines to $\Delta_W(Q'', x_w)$ and tie line, each tie line accounting for an equilibrium stage. The algorithm developed for the determination of number of stages has been described below.

Algorithm :

(1) For the known Q', x_D and reflux ratio, R, the value of x_1 (or L_1) is calculated as explained further. For a total condenser x_o(or L_o) and y_1 (or V_1) are equal to x_D (or D).

(2) From the known equation of y in terms of f(x), i.e., $y = f(x)$, the value of x which satisfies the equation for known value of y_1 (or V_1) is calculated by Newton-Raphson method.

(3) Extending the vertical from x, calculated above, such that it intersects the $H_L x$ line at a point, which is $x = x_1$ (or L_1).

(4) From the two point (x_1, H_L at x_1) and (x_D, Q'), a straight line is drawn such that it intersects a H_G-y line, and y_2 is obtained by linear regression method.

(5) Now, for known value of y_2 (or V_2) value of x_2 (or L_2) is obtained by steps 1 and 2 and value of y_3 (or V_3) is obtained by step 3. This procedure is repeated

for particular number of iterations (i) for which x_i reaches the composition of feed. These number of iterations give the number of stages or trays in enriching section.

(6) Starting with the value of x_F (the composition of feed as obtained above), or F, and known values Q", the value of x is obtained which satisfies the value of equation y = f(x) for known value of y_{F+1}(or V_{F+1}) by Newton-Raphson method.

(7) Extending the vertical from x_{F+1}(or L_{F+1}) such that it intersects the H_L-x line at a point which is $x = x_{F+1}$.

(8) From the two point (x_{F+1},H_L at x_{F+1}) and (x_w, Q") a straight line is drawn such that it intersects a H_G-y line and y_{F+2}(or V_{F+2}) is obtained by linear regression method.

(9) Now for known value of y_{F+2} (or V_{F+2}), the value or x_{F+2} (or L_{F+2}) is obtained by steps 5 and 6 and value of y_{F+3} is obtained by step 3. This procedure is repeated for particular number of iteration (j) for which x_j reaches the composition of residue. These number of iterations give the number of plates in stripping section. Number of plates in enriching section and stripping section minus one gives number of plates in the column.

3.6 DETERMINATION OF COMPRESSOR WORK IN HEAT PUMP ASSISTED DISTILLATION COLUMN

Ideal gas equations cannot be applied to the gases or vapours at very high pressures. Therefore, Lee and Kesler generalised correlations for determination of residual properties (residual enthalpy and residual entropy), which along with virial coefficients are used for the determination of compressor -work. As evident from Eq. (3.26), the properties for the real gases at high pressure can be calculated if the properties for the gases at ideal state and residual properties are known. Eq. (3.26) is applicable for enthalpy and entropy of the gas

$$H = H^{ig} + H^R$$

$$S = S^{ig} + S^R \tag{3.26}$$

where $H^{ig} = H_0^{ig} + \int_{T_0}^{T} C_p^{ig}\, dT$ (3.27)

and $S^{ig} = S_0^{ig} + \int_{T_0}^{T} C_p^{ig} \frac{dT}{T} - R\ln\frac{P}{P_0}$ (3.28)

Substituting into the preceding equation gives

$$H = H_0^{ig} + \int_{T_0}^{T} C_p^{ig}\, dT + H^R \tag{3.29}$$

and $S = S_0^{ig} + \int_{T_0}^{T} C_p^{ig} \frac{dT}{T} - R\ln\frac{P}{P_0} - S^R$ (3.30)

Eq (3.29) and Eq (3.30) may be expressed alternatively to include mean heat capacities

$$H = H_0^{ig} + <C_p^{ig}>_H (T - T_0) + H^R \tag{3.31}$$

$$H = S_0^{ig} + <C_p^{ig}>_S \ln\frac{T}{T_0} - R\ln\frac{P}{P_0} + S^R \tag{3.32}$$

where H^R and S^R are given by (3.33) and (3.34)

$$\frac{H^R}{RT_c} = \frac{(H^R)^o}{RT_c} + \frac{\omega (H^R)^1}{RT_c} \tag{3.33}$$

$$\frac{S^R}{R} = \frac{(S^R)^o}{R} + \frac{\omega (S^R)^1}{R} \tag{3.34}$$

Calculated values of the quantities $(H^R)^o/RT_c$, $(H^R)^1/RT_c$, $(S^R)^o/R$ and $(S^R)^1/R$ as determined by Lee and Kesler are given as function of T_r and P_r (reduced temperature and pressure) in Tables B.7.1 through B.7.4 in Appendix-B. These values, together with Eq. (3.33) and Eq. (3.34) allow estimation of residual enthalpies and entropies on the basis of three parameter corresponding states principle as developed by Lee and Kesler.

As with the generalised compressibility factor correlation, the complexity of the functions $(H^R)^o/RT_c$, $(H^R)^1/RT_c$, $(S^R)^o/R$ and $(S^R)^1/R$ precludes their general representation by simple equation.

However, the correlation of Z based on generalized virial coefficients and valid at low pressure can be extended to the residual properties. The equation relating Z to the function B^o and B^1 is

$$Z = 1 + B^o \frac{P_r}{T_r} + \omega B^1 \frac{P_r}{T_r} \tag{3.35}$$

B^o and B^1 are functions of temperature only. The residual enthalpy and entropy based on the virial coefficient [27] is given as

$$\frac{H^R}{RT_c} = P_r \left[B^o - T_r \frac{dB^1}{dT_r} + \omega \left(B^1 - T_r \frac{dB^1}{dT_r} \right) \right] \tag{3.36}$$

and $$\frac{S^R}{R} = -P_r \left(\frac{dB^o}{dT_r} + \omega \frac{dB^1}{dT_r} \right) \tag{3.37}$$

The dependence of B^o and B' on reduced temperature is given by Eq (3.38) and Eq (3.40). Differentiation of these equations provide expression for dB^o/dT_r and dB^1/dT_r given by Eq (3.39) and Eq (3.41). Thus, the four correlations required for application of Eq. (3.36) and (3.37) are :

$$B^o = 0.083 - \frac{0.422}{T_r^{1.6}} \tag{3.38}$$

$$\frac{dB^o}{dT_r} = \frac{0.675}{T_r^{2.6}} \tag{3.39}$$

$$B^1 = 0.139 - \frac{0.172}{T_r^{4.2}} \tag{3.40}$$

$$\frac{dB^1}{dT_r} = \frac{0.722}{T_r^{5.2}} \tag{3.41}$$

The generalized correlations for H^R and S^R, together with ideal gas heat capacities, allow calculation of enthalpy and entropy values of gases at any temperature and pressure by Eq. (3.31) and Eq (3.32). For a change from state 1 to state 2, Fig. 3.2, we can write Eq. 3.31 for both states

$$H_2 = H_o^{ig} + \int_{T_1}^{T_2} C_p^{ig}\, dT + H_2^R \tag{3.42}$$

$$H_1 = H_o^{ig} + \int_{T_1}^{T_2} C_p^{ig}\, dT + H_1^R \tag{3.43}$$

The enthalpy change for the process, $\Delta H = H_2 - H_1$ is given by the difference between these two equations

$$\Delta H = \int_{T_1}^{T_2} C_p^{ig}\, dT + H_2^R - H_1^R \tag{3.44}$$

Similarly by Eq. (3.32) for entropy we get

$$\Delta S = \int_{T_1}^{T_2} C_p^{ig} \frac{dT}{T} - R \ln \frac{P_2}{P_1} + S_2^R - S_1^R \tag{3.45}$$

Again these equations may be written in alternative form

$$\Delta H = < C_p^{ig} >_H (T_2 - T_1) + H_2^R - H_1^R \tag{3.46}$$

$$\Delta S = < C_p^{ig} >_S \ln\left(\frac{T_2}{T_1}\right) - R \ln\left(\frac{P_2}{P_1}\right) + S_2^R - S_1^R \tag{3.47}$$

The compression work is given by Eq. (3.46).

3.7 COST ANALYSIS OF DISTILLATION COLUMN

Distillation columns are costly equipments and cannot be replaced easily until they have been used completely for their life period. On the other hand, steam and water costs form a heavy burden on the money bill, therefore it seems logical to consider the total cost of the utilities used in the conventional distillation column ,

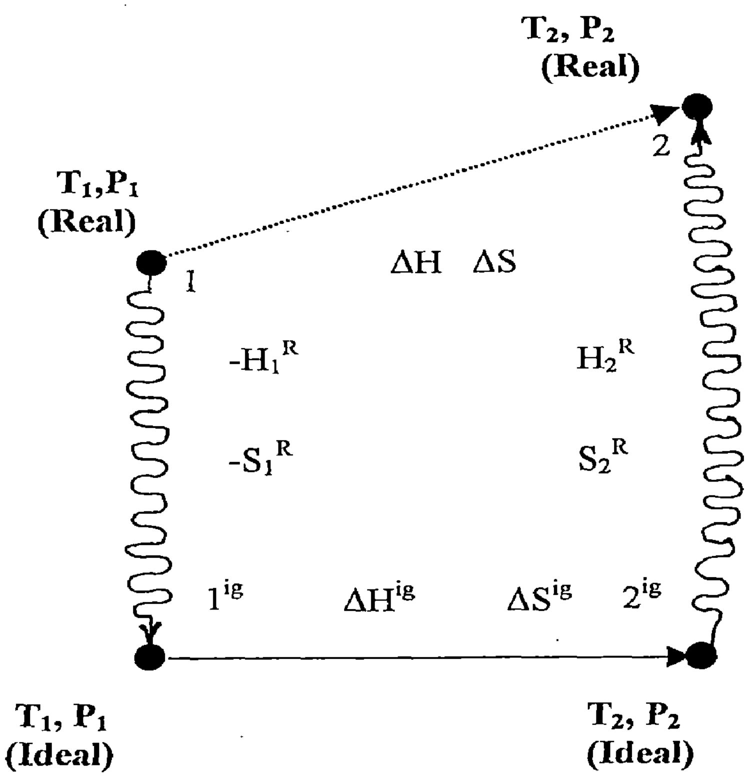

Fig 3.2 Calculational Path for property changes ΔH and ΔS

Fig 3.3, in addition to the fixed costs of condenser and reboiler. In the heat pump assisted distillation configuration, Fig 3.4, fixed cost of compressor will add to the fixed costs of the equipment and the electricity costs will add to the utility costs.

3.7.1 Cost of Compressor

Using the data available in the graph [8], an equation relating cost of compressor with its power has been developed. The equation has been converted to the present cost index. It is of the form

$$C_{Comp} = 145221\ W^{0.73} \tag{3.48}$$

It is assumed that the service life of the compressor is equal to n years and salvage value at the end of its life is zero. Cost of piping and instrumentation etc. are generally taken as 40% of the fixed cost of compressor. Annual maintenance cost of compressor is assumed as 10% of the fixed cost of compressor.

Therefore, $C_{Comp,A} = \dfrac{1.4 \times C_{Comp}}{n} + 0.1 \text{x}\ 1.4\ \text{x}\ C_{Comp}$

$$= 0.2 \text{ x } 1.4 \text{ x } 145221 \text{ x } W^{0.73} \tag{3.49}$$

3.7.2 Cost of Reboiler

Based on data available in graph form [8] for floating head type exchanger the cost equation is developed on the basis of present cost index :

$$C_R = 104420\ A_R^{0.602}$$

Annual cost of reboiler is based on n years of service life and no salvage value. Annual maintenance cost of the reboiler is assumed as 10% of fixed cost of reboiler.

Therefore, $C_{R,A} = \dfrac{C_R}{n} + 0.1 \text{x}\ C_R$

$$= 0.2 \text{ x } 104420 \text{ x } A_R^{0.602}$$

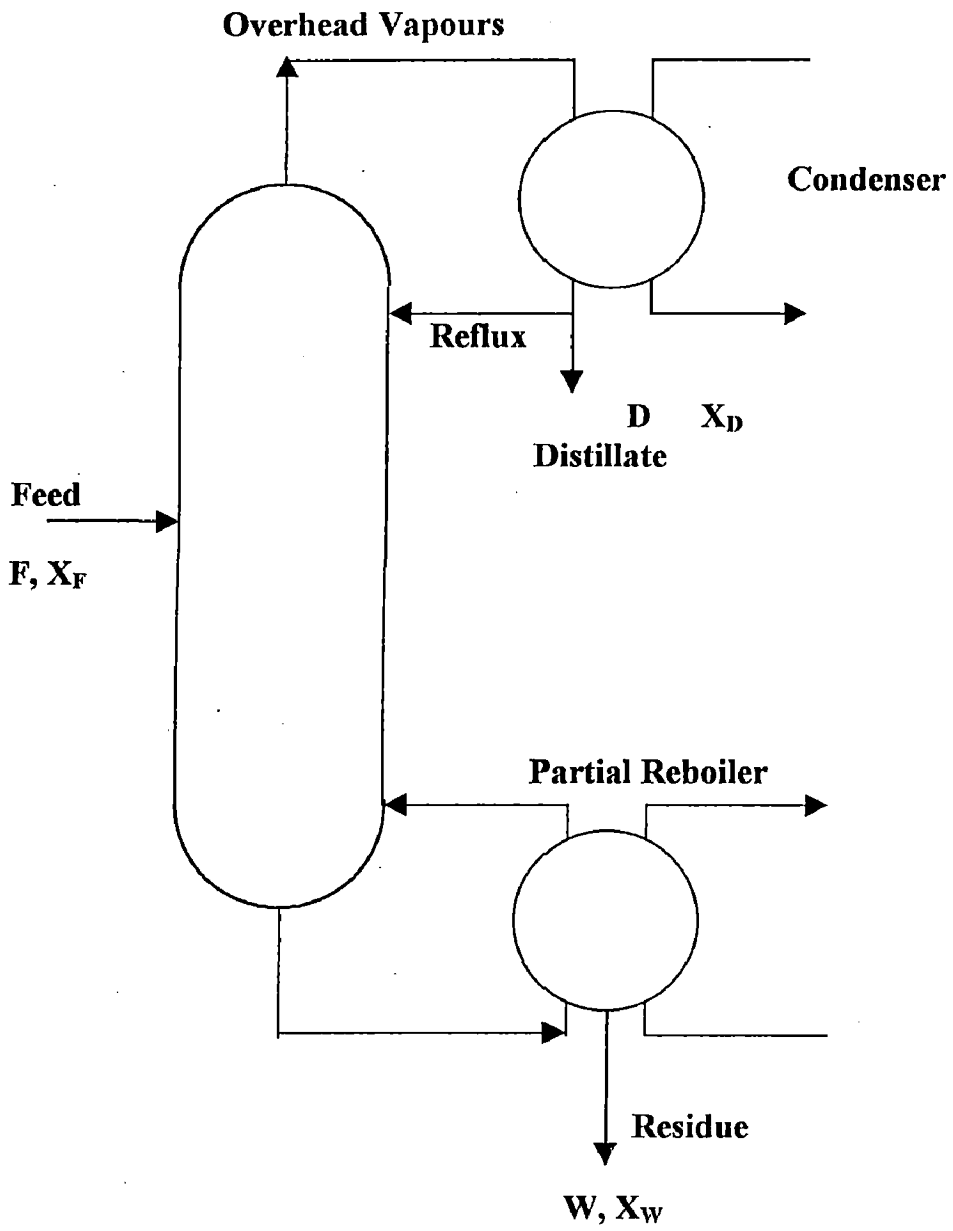

Fig 3.3 Conventional Distillation Column

$$L_j = \frac{D[H_{GD} - H_G(X_D)_{j+1}] + Q_C}{[H_G(x_j)_{j+1} - H_{Lj}]} \qquad (1 \le j \le F-2) \qquad (4.23)$$

Similarly

$$L_{F-1} = \frac{D[H_{GD} - H_G(X_D)_F] + V_f[H_G(y_f)_F - H_f] + Q_c}{[H_G(x_{F-1})_F - H_{L_{F-1}}]} \qquad (4.24)$$

and $$Q_C = L_o\left[H_G(x_0)_1 - H_{L0}\right] + D\left[H_G(X_D)_1 - H_{GD}\right. \qquad (4.25)$$

where the enthalpy expressions appearing in these equations are defined in a manner analogous to those stated below Eq. (4.22)

The flow rates in the stripping section may be determined by using enthalpy balances that enclose either the top of the bottom of the column. When the reboiler is enclosed, the following formula for the computation of the vapour rates is developed in a manner analogous to that demonstrated above.

$$V_{j+1} = \frac{W\left[H_L(x_W)_j - H_{LW}\right] + Q_R}{\left[H_{G_{j+1}} - H_L(y_{j+1})_j\right]} \qquad F \le j \le N \qquad (4.26)$$

where

$$H_L(x_W)_j = \sum_{i=1}^{2} H_{Lji}\, x_{Wi}$$

$$H_L(y_{j+1})_j = \sum_{i=1}^{2} H_{Lji}\, y_{j+1,i}$$

The reboiler duty Q_R is found by use of the overall enthalpy balance [The last expression given by Eq. (4.1)

The total flow rates of the vapour and liquid streams are related by the following total material balances, which are readily obtained by use of enclosures shown in Fig. 4.1.

$$\begin{aligned} V_{j+1} &= L_j + D & &(0 \le j \le F-2) \\ V_F + V_f &= L_{F-1} + D & & \\ L_j &= V_{j+1} + W & &(F \le j \le N) \qquad (4.27) \\ F &= D + W & & \end{aligned}$$

After the L_j's for the rectifying section and the $V_{j's}$ for the stripping section have been determined by use of the enthalpy balances the remaining total flow rates are found by use of Eq. (4.27). The most recent sets of values of the variable $\{T_{j,n+1}\}$, $\{V_{j,n+1}\}$ and $\{L_{j,n+1}\}$ are used to make the next trial through the column. The procedure described is repeated until values of the desired accuracy have been obtained.

4.6 ALGORITHM FOR SIMULATION

1. Assume a set of temperatures $\{T_j\}$ and a set of vapour rates $\{V_j\}$. [The set of liquid rates corresponding to one set of assumed vapour rates are found by use of the total material balances as shown in Eq. 4.27].
2. On the basis of the temperatures and flow rates assumed in step 1, compute the component flow rates by use of Eq. 4.10 for each component i.
3. Find that $\theta > 0$, that makes $g(\theta) = 0$ [see Eqs. 4.14 through 4.16]. [Newton's method always converges to the desired θ, provided that the first assumed value of θ is taken to be equal to zero.
4. Use equation 4.17 to compute the set of corrected x_{ji}'s for each component i and plate j.
5. Use the results of step 4 to compute the K_{jb} for each j by use of the first expression of Eq. 4.19. Use the K_{jb}'s so obtained to compute a new set of temperatures $\{T_{j,n+1}\}$ by use of Eq. 4.20.
6. Use the results of steps 4 and 5 to compute the new sets of total flow rates, $\{V_{j,n+1})$ and $\{L_{j,n+1}\}$ by use of Eqs. (4.23) through (4.27).
7. If θ, the T_j's and V_j's are within the prescribed tolerances, convergence has been achieved; otherwise repeat steps 2 through 6 on the basis of the most recent set of T_j's and V_j's.

The computer program for the simulation of distillation column (for benzene-toluene system) and its results are given in Appendix A.

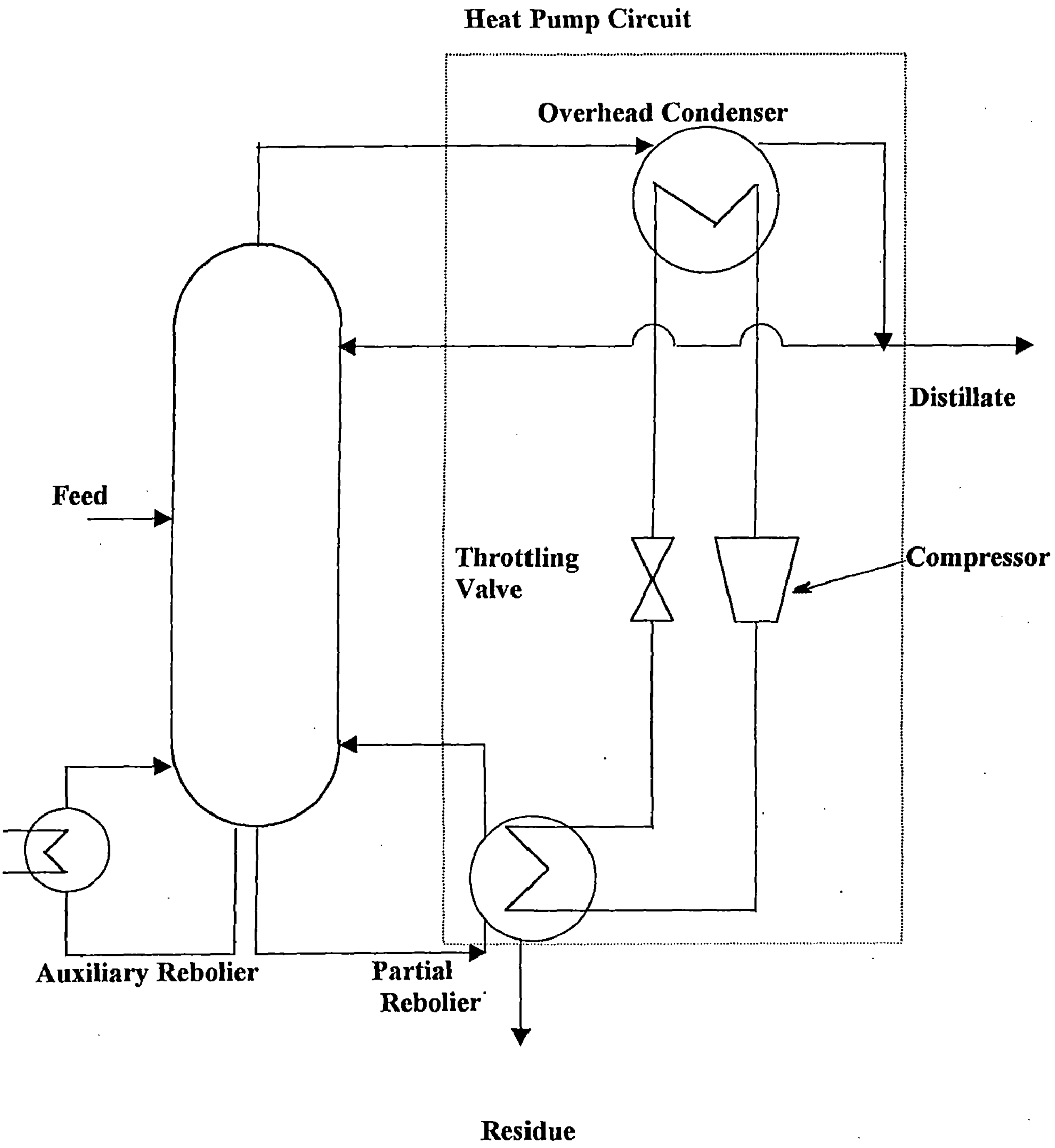

Fig 3.4 Distillation Column Coupled with Heat Pump

3.7.3 Cost of Condenser

Similarly, based on data available in graph form [8], the cost equation for condenser is developed on the basis of present cost index:

$$C_C = 78963.5\, A_C^{0.602}$$

Annual maintenance cost of the condenser is assumed as 10% of fixed cost of condenser.

$$C_{C,A} = \frac{C_C}{n} + 0.1 \text{ x } C_C$$

$$= 0.2 \text{ x } 78963.5 \text{ x } C_C$$

The cost of expansion valve and flash drum is generally quite less when compared to that of other equipments like reboiler and compressor. Therefore, these costs have not been considered here.

An inspection of Eq. 3.42 and 3.46 shows the work done by compressor depends on the value of ΔT_r where $\Delta T_r = T_2 - T_3$. For the fixed value of T_1 and T_3, as T_2 increases H_2 increases, and hence the compression work increases. Consequently cost of compressor, which is a function of work done, also increases. Thus, the cost of compressor increases with the increase in the value of ΔT_r. However, increase in the value of ΔT_r decreases the value of surface area, A_R, which in turn decreases the cost of reboiler. Thus, increase in ΔT_r has two counteracting effects – one is to increase the cost of compressor and another is to decrease the cost of reboiler. This suggests that there occurs a ΔT_r value for which the total cost of compressor and the reboiler becomes minimum.

CHAPTER - 4

SIMULATION OF DISTILLATION COLUMN

4.1 EQUILIBRIUM RELATIONSHIPS, MATERIAL BALANCES AND ENTHALPY BALANCES

For a distillation column at steady state operation, following specifications are to be made :

(1) number of plates in each section of the column

(2) quantity, composition, and thermal condition of feed

(3) the pressure maintained throughout the column

(4) type of overhead condenser (total or partial)

(5) reflux ratio, L_o/D or V_1 or L_o

(6) one specification on the distillate such as total flow rate D.

For this set of given conditions, the problem is to find the compositions of top and bottom products. Following equations apply to the distillation of binary mixture.

Equilibrium Relationships

$$\left\{\begin{array}{ll} y_{ji} = K_{ji}x_{ji} & i = 1, 2;\quad 0 \le j \le N+1 \\ \sum_{i=1}^{2} y_{ji} = 1 & 0 \le j \le N+1 \\ \sum_{i=1}^{2} x_{ji} = 1 & 0 \le j \le N+1 \end{array}\right. \tag{4.1}$$

Material Balance

$$\left\{\begin{array}{ll} V_{j+1}\, y_{j+1,i} = L_j\, x_{ji} + DX_{Di} & i = 1,2;\quad 0 \le F-2 \\ V_F\, y_{Fi} + V_f\, y_{fi} = L_{F-1}x_{F-1,i} + DX_{Di} & i = 1, 2; \\ V_{j+1}\, y_{j+1,i} = L_j x_{ji} - Wx_{Wi} & i = 1, 2;\quad F \le j \le N \\ FX_i = DX_{Di} + Wx_{Wi} & i = 1, 2 \end{array}\right. \tag{4.2}$$

Enthalpy Balances

$$\begin{cases} V_{j+1}\, H_{Gj+1} = L_j H_{Lj} + DH_D + Q_C & 0 \le j \le F-2 \\ V_F\, H_F + V_f H_f = L_{F-1} H_{LF-1} + DH_D + Q_C & \\ V_{j+1} H_{Gj+1} = L_j H_{Lj} - WH_{LW} + Q_R & F \le j \le N \\ FH = WH_{LW} + DH_D + Q_C - Q_R & \end{cases} \qquad (4.3)$$

A schematic representation of the component material balance is shown in Fig. 4.1 As the benzene and toluene form ideal solution, the enthalpy per mole of vapour and the enthalpy per mole of liquid leaving plate j are given by the following expression

$$H_{Gj} = \sum_{i=1}^{2} H_{Gji}\, y_{ji} \qquad \text{(vapour)}$$

$$H_{Lj} = \sum_{i=1}^{2} H_{Lji}\, x_{ji} \qquad \text{(liquid)}$$

where the enthalpy of each pure component i in the vapour and liquid streams leaving plate j are represented by H_{Gji} and H_{Lji} respectively. These enthalpies are, of course evaluated at the temperature and pressure of plate j. The meaning of H_D depends on the condenser used. In the system under study, the total condenser is used. For a total condenser, (D is withdrawn from the accumulator as a liquid at its bubble point temperature T_b at the column pressure, and $y_{1i} = x_{oi} = X_{Di}$),

$$H_D = \sum_{i=1}^{2} H_{L0i} X_{Di} = \sum_{i=1}^{2} H_{L0i}\, X_{0i} = H_{LO}$$

The enthalpy per mole of residue has double but equivalent representation, H_{LW} and H_{LN+1}, that is

$$H_{LW} = \sum_{i=1}^{2} H_{LW}\, X_{Wi} = \sum_{i=1}^{2} H_{LN+1,i}\, x_{N+1,i} = H_{LN+1}$$

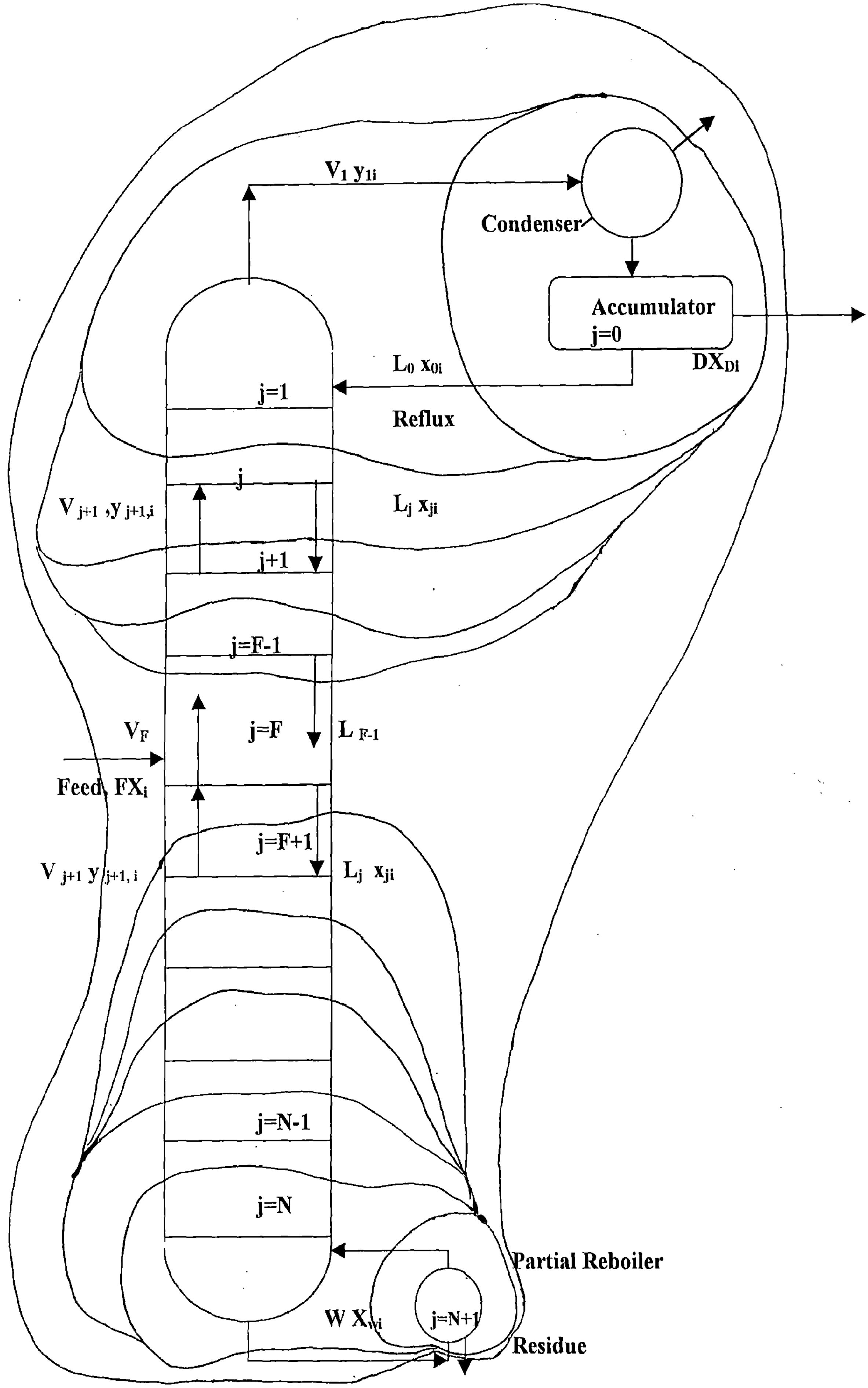

Fig 4.1: Representation of Component -Material Balance (given by Eqs. 4.1 to 4.3)

The symbols Q_C and Q_R are used to denote the condenser and reboiler duties, respectively. The condenser duty Q_C is equal to the net amount of heat removed per unit time by the condenser and the reboiler duty is equal to the net amount of heat introduced to the reboiler per unit time.

4.2 COMPONENT-MATERIAL BALANCE AND EQUILIBRIUM RELATIONSHIP AS A TRIDIAGONAL MATRIX

In the case of the component-material balances, a new set of variables, the component flow rates in the vapour and liquid phases are introduced, namely,

$$v_{ji} = V_j y_{ji} \quad \text{and} \quad l_{ji} = L_j x_{ji} \tag{4.4}$$

Also, the flow rates of component i in the distillate and residue are represented by

$$d_i = DX_{Di} \quad \text{and} \quad w_i = Wx_{Wi}$$

and the flow rates of component i in the vapour and liquid parts of the feed are represented by

$$v_{fi} = V_f y_{fi} \quad \text{and} \quad l_{fi} = L_f x_{fi}$$

The equilibrium relationship $y_{ji} = K_{ji} x_{ji}$ may be restated in an equivalent form in terms of component flow rates v_{ji} and l_{ji} as follows. First, observe that the expression $y_{ji} = K_{ji} x_{ji}$ may be restated in the form

$$V_j y_{ji} = \left(\frac{V_j K_{ji}}{L_j} \right) L_j x_{ji}$$

and from Eq. (3.4) it follows that

$$v_{ji} = S_{ji} l_{ji} \text{ and } l_{ji} = A_{ji} v_{ji} \tag{4.5}$$

where $A_{ji} = \dfrac{1}{S_{ji}} = \dfrac{L_j}{K_{ji} V_j}$

Instead of enclosing the end of the column and the respective plates in each section of the column as demonstrated by Eq. (4.1) through Eq. (4.3) and Fig. 4.1, an equivalent set of component balance is obtained by enclosing each plate (j = 0, 1, 2, ..., N, N+1) by a component material balance as demonstrated in Fig. 4.2.

The corresponding set of material balance for each component i are as follows :

$$\begin{cases} -l_{0i} - d_i + v_{1i} = 0 \\ l_{j-1,i} - v_{ji} - l_{ji} + v_{j+1,i} = 0 \quad (1 \le j \le F-2) \\ l_{F-2,i} - v_{F-1,i} - l_{F-1,i} + v_{Fi} = -v_{fi} \\ l_{F-1,i} - v_{F,i} - l_{F,i} + v_{F+1,i} = -l_{fi} \\ l_{j-1,i} - v_{ji} - l_{ji} + v_{j+1,i} = 0 \quad (F+1 \le j \le N) \\ l_{Ni} - v_{N+1,i} - w_i = 0 \end{cases} \tag{4.6}$$

Except for the first expression of (4.6), the l_{ji},s may be eliminated from equation (4.6) by use of equilibrium relationship, Eq. (4.5). For the total condenser, l_{o1} and d_i have the same compositions, and thus,

$$l_{oi} = \left(\frac{L_o}{D}\right) d_i \tag{4.7}$$

$$l_{oi} = A_{oi}\, d_i \tag{4.8}$$

where, $A_{oi} = \frac{L_o}{D}$

Also, the form of $A_{N+1,i}$ differs slightly from that for A_{ji} because of the double representation by the subscripts "N+1 " and "W" that is

$$\left.\begin{array}{l} V_{N+1,i}\, y_{N+1,i} = \left(\dfrac{V_{N+1} K_{N+1,i}}{W}\right) Wx_{Wi} \\ \text{or} \quad w_i = A_{N+1,i}\, v_{N+1,i} \end{array}\right] \tag{4.9}$$

where $A_{N+1,i} = \dfrac{W}{K_{N+1,i}\, V_{N+1}}$

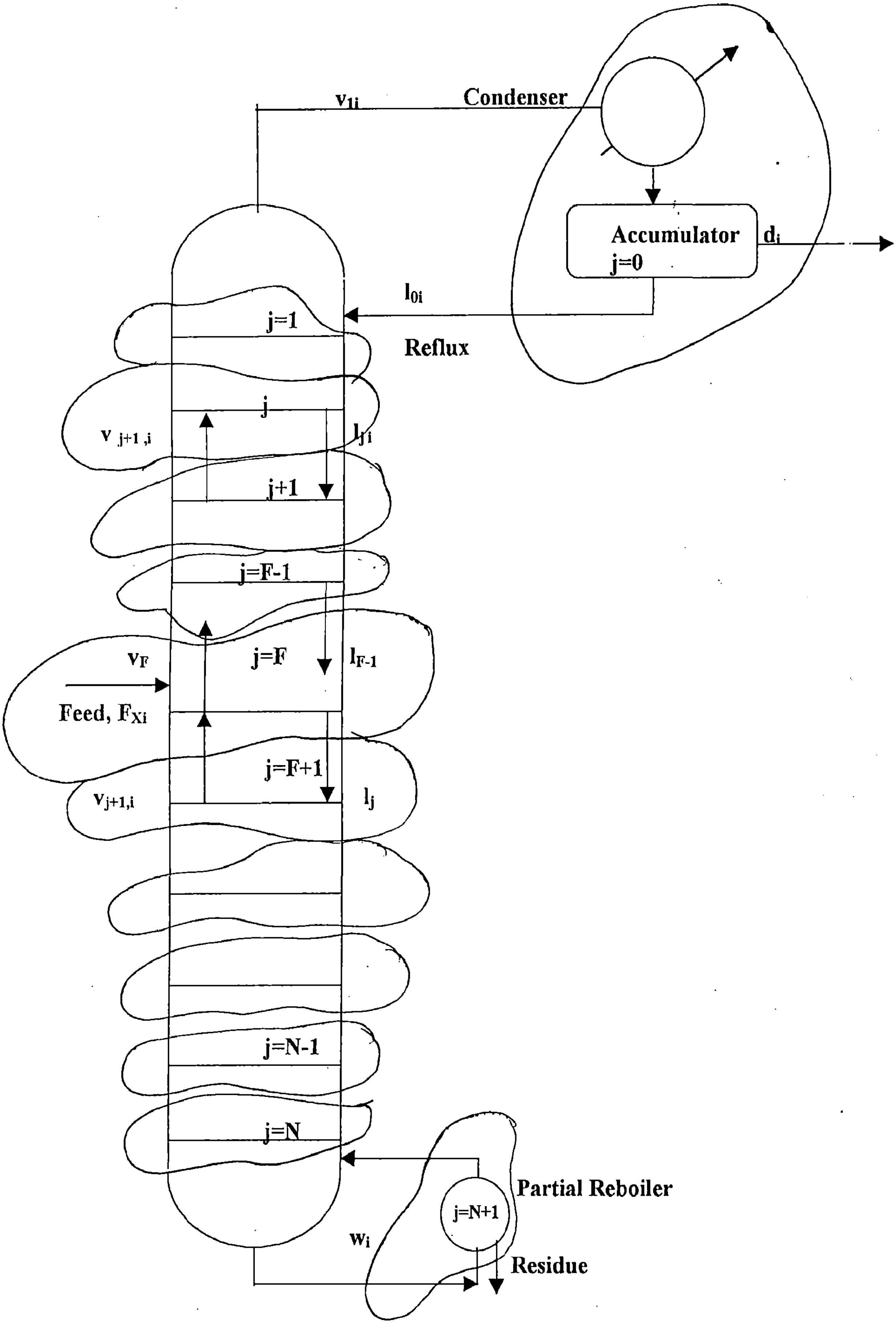

Fig 4.2 Representation of Component -Material Balance (given by Eq 4.6)

when the l_{ji}'s and w_i are eliminated from Eq. (4.6) by use of Eq. (4.5), (4.7), (4.8) and (4.9), the following results is obtained.

$$\begin{cases} -(A_{oi}+1)d_i + v_{1i} = 0 \\ A_{j-1,i}\, v_{j-1,i} - (A_{ji}+1)v_{ji} + v_{j+1,i} = 0 \qquad (1 \le j \le F-2) \\ A_{F-2,i}\, v_{F-2,i} - (A_{F-1}+1)v_{F-1,i} + v_{Fi} = -v_{fi} \\ A_{F-1,i}\, v_{F-1,i} - (A_{F,i}+1)v_{F,i} + v_{F+1,i} = -l_{fi} \\ A_{j-1,i}\, v_{j-1,i} - (A_{ji}+1)v_{ji} + v_{j+1,i} = 0 \qquad (F+1 \le j \le N) \\ A_{Ni}\, v_{Ni} - (A_{N+1,i}+1)\, v_{N+1,i} = 0 \end{cases}$$

This set of equations may be stated in the matrix form as

$$A_i v_i = -\zeta_i \tag{4.10}$$

where

$$A_i = \begin{bmatrix} -\rho_{oi} & & 1 & 0 & 0 & \cdots & \cdots & \cdots & \cdots & 0 \\ A_{oi} & & -\rho_{1i} & 1 & 0 & \cdots & \cdots & \cdots & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & \cdots & 0 & A_{F-2,i} & -\rho_{F-1,i} & 1 & 0 & 0 & \cdots & 0 \\ 0 & \cdots & 0 & 0 & A_{F-1,i} & -\rho_{Fi} & 1 & 0 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & \cdots & \cdots & \cdots & \cdots & 0 & A_{N-1,i} & -\rho_{Ni} & \cdots & 1 \\ 0 & \cdots & \cdots & \cdots & \cdots & 0 & 0 & A_{Ni} & \cdots & -\rho_{N+1,i} \end{bmatrix}$$

$$v_i = [d_i, v_{1i}, v_{2i}, \ldots\ldots\ldots, v_{F-1,i}, v_{F,i} \ldots\ldots, v_{Ni}, v_{N+1,i}]^T$$

$$\zeta_i = [0 \quad 0 \quad 0 \ldots\ldots\ldots v_{fi}\, l_{fi} \ldots\ldots\ldots 0 \quad 0]^T$$

$$\rho_{ji} = A_{ji} + 1$$

The remainder of the development of the calculation procedure is ordered in the same sequence in which the calculations are carried out. The calculational procedure is initiated by the assumption of a set of temperatures $\{T_j\}$ and a set of vapour rates $\{V_j\}$ from which the corresponding set of liquid rates $\{L_j\}$ is found by using the total material balances enumerated below. This particular choice of variables was proposed by Thiele and Geddes. On the basis of the assumed temperatures and total flow rates, the absorption factors {Aji} appearing in Eq. (4.10) may be evaluated for component i on each plate j. Since matrix A_i in Eq. (4.10) is of tridiogonal form, this matrix equation may be solved for calculated values of the vapour rates for component i [denoted by (v_{ji})] by use of the Thomas algorithm. Consider the following set of linear equation in the variables x_o, $x_1, \ldots\ldots,$ x_N, x_{N+1}, whose coefficient form a tridiogonal matrix of the following form

$$
\begin{aligned}
&B_{o,i}\,x_o + C_{o,i}x_1 = D_{o,i} \\
&A_{1,i}x_o + B_{1,i}x_1 + C_{1,i}x_2 = D_{1,i} \\
&A_{2i}x_1 + B_{2,i}x_2 + C_{2,i}x_3 = D_{2,i} \\
\\
&A_{N,i}x_N + B_{N,i}x_N + C_{N,i}x_{N+1} = D_{N,i} \\
&A_{N+1,i}\,x_N + B_{N+1,i}\,x_{N+1} = D_{N+1,i}
\end{aligned}
$$

For each component, the following coefficients are determined.

$$a_{oi} = B_{oi} \qquad\qquad b_{oi} = D_{oi}/B_{oi}$$

$$
\left.
\begin{aligned}
a_{ji} &= B_{ji} - \frac{Aji.C_{j-1,i}}{a_{j-1,i}} \\
b_{ji} &= \frac{D_{ji} - A_{ji}.b_{j-1,i}}{a_{ji}}
\end{aligned}
\right\} \quad 1 \le j \le N+1
$$

$$x_{N+1} = v_{N+1,i} = b_{N+1,i} \qquad i = 1, 2$$

$$x_j = v_{ji} = b_{ji} - \frac{C_{ji}.v_{j+1,i}}{a_{ji}} \qquad i = 1, 2;\quad 0 \le j \le N$$

$$d_i = v_{oi}$$

After these recurrence formulas have been applied for each component i and the complete set of vapour rates $\{(v_{ji})_{Ca}\}$ has been found, the corresponding set of liquid rates $\{(l_{ji})_{Ca}\}$ is then found by use of Eq. (4.5). These sets of calculated flow rates can be used in conjunction with the θ-method of convergence and the K_b method in the determination of an improved set of temperatures.

4.3 FORMULATION OF THE θ-METHOD OF CONVERGENCE

In this application of the θ-method of convergence, it is used to weight the mole fractions that are employed in the K_b method for computing a new temperature profile. The corrected set of product rates is used as weight factors in the calculation of improved sets of mole fractions. The corrected terminal rates are selected so that they are both in overall component-material balance and in agreement with the specified value of D, that is

$$FX_i = (d_i)_{co} + (w_i)_{co} \tag{4.11}$$

and

$$\sum_{i=1}^{2} (d_i)_{co} = D \tag{4.12}$$

These two conditions may be satisfied simultaneously by suitably choosing the multiplier θ, which is defined by

$$\left(\frac{w_i}{d_i}\right)_{co} = \theta\left(\frac{w_i}{d_i}\right)_{ca} \tag{4.13}$$

The subscripts 'co" and "ca" are used throughout this discussion to distinguish between the corrected and calculated values of a variable, respectively.

Elimination of $\left(\frac{w_i}{d_i}\right)_{ca}$ from Eq. (4.11) and (4.13) yields the formula $(d_i)_{co}$, namely

$$(d_i)_{co} = \frac{FX_i}{1+\theta\left(\frac{w_i}{d_i}\right)_{ca}} \tag{4.14}$$

Since the specified values of $(d_i)_{co}$ are to have a sum equal to the specified value of D, the desired value of θ is that $\theta > 0$ that makes $g(\theta) = 0$, where

$$g(\theta) = \sum_{i=1}^{2} (d_i)_{ca} - D \tag{4.15}$$

In the determination of θ by Newton's method, the following formula for the first derivative $g'(\theta)$ is needed.

$$g'(\theta) = \sum_{i=1}^{2} \frac{d(d_i)_{ca}}{d\theta} = -\sum_{i=1}^{2} \frac{\left(\dfrac{w_i}{d_i}\right)_{ca} FX_i}{\left[1+\theta\left(\dfrac{w_i}{d_i}\right)_{ca}\right]^2} \tag{4.16}$$

After the desired value of θ has been obtained, $(w_i)_{co}$ may be computed by Eq. (4.13). Note that Newton's method converges to the positive root of $g(\theta)$, provided that $\theta = 0$ is taken to be the first trial value.

The corrected mole fractions for the liquid and vapour phases are computed as follows :

$$x_{ji} = \frac{\left(\dfrac{l_{ji}}{d_i}\right)_{ca} (d_i)_{co}}{\sum_{i=1}^{2}\left(\dfrac{l_{ji}}{d_i}\right)_{ca} (d_i)_{co}} \tag{4.17}$$

$$y_{ji} = \frac{\left(\dfrac{v_{ji}}{d_i}\right)_{ca} (d_i)_{co}}{\sum_{i=1}^{2}\left(\dfrac{v_{ji}}{d_i}\right)_{ca} (d_i)_{co}} \tag{4.18}$$

These expressions are consistent with the definition of θ given by Eq. (4.13).

4.4 DETERMINATION OF AN IMPROVED SET OF TEMPERATURES BY USE OF THE K_b METHOD

On the basis of the mole fractions given by Eq. (4.17) and (4.18) and the last temperature profile (the one assumed to make the nth trial), the new temperature profile is found by using the K_b method in the following manner

For any plate j,

$$\left. \begin{aligned} K_{jb}\Big|_{T_{j,n+1}} &= \frac{1}{\sum_{i=1}^{2} \alpha_{ji}\Big|_{T_{jn}} x_{ji}} \\ \text{or } K_{jb}\Big|_{T_{j,n+1}} &= \sum_{i=1}^{2} \frac{y_{ji}}{\alpha_{ji}\Big|_{T_{jn}}} \end{aligned} \right] \qquad (4.19)$$

where

$\alpha_{ji} = K_{ji}/K_{jb}$, the relative volatility of component i at the temperature of plate j. The rate of convergence of the entire calculational procedure is dependent upon the precise choice of K_{jb}.

It can be shown that the x_{ji}'s and y_{ji}'s defined by Eq. (4.17) and (4.18) respectively, form a consistent set in that they give the same value of K_{jb}. Component b represents a hypothetical base component whose K value is given by

$$\log_e K_{jb} = \frac{a}{T_j} + b \qquad (4.20)$$

where the constants a and b are evaluated on the basis of the values of K at the upper and lower limits of the curve fits of the mid boiling component of the mixture or one just lighter. Thus after K_{jb} has been computed by use of Eq. (4.19), one temperature $T_{j,n+1}$ to be assumed for the next trial is calculated directly by use of Eq. (4.20).

The corrected compositions and the new temperatures are used in the enthalpy balances to determine the total flow rates to be used for the next trial through the column.

4.5 DETERMINATION OF AN IMPROVED SET OF TOTAL FLOW RATES BY USE OF THE CONSTANT COMPOSITION METHOD

In the constant composition method, one total flow rate (V_j or L_j) is eliminated from each of the enthalpy balances given by Eq. (4.3) by use of set of the component material balances given by Eq. (4.3). To illustrate the development of these equations, consider the enthalpy balance enclosing any plate j of the rectifying section, namely

$$V_{j+1}H_{Gj+1} = L_jH_{Lj} + DH_D + Q_C \quad (0 \le j \le F-2) \tag{4.21}$$

The total flow rate V_{j+1} is eliminated from Eq. (4.21) by use of component material balance enclosing plate

$$v_{j+1,i} = l_{ji} + d_i \qquad (0 \le j \le F-2)$$

as follows

$$\begin{aligned} V_{j+1}H_{Gj+1} &= \sum_{i=1}^{2} H_{Gj+1,i}\, v_{j+1,i} = \sum_{i=1}^{2} H_{Gj+1}(l_{ji} + d_i) \\ &= L_j \sum_{i=1}^{2} H_{Gj+1,i}x_{ji} + D\sum_{i=1}^{2} H_{Gj+1,i}X_{Di} \\ &= L_j\, H_G(x_j)_{j+1} + DH_G(X_D)_{j+1} \end{aligned} \tag{4.22}$$

where $H_G(x_j)_{j+1} = \sum_{i=1}^{2} H_{Gj+1,i}\, x_{ji}$

$$H_G(X_D)_{j+1} = \sum_{i=1}^{2} H_{Gj+1}\, X_{Di}$$

Elimination of $V_{j+1}H_{g_{j+1}}$ from equations 4.21 and 4.22 yields

CHAPTER - 5

RESULTS AND DISCUSSIONS

This chapter discusses results and interpretations of the analysis of a conventional distillation configuration. Benzene-toluene system has been considered for conventional distillation column as well as heat pump assisted distillation configurations.

5.1 COMPARISON OF HEAT LOADS

The condenser and reboiler duty as calculated by Ponchon-Savarit method compared with that calculated by the simulation of distillation column (for benzene-toluene system)

Table 5.1: Comparison of heat loads

Type of heat load	By Ponchon-Savarit method	By Simulation
Condenser Duty, kW	596.882	593.796
Reboiler Duty, kW	661.418	672.954

Therefore, as evident from the table, it can be inferred that the heat loads as calculated by the graphical method (Ponchon-Savarit method) are very close to that obtained by simulation of the column for the benzene-toluene system.

5.2 ECONOMICAL ANALYSIS OF HEAT PUMP

In distillation column coupled with heat pump, the temperature difference between the bottoms of the column and the compressed vapour stream in reboiler, ΔT_r plays an important role in determining whether the use of heat pump is economically feasible or not. The annual costs of reboiler and that of compressor are directly related to ΔT_r . In the case of reboiler, it decreases continuously with increase in ΔT_r whereas for compressor , it increases. The annual electricity charges depends on the power of compressor, and hence depends on ΔT_r. These costs have been plotted in Fig 5.1 for a given set of economic data. The total costs, as seen, from the figure, passes through a point of minima. This point represent the optimum value of ΔT_r. It may be mentioned here that the value of optimum ΔT_r is valid only for the set of economic data used in this investigation.

The total annual cost of the conventional distillation system has been compared with that of system coupled with heat pump to determine the range of ΔT_r for which application of heat pump is justified economically. This plot is shown in Fig. 5.2. The dotted line in this figure represents the total annual cost of the conventional column whereas firm line represents that of column with heat pump. The region abc of firm line lying below the dotted line represents the range of ΔT_r for which the cost of column with heat pump is less than that of the conventional column. Therefore, this region establishes the range of ΔT_r for the applicability of heat pump in distillation unit. For the present data, range of ΔT_r is found to be 1 °C to 8.5 °C. Although use of heat pump has been found to be profitable in this range, yet the system should be examined for its normal operation.

It is important to mention here that the above range of ΔT_r is valid only for the fixed cost of reboiler, condenser, compressor and cost of electric energy used in this investigation. Costs are never static in nature. They, as present day trend indicates, increase continuously depending upon inflation. Therefore, this analysis of determining the range of ΔT_r for the applicability of heat pump has been

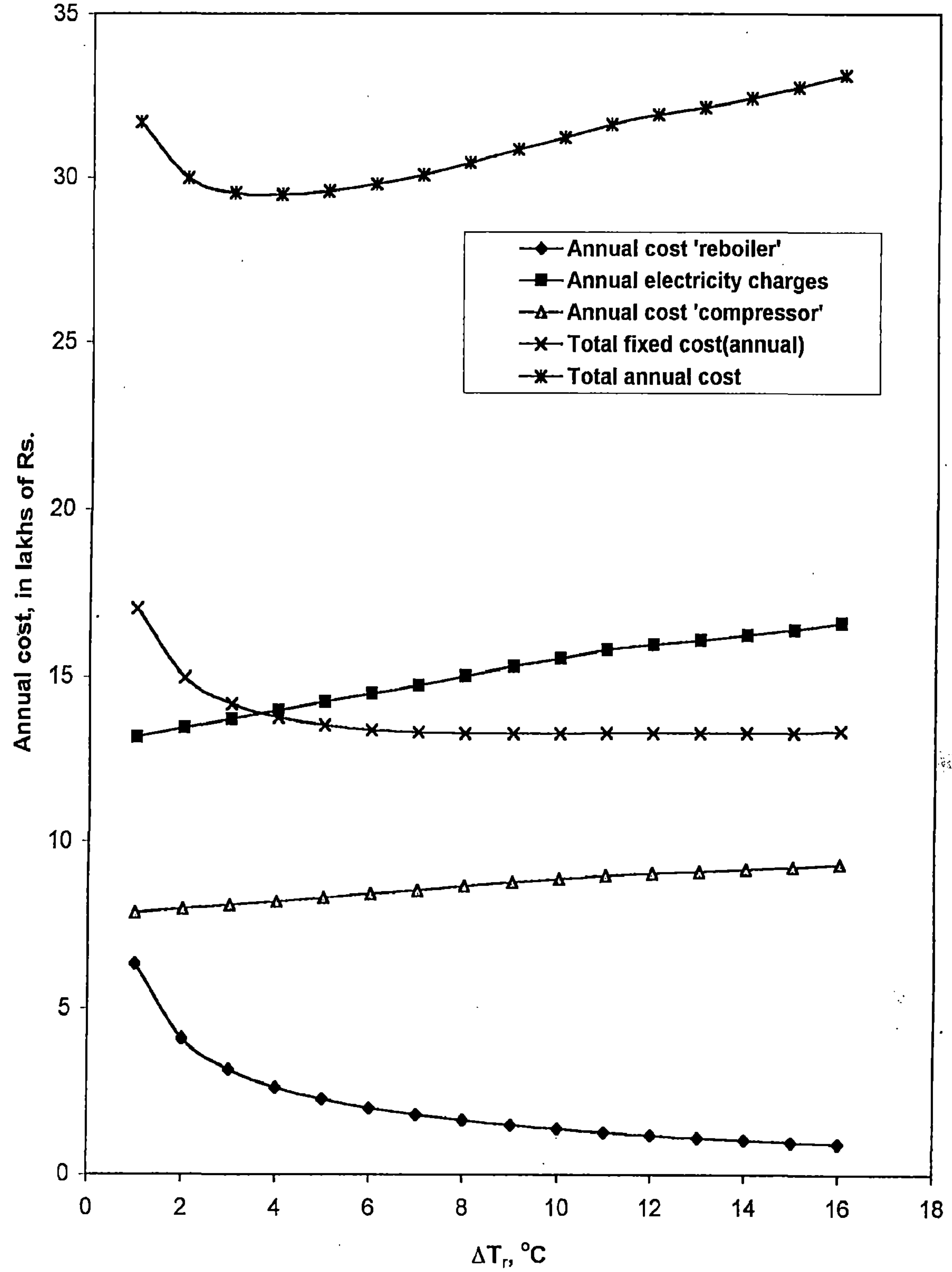

Fig. 5.1 : Variation of annual fixed costs and electricity charges for heat pump with ΔT_r

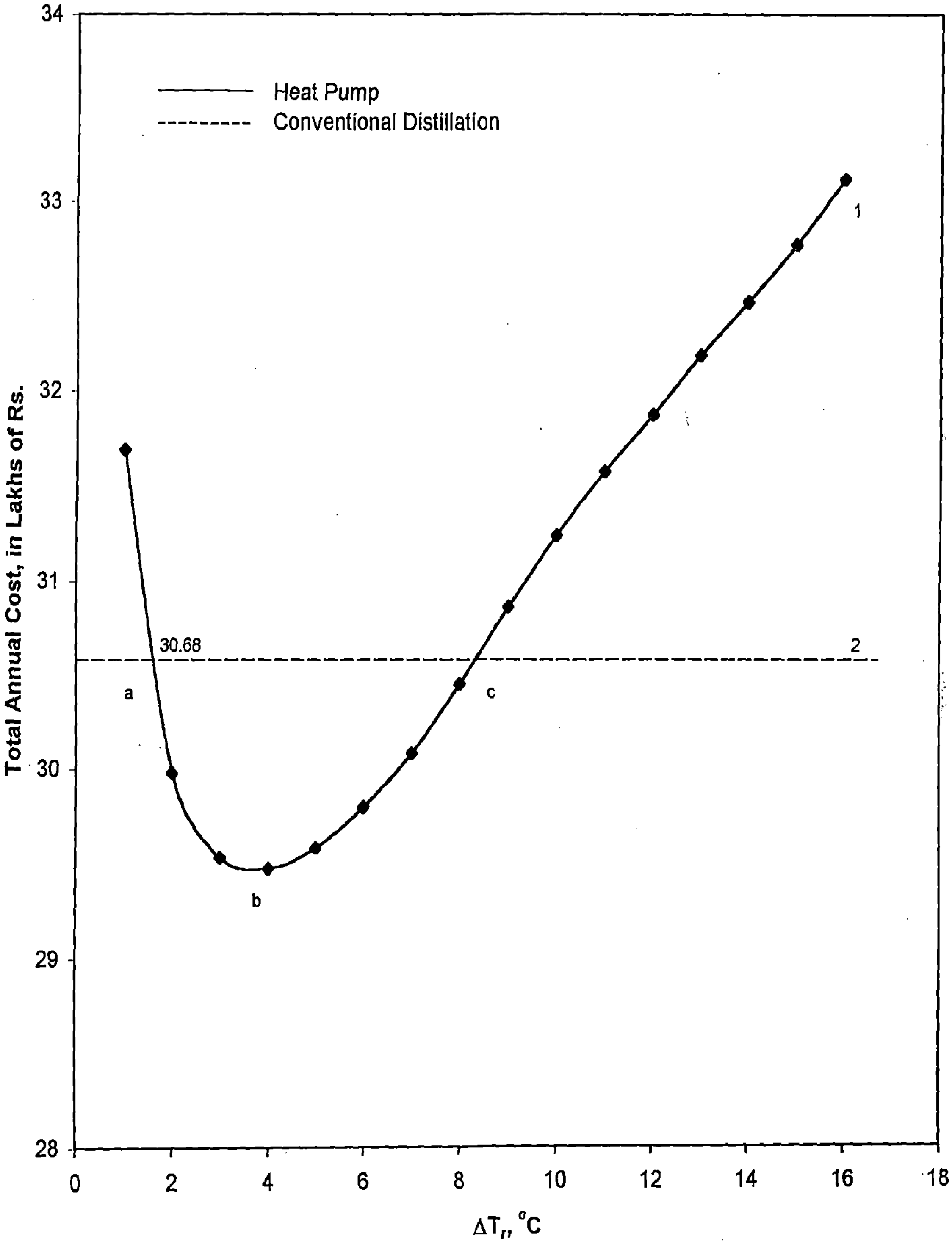

Fig. 5.2 : Variation of total annual cost for column coupled with heat pump with ΔT_r

extended to futuristic utilities and fixed costs. This has been carried out by defining two cost indices, as given below :

$$\text{Fixed cost index (FCI)} = \frac{\text{Prevalent fixed cost of equipment}}{\text{Reference fixed cost of equipment}}$$

and $$\text{Utility cost index (UCI)} = \frac{\text{Prevalent cost of equipment}}{\text{Reference cost of equipment}}$$

In the present investigation, reference cost of utilities and equipment has been taken as those used in Fig. 5.2.

To determine the effect of variation of UCI on the applicability range of ΔT_r, a plot between annual cost of both the cases (column with and without heat pump) and ΔT_r with UCI has been shown in Fig. 5.3. This plot is for a given value of FCI. The dotted lines of the plot represent the case of conventional column (at minimum ΔT_r for a particular value of UCI and FCI) whereas the firm lines of column coupled with heat pump (for the range of ΔT_r). From this plot, following salient features are noted.

(1) For a given value of FCI and UCI, there exists a unique range of ΔT_r for which the use of heat pump is economically justified.

(2) For a given value of FCI, an increase in the cost of utilities (UCI) increases the applicability range of ΔT_r. However, the optimal value of ΔT_r suffers a little decrease.

These points suggest that the use of heat pump in distillation is favoured when cost of utilities rises due to inflation as it corresponds to a large range of ΔT_r.

Fig. 5.4 also contains a plot similar to that of Fig. 5.3 but for FCI = 2.0, this plot has the same trend as that observed earlier.

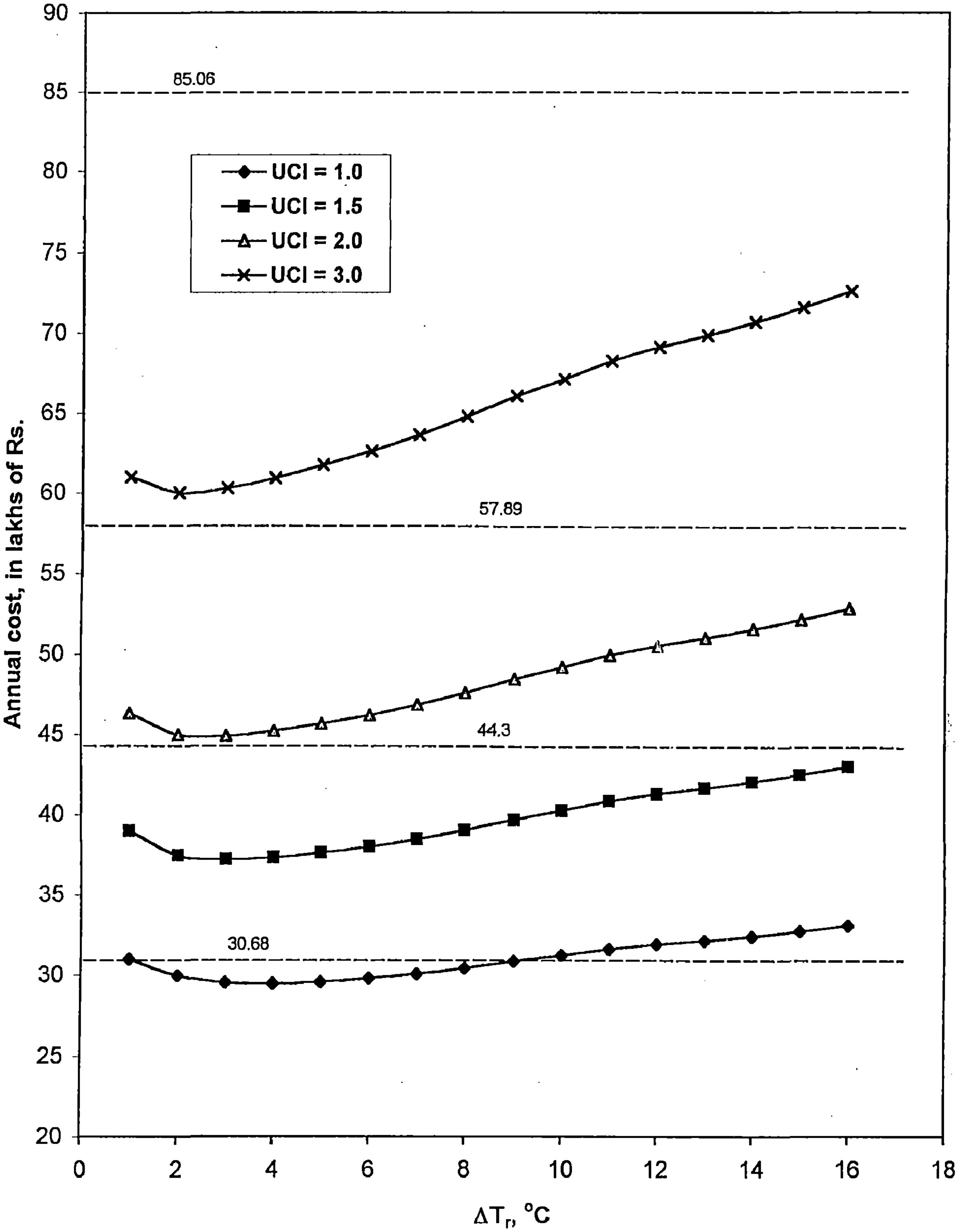

Fig. 5.3 : Variation of total annual cost for heat pump assisted distillation column with ΔT_r, for various UCI (FCI = 1.0)

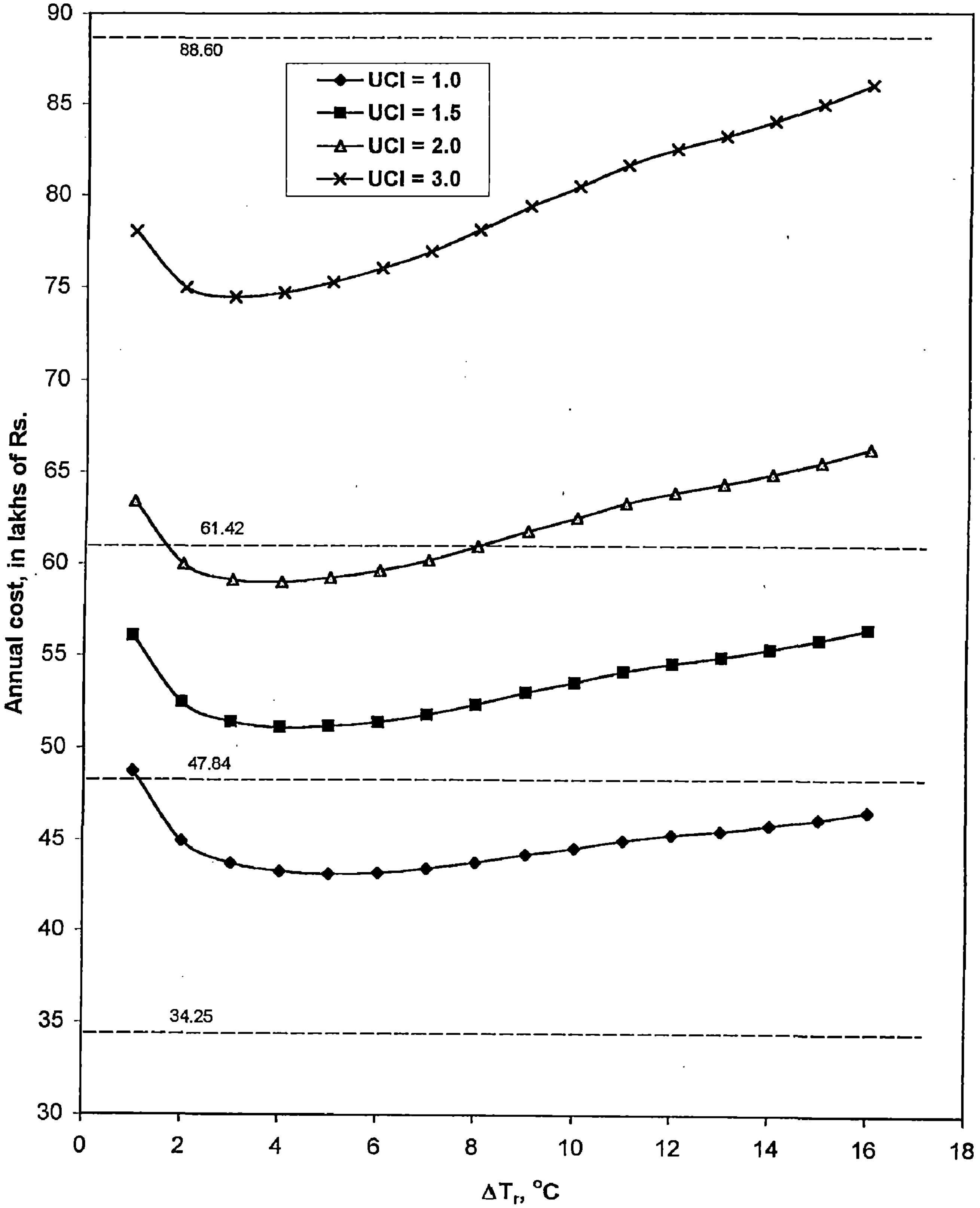

Fig. 5.4 : Variation of total annual cost for heat pump assisted distillation column with ΔT_r, for various UCI (FCI = 2.0)

To obtain the parametric effect of variation of FCI on applicability range of ΔT_r, plot between annual total cost of column with heat pump and ΔT_r with FCI as a parameter has been drawn in Fig. 5.5 and 5.6. These plots also contain annual total cost data conventional column. They are for 1.0 and 2.0 values of UCI respectively.

An examination of the plot contained in Fig. 5.5 shows that the column coupled with heat pump for which the value of FCI is equal to 1.0, has an applicability range of ΔT_r from 1 to 8.5 °C. However, systems having values of FCI equal to 1.5 and higher always show annual total cost to be higher than that of conventional column. Therefore, the use of heat pump for columns having FCI more than 1.5 and UCI equal to 1.0 is not recommended. The plot of Fig. 5.6 clearly shows that for the value of UCI equal to 2.0, there exists applicability ranges of ΔT_r for FCI = 2.0. The range of ΔT_r goes on shrinking as the value of FCI increases. In the case of FCI = 3.0, use of heat pump is not recommended.

Tables given in Appendix-D provide applicability range of ΔT_r for various values of FCI and UCI. These tables are of immense utility to energy conscious plant managers to determine the range of ΔT_r for which use of heat pump in distillation is economically viable for various values of fixed and utility costs.

For the value of ΔT_r at which the total costs of utilities and equipments taken together, are minimum, the comparison of costs of utilities and equipments is shown in the table given below :

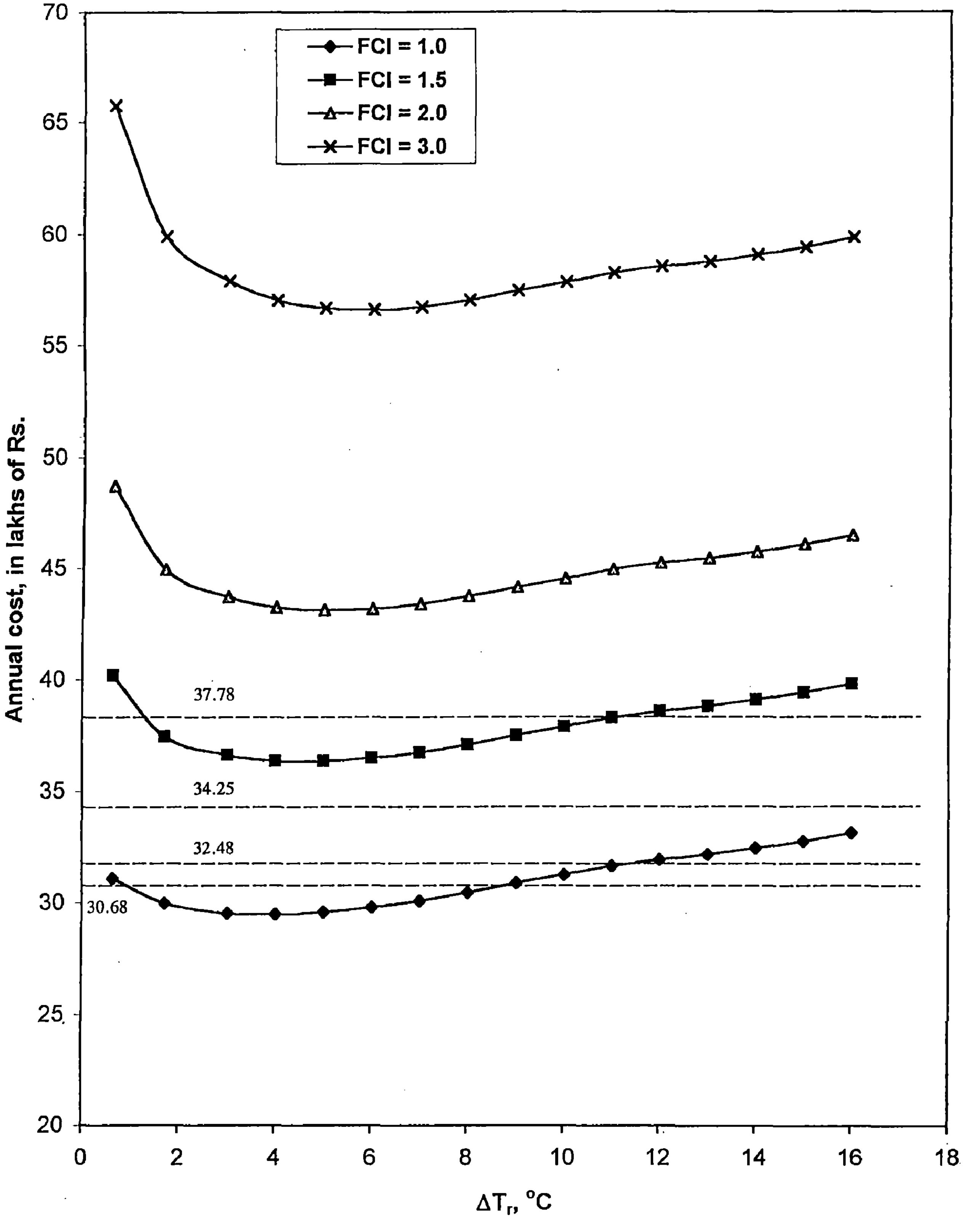

Fig. 5.5 : Variation of total annual cost for heat pump assisted distillation column with ΔT_r, for various FCI (UCI = 1.0)

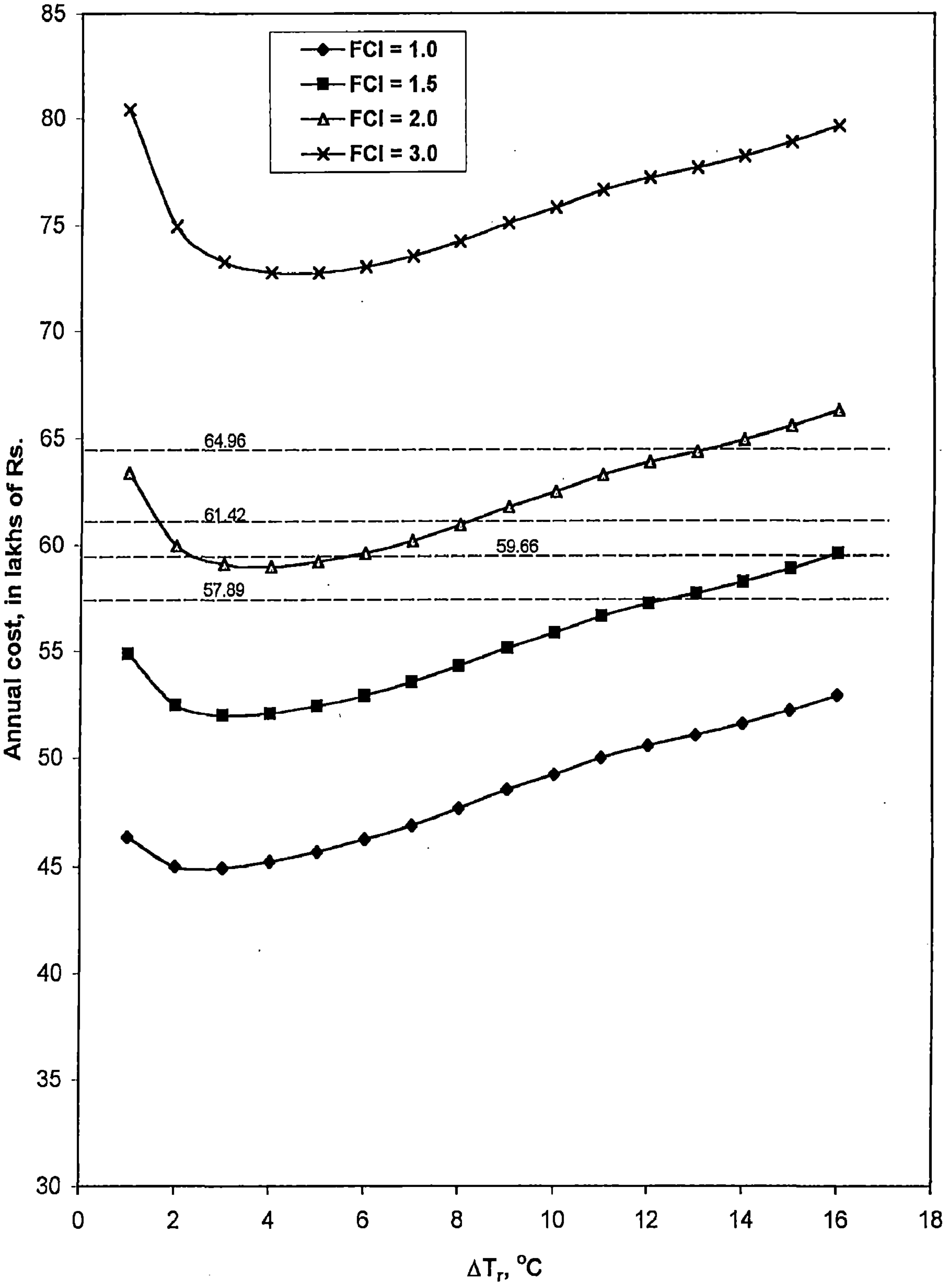

Fig. 5.6 : Variation of total annual cost for heat pump assisted distillation column with ΔT_r, for various FCI (UCI = 2.0)

Table 5.2 : Comparison of Costs of Utilities and Equipments (in Rs.) for Conventional Distillation Column and Heat Pump Assisted Distillation Column

Utility/Equipment	Conventional distillation column	Heat pump assisted distillation column
Cooling water	3,44,573.44	
Steam	21,45,194.99	1,73,776.00
Electricity	-	16,80,000.00
Condenser	96,639.92	2,22,434.00
Reboiler	4,81,992.01	2,64,934.06
Auxiliary reboiler		61,904.70
Compressor		5,44,950.59
Total	30,67,999.96	29,47,999.35

From the table given above, it is evident that annual total cost for the column coupled with heat pump is less than that for conventional distillation. So, it can be concluded that heat pump assisted distillation column is economically feasible for $\Delta T_r = 4°C$.

CONCLUSIONS AND RECOMMENDATIONS

It can be concluded from the present investigation pertaining to energy management in distillation that the heat pump assisted distillation configuration which use external refrigerant, can be recommended. The range of ΔT_r for which the use of heat pump is economically justified, has been determined for a given set of economic and process data. The present analysis has also considered inflation in the cost of steam and cooling water. This analysis has been extended to futuristic costs by properly accommodating the inflation in the costs of equipments and of utilities.

Following recommendations are made for further studies

(1) The non-ideal solutions like methanol-water, etc. should be analyzed to obtain the generalized behaviour.

(2) The economic analysis of other heat pump assisted distillation configurations should be carried out. These configurations are mentioned below :

   (i) Heat pump with recompression of overhead vapour.
   (ii) Heat pump with reboiler liquid flashing
   (iii) Heat pump with intermediate condensers and reboilers.

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APPENDIX-A

SOFTWARE LISTING

/* BENZENE-TOLUENE SYSTEM */

PROGRAM NO. 1

```
/* PROGRAM TO CALCULATE VAPOUR COMPOSITION, BUBBLE-POINT TEMPERATURE*/
/* AND ENTHALPY OF LIQUID MIXTURE AND ENTHALPY OF VAPOUR MIXTURE*/
/* FOR A LIQUID COMPOSITION*/
#include<stdio.h>
#include<math.h>
#include<conio.h>
void main()
{
int i;
float p1sat,p2sat,x,pt=1.0,d,t,sum=0,y,Cben,Ctol,Cmix,t0=273.16;
float hl,hg,latb,latt,T[3],X[3];
clrscr();
printf("ENTER THE COMPOSITION OF RESIDUE, FEED AND DISTILLATE:");
for(i=0;i<=2;i++)
{
scanf("%f",&X[i]);
}
printf("     X           Y            T             HL             HG\n");
for(x=0.0;x<=1.1;x=x+0.1)
{
t=350;
d=10;
aa:
p1sat=exp(15.9008-2788.51/(t-52.36))/760;
p2sat=exp(16.0137-3096.52/(t-53.67))/760;

sum=(x*p1sat+(1-x)*p2sat)/pt;
if(fabs(sum-1)>0.00001)
{
 if(sum<1) { t=t+d; goto aa; }
 if(sum>1) { t=t-d; d=d*0.1; goto aa;}
}
y=p1sat*(1-p2sat)/(p1sat-p2sat);
Cben=155.6259*(t-t0)-0.2710512*(t*t-t0*t0)/2.0+6.750819*pow(10,-
4)*(pow(t,3)-pow(t0,3))/3.0;
Ctol=147.0419*(t-t0)-0.1140537*(t*t-t0*t0)/2.0+4.896709*pow(10,-
4)*(pow(t,3)-pow(t0,3))/3.0;
Cben=Cben/(t-t0);
Ctol=Ctol/(t-t0);
Cmix=x*Cben+(1-x)*Ctol;
hl=Cmix*(t-t0);
latb=30.761*pow((562-t)/208.69,0.38);
latt=33.179*pow((593.1-t)/209.37,0.38);
hg=y*(Cben*(t-t0)+latb*pow(10,3))+(1-y)*(Ctol*(t-t0)+latt*pow(10,3));
printf("  %.2f    %f    %.3f    %.3f     %.3f\n",x,y,t,hl,hg);
}
```

```
printf("\n\n\n");
printf("\nResidue-1             Feed-2            Distillate-3\n\n");
printf("        X          Y          T               HL
HG\n");
for(i=0;i<=2;i++)
{
T[i]=350;
d=10;
bb:
p1sat=exp(15.9008-2788.51/(T[i]-52.36))/760;
p2sat=exp(16.0137-3096.52/(T[i]-53.67))/760;

sum=(X[i]*p1sat+(1-X[i])*p2sat)/pt;
if(fabs(sum-1)>0.00001)
{
 if(sum<1)  { T[i]=T[i]+d; goto bb; }
 if(sum>1)  { T[i]=T[i]-d; d=d*0.1; goto bb;}
}
y=p1sat*(1-p2sat)/(p1sat-p2sat);
Cben=155.6259*(T[i]-t0)-0.2710512*(T[i]*T[i]-
t0*t0)/2.0+6.750819*pow(10,-4)*(pow(T[i],3)-pow(t0,3))/3.0;
Ctol=147.0419*(T[i]-t0)-0.1140537*(T[i]*T[i]-
t0*t0)/2.0+4.896709*pow(10,-4)*(pow(T[i],3)-pow(t0,3))/3.0;
Cben=Cben/(T[i]-t0);
Ctol=Ctol/(T[i]-t0);
Cmix=X[i]*Cben+(1-X[i])*Ctol;
hl=Cmix*(T[i]-t0);
latb=30.761*pow((562-T[i])/208.69,0.38);
latt=33.179*pow((593.1-T[i])/209.37,0.38);
hg=y*(Cben*(T[i]-t0)+latb*pow(10,3))+(1-y)*(Ctol*(T[i]-
t0)+latt*pow(10,3));
printf("%d  %f    %f     %.3f      %.3f
%.3f\n",i+1,X[i],y,T[i],hl,hg);
}
getche();
}
```

PROGRAM NO. 2

```
/*PROGRAM TO DETERMINE THE Q-MIN LINE*/
#include<stdio.h>
#include<math.h>
#include<conio.h>
void main()
{ float t,p1sat,p2sat,x,hl,y,hg,theta1,theta2,hf;
float a11,a12,a13,a21,a22,a23,c1,c2,sum,xf,hfc,d,t1,t2;
clrscr();
printf("ENTER THE COMPOSITION OF FEED:");
scanf("%f",&xf);
printf("ENTER THE ENTHALPY OF FEED CALCULATED BY GRAPHICAL METHOD:");
scanf("%f",&hfc);
printf("ENTER THE TEMPERATURE RANGE WHERE THE Q_MIN LINE IS EXPECTED
IN KELVIN:\n");
printf("        S U G G E S T I O N\n");
printf("Q-MIN LINE LIES SOMEWHERE BETWEEN 366 K-367 K:\n");
printf("FIRST ENTER LOWER TEMPERATURE\n");
scanf("%f%f",&t1,&t2);
for(t=t2;t>=t1;t=t-0.0001)
{
p1sat=exp(15.9008-2788.51/(t-52.36))/760;
p2sat=exp(16.0137-3096.52/(t-53.67))/760;
x=(1.0-p2sat)/(p1sat-p2sat);
hl=17527.6-6920.65*x;
y=p1sat*(p2sat-1)/(p2sat-p1sat);
hg=51282.2-9423.89*y;
theta1=atan2((hg-hl),(y-x));
theta2=atan2((hl-hfc),(x-xf));
theta1=180*theta1/3.14159;
theta2=180*theta2/3.14159;
sum=0;
a11=2;a12=sum+x+y;
a21=sum+x+y; a22=sum+x*x+y*y;
a13=sum+hg+hl;  a23=sum+x*hl+y*hg;
c2=(a13*a21-a11*a23)/(a12*a21-a11*a22);
c1=(a12*a23-a22*a13)/(a12*a21-a11*a22);
hf=c2*xf+c1;
if(fabs(hf-hfc)<=0.2)
{
printf("\nISOTHERM LINE FOR QMIN PASSES THROUGH=%.3f\n",t);
printf("\nQMIN INTERSECTS HL-x LINE AT  x=%f  AND HL=%.3f\n",x,hl);
printf("\nQMIN INTERSECTS HG-y LINE AT  y=%f  AND HG=%.3f\n",y,hg);
printf("\nEQUATION OF Q-MIN LINE: H=%.3fx%.3f\n ",c2,c1);
printf("\ntheta1=%f  theta2=%f\n",theta1,theta2);
printf("\nENTHALPY OF FEED=%.3f\n",hf);
}
}
getche();
}
```

PROGRAM NO. 3

```
/*PROGRAM TO CALCULATE NO. OF STAGES IN DISTILLATION COLUMN FOR */
/*BENZENE -TOLUENE SYSTEM*/
#include<stdio.h>
#include<math.h>
#include<conio.h>
void main()
{int stage1,stage2,i,j;
float x,x_old,fx,dfx,a0,a1,a2,a3,a4,a5;
float y,a11,a12,a13,a21,a22,a23,h,Q,xd,C2,C1,c2,c1,sum,hF,hg1,hl0;
float X,xw,Qw,F,D,W,R,hW,hD,Qc,Qr,xmin;
clrscr();
printf("ENTER COMPOSITION OF RESIDUE AND DISTILLATE:");
scanf("%f%f",&xw,&xd);
printf("ENTER MOLAR FLOW RATES OF RESIDUE, FEED AND DISTILLATE:");
scanf("%f%f%f",&W,&F,&D);
printf("ENTER ENTHALPY OF RESIDUE, FEED AND DISTILLATE:");
scanf("%f%f%f",&hW,&hF,&hD);
printf("ENTER REFLUX RATIO:");
scanf("%f",&R);
printf("ENTER THE ENTHALPY OF OVERHEAD VAPOURS LEAVING TOP PLATE:");
scanf("%f",&hg1);
printf("ENTER THE ENTHALPY OF LIQUID ENTERING THE TOP PLATE AS
REFLUX:");
scanf("%f",&hl0);
printf("ENTER THE VALUE OF x AT WHICH Q-MIN LINE INTERSECTS HL-x
LINE:");
scanf("%f",&xmin);
printf("      Stage        X                  Y\n");
Q=R*(hg1-hl0)+hg1;
Qc=(Q-hD)*D/3600;

C2=-9423.89;C1=51282.2;
a0=3.41329*pow(10,-5);a1=2.33928;
a2=-2.71257;a3=2.34031;
a4=-1.29036;a5=0.323333;
y=xd;
do
{
x_old=x;
fx=a0+a1*x+a2*x*x+a3*pow(x,3)+a4*pow(x,4)+a5*pow(x,5)-y;
dfx=a1+2.0*a2*x+3.0*a3*x*x+4.0*a4*pow(x,3)+5.0*a5*pow(x,4);
x=x-fx/dfx;
}
while((fabs(x-x_old)>=0.0000001)&&(dfx!=0));
Qw=(F*hF-D*Q)/W;
Qr=(hW-Qw)*W/3600;
printf("\t%d       %f          %f\n",1,x,y);
stage1=0;
i=0;
do
{
stage1=stage1+1;
i=i+1;
h=17527.6-6920.65*x;
sum=0;
a11=2;a12=sum+xd+x;
a21=sum+xd+x; a22=sum+x*x+xd*xd;
```

```
a13=sum+Q+h; a23=sum+xd*Q+x*h;
c2=(a13*a21-a11*a23)/(a12*a21-a11*a22);
c1=(a12*a23-a22*a13)/(a12*a21-a11*a22);
y=(c1-C1)/(C2-c2);
do
{
x_old=x;
fx=a0+a1*x+a2*x*x+a3*pow(x,3)+a4*pow(x,4)+a5*pow(x,5)-y;
dfx=a1+2.0*a2*x+3.0*a3*x*x+4.0*a4*pow(x,3)+5.0*a5*pow(x,4);
x=x-fx/dfx;
}
while((fabs(x-x_old)>=0.0000001)&&(dfx!=0));
printf("\t%d        %f            %f\n",i+1,x,y);
}
while(x_old>=xmin);
x=x_old;
C2=-9423.89;C1=51282.2;
a0=3.41329*pow(10,-5);a1=2.33928;
a2=-2.71257;a3=2.34031;
a4=-1.29036;a5=0.323333;
j=i;
stage2=0;
do
{
j=j+1;
stage2=stage2+1;
h=17527.6-6920.65*x;
sum=0;
a11=2;a12=sum+xw+x;
a21=sum+xw+x; a22=sum+x*x+xw*xw;
a13=sum+Qw+h; a23=sum+xw*Qw+x*h;
c2=(a13*a21-a11*a23)/(a12*a21-a11*a22);
c1=(a12*a23-a22*a13)/(a12*a21-a11*a22);
y=(c1-C1)/(C2-c2);
do
{
x_old=x;
fx=a0+a1*x+a2*x*x+a3*pow(x,3)+a4*pow(x,4)+a5*pow(x,5)-y;
dfx=a1+2.0*a2*x+3.0*a3*x*x+4.0*a4*pow(x,3)+5.0*a5*pow(x,4);
x=x-fx/dfx;
}
while((fabs(x-x_old)>=0.0000001)&&(dfx!=0));
printf("\t%d        %f            %f\n",j+1,x,y);
}
while(x_old>=xw);
printf("NO OF STAGES EXCLUDING REBOILER STAGE=%d\n\n",stage1+stage2);
printf("CONDENSER DUTY=%.3f kW       REBOILER DUTY=%.3f kW\n",Qc,Qr);
getche();
}
```

PROGRAM NO. 4

```
/* SIMULATION OF BENZENE-TOLUENE SYSTEM */
#include<stdio.h>
#include<conio.h>
#include<math.h>
void main()
{int i,j,N,feed,k,count;
float
T[20],L[20],V[20],delV,D,W,F,VF,pt=1.0,To[20],temp,Lo[20],Vo[20];
float K1[20],K2[20],A1[20],A2[20],v1[20],v2[20];
float XD,XF,XW,d1,d2,w1,w2,lF1,lF2,tfo,tr;
float vF1,vF2,theta,ftheta,dftheta;
float d1co,d2co,x1[20],x2[20],l1[20],l2[20];
float C1[20],C2[20],D1[20],D2[20],a1[20],a2[20],b1[20],b2[20];
float AA1[20],AA2[20],B1[20],B2[20];
float alpha1[20],alpha2[20],Kb[20],KB1,KB2,Ti,Tf;
float a11,a12,a13,a21,a22,a23,a,b,sum,Tn[20];
float t0,Cp1[20],Cp2[20],Cmix[20],hl[20],y1[20],y2[20];
float lat1[20],lat2[20],ps1[20],ps2[20];
float hg1[20],hg2[20],hg[20],hl1[20],hl2[20],Rex,sum1[20];
float
XD1,XD2,hD,Qc,QL[20],XW1,XW2,hW,Qw,hF,diffT[20],diffL[20],diffV[20];
clrscr();

N=18;feed=7;
D=26.355124;F=58.163082; W=31.807959;
XF=0.440209;
lF1=F*XF;  lF2=F*(1-XF);
vF1=0;  vF2=0;     /* LIQUID FEED */
printf("Enter the External Reflux Ratio:");
scanf("%f",&Rex);
/*ASSUMPTION OF TEMPERATURE */
for(j=0;j<=N+1;j++)
{  T[j]=390;
}


/*ASSUMPTION OF TOTAL VAPOUR FLOW RATES*/
for(j=1;j<=N+1;j++)
{  V[j]=100;
}

/*CALCULATION OF TOTAL LIQUID FLOW RATES*/
for(j=0;j<=feed-2;j++)
{
L[j]=V[j+1]-D;
}
VF=0;
L[feed-1]=V[feed]+VF-D;
for(j=feed;j<=N;j++)
{L[j]=V[j+1]+W;
}


/*LOOP STARTS HERE */
 count=0;
do
{ count=count+1;
```

```
/*ASSIGNMENT*/
for(j=0;j<=N+1;j++)
{  To[j]=T[j];
}

/*ASSIGNMENT */
for(j=0;j<=N+1;j++)
{  Lo[j]=L[j];
}

/*ASSIGNMENT */
for(j=0;j<=N+1;j++)
{  Vo[j]=V[j];
}
/*CALCULATION OF K-VALUES */
for(j=0;j<=N+1;j++)
{
ps1[j]=exp(15.9008-2788.51/(T[j]-52.36))/760;
ps2[j]=exp(16.0137-3096.52/(T[j]-53.67))/760;
K1[j]=ps1[j]/pt;
K2[j]=ps2[j]/pt;
}

/*CALCULATION OF  A FOR COMPONENTS*/
AA1[0]=L[0]/D;
AA2[0]=L[0]/D;

for(j=1;j<=N;j++)
{
AA1[j]=L[j]/(K1[j]*V[j]);
AA2[j]=L[j]/(K2[j]*V[j]);
}
AA1[N+1]=W/(K1[N+1]*V[N+1]);
AA2[N+1]=W/(K2[N+1]*V[N+1]);


/*SOLUTION OF THOMAS ALGORITHM FOR DETERMINATION OF COMPONENT VAPOUR
FLOW RATES*/
for(j=1;j<=N+1;j++)
{ A1[j]=AA1[j-1];
A2[j]=AA2[j-1];
}
for(j=0;j<=N+1;j++)
{
B1[j]=-(AA1[j]+1);
B2[j]=-(AA2[j]+1);
}

for(j=0;j<=N;j++)
{ C1[j]=1;  C2[j]=1;
}
for(j=0;j<=feed-2;j++)
{ D1[j]=0; D2[j]=0;
}
D1[feed-1]=-vF1;  D2[feed-1]=-vF2;
D1[feed]=-lF1;    D2[feed]=-lF2;

for(j=feed+1;j<=N+1;j++)
{D1[j]=0; D2[j]=0;
```

```
}
a1[0]=B1[0];
a2[0]=B2[0];

b1[0]=D1[0]/B1[0];
b2[0]=D2[0]/B2[0];

for(j=1;j<=N+1;j++)
{ a1[j]=B1[j]-A1[j]*C1[j-1]/a1[j-1];
  a2[j]=B2[j]-A2[j]*C2[j-1]/a2[j-1];

b1[j]=(D1[j]-A1[j]*b1[j-1])/a1[j];
b2[j]=(D2[j]-A2[j]*b2[j-1])/a2[j];
}

v1[N+1]=b1[N+1];
v2[N+1]=b2[N+1];

for(j=N;j>=0;j--)
{
v1[j]=b1[j]-C1[j]*v1[j+1]/a1[j];
v2[j]=b2[j]-C2[j]*v2[j+1]/a2[j];
}
d1=v1[0];
d2=v2[0];

w1=AA1[N+1]*v1[N+1];
w2=AA2[N+1]*v2[N+1];

l1[0]=v1[1]-d1;
l2[0]=v2[1]-d2;

for(j=1;j<=feed-2;j++)
{
l1[j]=v1[j+1]-v1[j]+l1[j-1];
l2[j]=v2[j+1]-v2[j]+l2[j-1];
}
l1[feed-1]=v1[feed]-v1[feed-1]+l1[feed-2]+vF1;
l2[feed-1]=v2[feed]-v2[feed-1]+l2[feed-2]+vF2;

l1[feed]=v1[feed+1]-v1[feed]+l1[feed-1]+lF1;
l2[feed]=v2[feed+1]-v2[feed]+l2[feed-1]+lF2;

for(j=feed+1;j<=N;j++)
{
l1[j]=v1[j+1]-v1[j]+l1[j-1];
l2[j]=v2[j+1]-v2[j]+l2[j-1];
}

l1[N+1]=w1;
l2[N+1]=w2;
/*DETERMINATION OF THETA*/
theta=0;
do
{
ftheta=(F*XF)/(1+theta*w1/d1)+F*(1-XF)/(1+theta*w2/d2)-D;
dftheta=(w1*F*XF/d1)/pow(1+theta*w1/d1,2)+
      (w2*F*(1-XF)/d2)/pow(1+theta*w2/d2,2);
dftheta=-dftheta;
```

```
theta=theta-ftheta/dftheta;
}
while((ftheta>=0.000001)&&(dftheta!=0));

d1co=F*XF/(1+theta*w1/d1);
d2co=F*(1-XF)/(1+theta*w2/d2);

for(j=0;j<=N+1;j++)
{
x1[j]=(l1[j]*d1co/d1)/(l1[j]*d1co/d1+l2[j]*d2co/d2);
x2[j]=(l2[j]*d2co/d2)/(l1[j]*d1co/d1+l2[j]*d2co/d2);
}

/*BASE COMPONENT FOR CALCULATION OF RELATIVE VOLATILITY IS N-HEPTANE*/
for(j=0;j<=N+1;j++)
{
alpha1[j]=exp(15.9008-2788.51/(T[j]-52.36))/
       exp(15.8737-2911.32/(T[j]-56.51));
alpha2[j]=exp(16.0137-3096.52/(T[j]-53.67))/
       exp(15.8737-2911.32/(T[j]-56.51));
}
for(j=0;j<=N+1;j++)
{
Kb[j]=1/(alpha1[j]*x1[j]+alpha2[j]*x2[j]);
}
sum=0;
Ti=270;
Tf=400;
KB1=exp(15.8737-2911.32/(Ti-56.51))/(760*pt);
KB2=exp(15.8737-2911.32/(Tf-56.51))/(760*pt);

a11=2;a12=sum+1/Tf+1/Ti;
a21=sum+1/Tf+1/Ti;a22=sum+pow(1/Tf,2)+pow(1/Ti,2);
a13= sum+log(KB1)+log(KB2); a23=sum+log(KB1)*(1/Ti)+log(KB2)*(1/Tf);
a=(a13*a21-a11*a23)/(a12*a21-a11*a22);
b=(a12*a23-a22*a13)/(a12*a21-a11*a22);

for(j=0;j<=N+1;j++)
{
Tn[j]=a/(log(Kb[j])-b);
}

t0=273.16;
for(j=0;j<=N+1;j++)
{
Cp1[j]=155.6259*(Tn[j]-t0)-0.2710512*(Tn[j]*Tn[j]-t0*t0)/2.0+
       6.750819*pow(10,-4)*(pow(Tn[j],3)-pow(t0,3))/3.0;
Cp2[j]=147.0419*(Tn[j]-t0)-0.1140537*(Tn[j]*Tn[j]-t0*t0)/2.0+
       4.896709*pow(10,-4)*(pow(Tn[j],3)-pow(t0,3))/3.0;
Cp1[j]=Cp1[j]/(Tn[j]-t0);
Cp2[j]=Cp2[j]/(Tn[j]-t0);

Cmix[j]=x1[j]*Cp1[j]+x2[j]*Cp2[j];
hl[j]=Cmix[j]*(Tn[j]-t0);
hl1[j]=Cp1[j]*(Tn[j]-t0);
hl2[j]=Cp2[j]*(Tn[j]-t0);
lat1[j]=30.761*pow((562-Tn[j])/208.69,0.38);
lat2[j]=33.179*pow((593.1-Tn[j])/209.37,0.38);
ps1[j]=exp(15.9008-2788.51/(Tn[j]-52.36))/760;
```

```
ps2[j]=exp(16.0137-3096.52/(Tn[j]-53.67))/760;
K1[j]=ps1[j]/pt;
K2[j]=ps2[j]/pt;
y1[j]=K1[j]*x1[j];
y2[j]=K2[j]*x2[j];
hg[j]=y1[j]*(Cp1[j]*(Tn[j]-t0)+lat1[j]*pow(10,3))+
            y2[j]*(Cp2[j]*(Tn[j]-t0)+lat2[j]*pow(10,3));
hg1[j]=y1[j]*(Cp1[j]*(Tn[j]-t0)+lat1[j]*pow(10,3));
hg2[j]=y2[j]*(Cp2[j]*(Tn[j]-t0)+lat2[j]*pow(10,3));
}
hD=(x1[0]*Cp1[0]+x2[0]*Cp2[0])*(Tn[0]-t0);
for(j=1;j<=N;j++)
{QL[j]=0;
}
L[0]=Rex*D;
Qc=L[0]*(hg1[1]*x1[0]+hg2[1]*x2[0]-hl[0])+
      D*(hg1[1]*x1[0]+hg2[1]*x2[0]-hD);

for(j=1;j<=feed-2;j++)
{
L[j]=(D*(hD-(hg1[j+1]*x1[0]+hg2[j+1]*x2[0]))+Qc+QL[j])/
      (hg1[j+1]*x1[j]+hg2[j+1]*x2[j]-hl[j]);
}
L[feed-1]=(D*(hD-(hg1[feed]*x1[0]+hg2[feed]*x2[0]))+Qc+QL[j])/
      (hg1[feed]*x1[feed-1]+hg2[feed]*x2[feed-1]-hl[feed-1]);

Tn[feed]=342.45;
tfo=303.16;
Cp1[feed]=155.6259*(Tn[feed]-tfo)-0.2710512*(Tn[feed]*Tn[feed]-
tfo*tfo)/2.0+
      6.750819*pow(10,-4)*(pow(Tn[feed],3)-pow(tfo,3))/3.0;
Cp2[feed]=147.0419*(Tn[feed]-tfo)-0.1140537*(Tn[feed]*Tn[feed]-
tfo*tfo)/2.0+
      4.896709*pow(10,-4)*(pow(Tn[feed],3)-pow(tfo,3))/3.0;
Cp1[feed]=Cp1[feed]/(Tn[feed]-tfo);
Cp2[feed]=Cp2[feed]/(Tn[feed]-tfo);
hF=(x1[feed]*Cp1[feed]+x2[feed]*Cp2[feed])*(Tn[feed]-t0);
tr=318.16;
Cp1[N+1]=155.6259*(Tn[N+1]-tr)-0.2710512*(Tn[N+1]*Tn[N+1]-tr*tr)/2.0+
      6.750819*pow(10,-4)*(pow(Tn[N+1],3)-pow(tr,3))/3.0;
Cp2[N+1]=147.0419*(Tn[N+1]-tr)-0.1140537*(Tn[N+1]*Tn[N+1]-tr*tr)/2.0+
      4.896709*pow(10,-4)*(pow(Tn[N+1],3)-pow(tr,3))/3.0;
Cp1[N+1]=Cp1[N+1]/(Tn[N+1]-tr);
Cp2[N+1]=Cp2[N+1]/(Tn[N+1]-tr);
hW=(x1[N+1]*Cp1[N+1]+x2[N+1]*Cp2[N+1])*(Tn[N+1]-t0);
Qw=W*hW+D*hD+Qc-F*hF;

for(j=feed;j<=N;j++)
{
V[j+1]=(W*(hl1[j]*x1[N+1]+hl2[j]*x2[N+1]-hW)+Qw-QL[j])/
      (hg[j+1]-(hl1[j]*y1[j+1]+hl2[j]*y2[j+1]));
}

for(j=0;j<=feed-2;j++)
{
V[j+1]=L[j]+D;
}
VF=0;
```

```
 V[feed]=L[feed-1]-VF+D;

 for(j=feed;j<=N;j++)
 {L[j]=V[j+1]+W;
 }
 /*ASSIGNMENT */
 for(j=0;j<=N+1;j++)
 {   T[j]=Tn[j];
 }
 /*DIFFERENCES OF OLD AND NEW VALUES OF T*/
 for(j=0;j<=N+1;j++)
 { diffT[j]= fabs(To[j]-Tn[j]);
 }
 temp=0;
 for(j=0;j<=N;j++)
 {
 if(diffT[j]<diffT[j+1])
 {   temp=diffT[j];
     diffT[j]= diffT[j+1];
     diffT[j+1]=temp;
      }
 }

  temp=0;
  for(j=0;j<=N+1;j++)
 { diffL[j]= fabs(Lo[j]-L[j]);
 }
 for(j=0;j<=N;j++)
 {
 if(diffL[j]<diffL[j+1])
 {   temp=diffL[j];
     diffL[j]= diffL[j+1];
     diffL[j+1]=temp;
      }
 }

 temp=0;
  for(j=0;j<=N+1;j++)
 { diffV[j]= fabs(Vo[j]-V[j]);
 }
 for(j=0;j<=N;j++)
 {
 if(diffV[j]<diffV[j+1])
 {   temp=diffV[j];
     diffV[j]= diffV[j+1];
     diffV[j+1]=temp;
      }
 }
 }
while((diffT[0]>=0.000001)&&(diffL[0]>=0.000001)&&(diffV[0]>=0.000001)
);
/*OUTPUT STATEMENTS*/
printf("\n\n\n");
printf("      Temp             Stage            V          Stage
L\n");
for(j=1;j<=N+1;j++)
{
printf("\t%.5f    %d    %f    %d    %f\n" ,Tn[j-1],j,V[j],j-1,L[j-1]);
}
```

```
getche();
clrscr();

printf("      Stage                 K1              K2\n");
for(j=1;j<=N+1;j++)
{
printf("\t%d          %f          %f\n"   ,j,K1[j],K2[j]);
}
printf("\n\n\n");
printf("      Stage            AA1              AA2\n");
for(j=0;j<=N+1;j++)
{
printf("\t%d          %f            %f\n ",j,AA1[j],AA2[j]);
}
getche();
clrscr();
printf("      Stage            A1               A2 \n");

for(j=1;j<=N+1;j++)
{
printf("\t%d          %f            %f\n",j,A1[j],A2[j]);
}
printf("\n\n\n");
printf("      Stage            B1               B2\n");

for(j=0;j<=N+1;j++)
{
printf("\t%d          %f            %f\n",j,B1[j],B2[j]);
}
getche();
clrscr();
printf("                         d1              d2\n");
printf("\t        %f            %f\n",d1,d2);
printf("      Stage              v1              v2\n");
for(j=1;j<=N+1;j++)
{
printf("\t%d          %f           %f\n",j,v1[j],v2[j]);
}
printf("                         w1              w2\n");
printf("\t        %f            %f\n",w1,w2);
getche();
clrscr();
printf("      Stage              l1              l2\n");
for(j=0;j<=N;j++)
{
printf("\t%d          %f           %f\n",j,l1[j],l2[j]);
}
printf("\n\n\n");
printf("      Stage            x1               x2\n");
for(j=0;j<=N+1;j++)
{
printf("\t%d          %f           %f        \n",j,x1[j],x2[j]);
}
getche();
clrscr();
printf("\n\n\n");
printf("      Stage            y1               y2\n");
for(j=0;j<=N+1;j++)
{
```

```
printf("\t%d          %f             %f       \n",j,y1[j],y2[j]);
}
getche();
clrscr();
printf("    Stage             Kb\n");
for(j=0;j<=N+1;j++)
{
printf("\t%d          %f\n",j,Kb[j]);
}
printf("\na=%f          b=%f",a,b);
printf("\n\n\n");
printf("    Stage             Tn\n");
for(j=0;j<=N+1;j++)
{
printf("\t%d          %f\n",j,Tn[j]);
}
getche();
clrscr();
printf("CONDENSER AND REBOILER DUTY IN kJ/hr\n");
printf("%f          %f\n\n",Qc,Qw);
printf("CONDENSER AND REBOILER DUTY IN kJ/sec\n");
printf("%f          %f\n\n",Qc/3600,Qw/3600);
printf("         PRESS ANY KEY TO RETURN TO PROGRAM");
getche();
}
```

```
Enter the External Reflux Ratio:


      Temp          Stage        V         Stage          L
      356.63403       1      68.523323      0         42.168198
      357.56158       2      74.757004      1         48.401878
      358.84216       3      85.116951      2         58.761826
      360.48489       4     101.898895      3         75.543770
      362.46420       5     127.602646      4        101.247520
      364.70605       6     162.356110      5        136.000992
      367.12512       7     206.226898      6        179.871780
      342.45001       8      70.094788      7        101.902748
      370.12015       9      69.822998      8        101.630959
      371.08728      10      69.357880      9        101.165840
      373.00723      11      69.131836     10        100.939796
      375.52094      12      69.192558     11        101.000519
      378.08438      13      69.437263     12        101.245224
      380.27206      14      69.726700     13        101.534660
      381.91595      15      69.975479     14        101.783440
      383.04718      16      70.157509     15        101.965469
      383.78165      17      70.278831     16        102.086792
      384.24142      18      70.355408     17        102.163368
      384.52310      19      70.402084     18        102.210045


     Stage          K1               K2
      1          1.139813         0.445226
      2          1.184168         0.464676
      3          1.243024         0.490619
      4          1.316940         0.523406
      5          1.404739         0.562637
      6          1.504504         0.607569
```

7	1.611901	0.656335
8	1.635524	0.667115
9	1.679660	0.687304
10	1.769996	0.728821
11	1.893871	0.786161
12	2.026950	0.848257
13	2.146088	0.904262
14	2.239081	0.948234
15	2.304839	0.979458
16	2.348315	1.000161
17	2.375848	1.013295
18	2.392836	1.021409
19	2.403181	1.026352

Stage	AA1	AA2
0	1.600000	1.600000
1	0.571617	1.455782
2	0.572072	1.453241
3	0.555140	1.408498
4	0.543518	1.378712
5	0.540031	1.369993
6	0.539602	1.369073
7	1.859314	5.040493
8	1.118932	2.820171
9	1.023362	2.552184
10	0.907676	2.232211
11	0.797553	1.932242
12	0.713207	1.705908
13	0.658081	1.559908
14	0.625589	1.474708
15	0.607634	1.427932
16	0.598071	1.403113
17	0.593062	1.390140
18	0.590445	1.383365
19	0.171560	0.401852

Stage	A1	A2
1	1.600000	1.600000
2	0.571617	1.455782
3	0.572072	1.453241
4	0.555140	1.408498
5	0.543518	1.378712
6	0.540031	1.369993
7	0.539602	1.369073
8	1.859314	5.040493
9	1.118932	2.820171
10	1.023362	2.552184
11	0.907676	2.232211
12	0.797553	1.932242
13	0.713207	1.705908
14	0.658081	1.559908
15	0.625589	1.474708
16	0.607634	1.427932
17	0.598071	1.403113
18	0.593062	1.390140
19	0.590445	1.383365

Stage	B1	B2
0	-2.600000	-2.600000
1	-1.571617	-2.455782
2	-1.572072	-2.453241
3	-1.555140	-2.408498
4	-1.543518	-2.378712
5	-1.540031	-2.369993
6	-1.539602	-2.369073
7	-2.859314	-6.040493
8	-2.118932	-3.820171
9	-2.023362	-3.552184
10	-1.907676	-3.232211
11	-1.797553	-2.932242
12	-1.713207	-2.705908
13	-1.658081	-2.559908
14	-1.625589	-2.474708
15	-1.607634	-2.427932
16	-1.598071	-2.403113
17	-1.593062	-2.390140
18	-1.590445	-2.383365
19	-1.171560	-1.401852

d1	d2
25.222685	0.294551

Stage	v1	v2
1	65.578979	0.765832
2	62.708740	1.409434
3	61.096596	2.342799
4	59.139870	3.594378
5	57.366264	5.250164
6	56.202248	7.487237
7	55.549519	10.545123
8	102.902779	20.888008
9	114.760002	26.643131
10	117.059746	35.733562
11	105.871078	47.500221
12	84.056519	59.517311
13	59.568413	69.266464
14	38.819614	75.784729
15	23.903898	79.495705
16	14.143575	81.249817
17	8.077619	81.738075
18	4.409291	81.362770
19	2.222203	80.289825

w1	w2
0.381241	32.264614

Stage	l1	l2
0	40.356293	0.471281
1	37.486053	1.114884
2	35.873909	2.048248
3	33.917183	3.299828
4	32.143578	4.955613
5	30.979561	7.192687
6	30.326832	10.250572

7	103.284004	53.152626
8	115.141228	58.907749
9	117.440971	67.998184
10	106.252304	79.764847
11	84.437744	91.781937
12	59.949638	101.531090
13	39.200840	108.049355
14	24.285124	111.760330
15	14.524800	113.514442
16	8.458844	114.002701
17	4.790517	113.627396
18	2.603429	112.554451

Stage	x1	x2
0	0.966684	0.033316
1	0.919309	0.080691
2	0.855796	0.144204
3	0.776924	0.223076
4	0.687287	0.312713
5	0.593400	0.406600
6	0.500619	0.499381
7	0.397017	0.602983
8	0.398424	0.601576
9	0.369172	0.630828
10	0.310991	0.689009
11	0.237647	0.762353
12	0.166716	0.833284
13	0.109475	0.890525
14	0.068580	0.931420
15	0.041555	0.958445
16	0.024525	0.975475
17	0.014084	0.985916
18	0.007777	0.992223
19	0.003988	0.996012

Stage	y1	y2
0	1.071574	0.014378
1	1.047841	0.035926
2	1.013406	0.067008
3	0.965735	0.109445
4	0.905116	0.163676
5	0.833572	0.228768
6	0.753183	0.303408
7	0.639953	0.395759
8	0.651632	0.401320
9	0.620084	0.433570
10	0.550453	0.502164
11	0.450072	0.599332
12	0.337925	0.706839
13	0.234943	0.805268
14	0.153555	0.883204
15	0.095777	0.938757
16	0.057592	0.975632
17	0.033462	0.999024
18	0.018608	1.013466
19	0.009583	1.022259

```
      Stage            Kb
        0           0.583473
        1           0.601956
        2           0.628275
        3           0.663434
        4           0.707954
        5           0.761350
        6           0.822674
        7           0.889431
        8           0.904215
        9           0.931931
        10          0.989037
        11          1.068143
        12          1.154118
        13          1.231925
        14          1.293187
        15          1.336782
        16          1.365727
        17          1.384107
        18          1.395468
        19          1.402393

 a=-4287.670898           b=11.483850


      Stage            Tn
        0           356.634033
        1           357.561584
        2           358.842163
        3           360.484894
        4           362.464203
        5           364.706055
        6           367.125122
        7           342.450012
        8           370.120148
        9           371.087280
        10          373.007233
        11          375.520935
        12          378.084381
        13          380.272064
        14          381.915955
        15          383.047180
        16          383.781647
        17          384.241425
        18          384.523102
        19          384.693878

 CONDENSER AND REBOILER DUTY IN kJ/hr
 2137666.750000          2422636.750000


 CONDENSER AND REBOILER DUTY IN kJ/sec
 593.796                 672.954

            PRESS ANY KEY TO RETURN TO PROGRAM
```

APPENDIX-B

VAPOUR PRESSURE OF VARIOUS SUBSTANCES

Antoine Equation:

$$\ln(p^*)=A-B/(C+T)$$

Table B.1 Coefficients of antoine equation

Name	Formula Wt. (kg/kmole)	Normal Boiling Point (K)	Range(K)	A	B	C
Benzene	78.11	353.26	280-377	15.9008	2788.51	-52.36
Toluene	92.13	383.78	280-410	16.0137	3096.52	-53.67
n-heptane	100.2	371.59	270-400	15.8737	2911.32	-56.51

HEAT CAPACITIES OF SUBSTANCES IN LIQUID STATE

Heat Capacity equation :

$$C_L=A+BT+CT^2$$

Table B.2 Coefficients of heat capacities equation in liquid state

Name	Range	A	B	$C \times 10^4$
Benzene	278.7-383.31	155.6259	-0.2710512	6.750819
Toluene	178-413.73	147.0419	-0.1140537	4.896709

HEAT CAPACITIES OF GASES IN IDEAL-GAS STATE

Heat Capacity Equation:

$$C_p/R=A+BT+CT^2$$

Table B.3 Coefficients of heat capacity equation of gases in ideal-gas state

Name	Tmax (K)	A	$B \times 10^3$	$C \times 10^6$
Benzene	1500	-0.206	39.064	-13.301
Toluene	1500	0.290	47.052	-15.716
Iso-butane	1500	1.677	37.853	-11.945

ENTHALPY OF VAPORISATION

Enthalpy of Vaporisation equation:

$$HVAP = HVAP1 \times \left[\frac{T_c - T}{T_c - T_1}\right]^{0.38}$$

Table B.4 Coefficients of equation for enthalpy of vaporisation

Name	HVAP1	T1	Tc
Benzene	30.761	353.31	562
Toluene	33.179	383.73	593.1

THERMODYNAMIC PROPERTIES OF BENZENE, TOLUENE AND ISOBUTANE

Table B.5.1 Thermodynamic properties of saturated benzene

T (K)	P (bar)	v_l X 10^{-3} m^3/kg	v_g, m^3/kg	h_l kJ/kg	h_g kJ/kg
330	0.4665	1.192	0.7379	442.1	852.4
340	0.6615	1.207	0.5332	460.8	863.6
350	0.9162	1.224	0.3938	479.6	875.0
360	1.2419	1.241	0.2965	498.7	886.7
370	1.6517	1.259	0.2233	518.1	898.6
380	2.1588	1.277	0.1767	537.7	910.6
390	2.7774	1.297	0.1393	557.6	922.9
400	3.5228	1.318	0.1112	577.9	935.2
410	4.4091	1.340	0.08972	598.6	947.8
420	5.454	1.363	0.07309	619.7	960.4

Table B.5.2 Thermodynamic properties of saturated toluene

T (K)	P (bar)	v_l X 10^{-3} m^3/kg	v_g, m^3/kg	h_l kJ/kg	h_g kJ/kg
330	0.1633	1.201	1.80	419.6	812.9
340	0.2416	1.215	1.25	437.4	825.2
350	0.3480	1.230	0.891	456.0	837.8
360	0.4894	1.245	0.698	475.1	850.7
370	0.6736	1.261	0.481	494.6	863.8
380	0.9090	1.277	0.364	514.4	877.2
390	1.2049	1.294	0.279	534.7	890.9
400	1.5713	1.312	0.218	555.4	904.8
410	2.0651	1.331	0.178	576.8	919.0
420	2.5589	1.350	0.137	598.1	933.1

Table B.5.3 Thermodynamic properties of saturated isobutane

T (K)	P (bar)	$v_l \times 10^3$ m^3/kg	v_g, m^3/kg	h_l kJ/kg	h_g kJ/kg
300	3.7365	1.824	0.104	381.1	708.4
310	4.934	1.868	0.0794	406.4	721.7
320	6.392	1.916	0.0614	432.4	734.8
330	8.140	1.971	0.0481	459.2	747.7
340	10.21	2.032	0.0380	486.9	760.0
350	12.64	2.103	0.0301	515.7	771.8
360	15.46	2.187	0.0240	545.6	782.7
370	18.72	2.289	0.0190	577.1	792.3
380	22.48	2.420	0.0150	610.6	799.8
390	26.82	2.604	0.0115	647.1	803.1
400	31.86	2.920	0.0083	689.6	799.6
408.1(T_c)	36.55	4.464	0.0045	752.5	752.5

CRITICAL PROPERTIES OF PURE SPECIES

Table B.6 Critical properties of pure species

Name	ω	Tc (K)	Pc (bar)	Zc	Vc cm^3/mol
Benzene	0.21	562.2	48.98	0.271	259
Toluene	0.262	591.8	41.06	0.264	316
Isobutane	0.181	408.1	36.48	0.282	262.7

LEE AND KESLER GENERALISED CORRELATIONS

Table B.7.1 Values of $(H^R)^0/RT_c$

Tr/Pr	0.01	0.05	0.1	0.2	0.4	0.6	0.8	1.0
0.30	-6.045	-6.043	-6.040	-6.034	-6.022	-6.011	-5.999	-5.987
0.35	-5.906	-5.904	-5.901	-5.895	-5.882	-5.870	-5.858	-5.845
0.40	-5.763	-5.761	-5.757	-5.751	-5.738	-5.726	-5.713	-5.700
0.45	-5.615	-5.612	-5.609	-5.603	-5.590	-5.577	-5.564	-5.551
0.50	-5.465	-5.463	-5.459	-5.453	-5.440	-5.427	-5.414	-5.401
0.55	-0.032	-5.312	-5.309	-5.303	-5.290	-5.278	-5.265	-5.252
0.60	-0.027	-5.162	-5.159	-5.153	-5.141	-5.129	-5.116	-5.104
0.65	-0.023	-0.118	-5.008	-5.002	-4.991	-4.980	-4.968	-4.956
0.70	-0.020	-0.101	-0.216	-4.848	-4.838	-4.828	-4.818	-4.808
0.75	-0.017	-0.088	-0.183	-4.687	-4.679	-4.672	-4.664	-4.655
0.80	-0.015	-0.078	-0.160	-0.345	-4.507	-4.504	-4.499	-4.494
0.85	-0.014	-0.069	-0.141	-0.300	-4.309	-4.313	-4.316	-4.316
0.90	-0.012	-0.062	-0.126	-0.264	-0.596	-4.074	-4.094	-4.108
0.93	-0.011	-0.058	-0.118	-0.246	-0.545	-0.960	-3.920	-3.953
0.95	-0.011	-0.056	-0.113	-0.235	-0.516	-0.885	-3.763	-3.825
0.97	-0.011	-0.054	-0.109	-0.225	-0.490	-0.824	-1.356	-3.658
0.98	-0.010	-0.053	-0.107	-0.221	-0.478	-0.797	-1.273	-3.544
0.99	-0.010	-0.052	-0.105	-0.216	-0.466	-0.773	-1.206	-3.376
1.00	-0.010	-0.051	-0.103	-0.212	-0.455	-0.750	-1.151	-2.584

Table B.7.2 Values of $(H^R)^1/RT_c$

Tr/Pr	0.01	0.05	0.1	0.2	0.4	0.6	0.8	1.0
0.30	-11.098	-11.096	-11.095	-11.091	-11.083	-11.076	-11.069	-11.062
0.35	-10.656	-10.655	-10.654	-10.653	-10.650	-10.646	-10.643	-10.640
0.40	-10.121	-10.121	-10.121	-10.120	-10.121	-10.121	-10.121	-10.121
0.45	-9.515	-9.515	-9.516	-9.517	-9.519	-9.521	-9.523	-9.525
0.50	-8.868	-8.869	-8.870	-8.872	-8.876	-8.880	-8.884	-8.888
0.55	-0.080	-8.211	-8.212	-8.215	-8.221	-8.226	-8.232	-8.238
0.60	-0.059	-7.568	-7.570	-7.573	-7.579	-7.585	-7.591	-7.596
0.65	-0.045	-0.247	-6.949	-6.952	-6.959	-6.966	-6.973	-6.980
0.70	-0.034	-0.185	-0.415	-6.360	-6.367	-6.373	-6.381	-6.388
0.75	-0.027	-0.142	-0.306	-5.796	-5.802	-5.809	-5.816	-5.824
0.80	-0.021	-0.110	-0.234	-0.542	-5.266	-5.271	-5.278	-5.285
0.85	-0.017	-0.087	-0.182	-0.401	-4.753	-4.754	-4.758	-4.763
0.90	-0.014	-0.070	-0.144	-0.308	-0.751	-4.254	-4.248	-4.249
0.93	-0.012	-0.061	-0.126	-0.265	-0.612	-1.236	-3.942	-3.934
0.95	-0.011	-0.056	-0.115	-0.241	-0.542	-0.994	-3.737	-3.712
0.97	-0.010	-0.052	-0.105	-0.219	-0.483	-0.837	-1.616	-3.470
0.98	-0.010	-0.050	-0.101	-0.209	-0.457	-0.776	-1.324	-3.332
0.99	-0.009	-0.048	-0.097	-0.200	-0.433	-0.722	-1.154	-3.164
1.00	-0.009	-0.046	-0.093	-0.191	-0.410	-0.675	-1.634	-2.471

Table B.7.3 Values of $(S^R)^0/R$

Tr/Pr	0.01	0.05	0.1	0.2	0.4	0.6	0.8	1.0
0.30	-11.614	-10.008	-9.319	-8.635	-7.961	-7.574	-7.304	-7.099
0.35	-11.185	-9.579	-8.890	-8.205	-7.529	-7.140	-6.869	-6.663
0.40	-10.802	-9.196	-8.506	-7.821	-7.144	-6.755	-6.483	-6.275
0.45	-10.453	-8.847	-8.157	-7.472	-6.794	-6.404	-6.132	-5.924
0.50	-10.137	-8.531	-7.841	-7.156	-6.479	-6.089	-5.816	-5.608
0.55	-0.038	-8.245	-7.555	-6.870	-6.193	-5.803	-5.531	-5.324
0.60	-0.029	-7.983	-7.294	-6.610	-5.933	-5.544	-5.273	-5.066
0.65	-0.023	-0.122	-7.052	-6.368	-5.694	-5.306	-5.036	-4.830
0.70	-0.018	-0.096	-0.206	-6.140	-5.467	-5.082	-4.814	-4.610
0.75	-0.015	-0.078	-0.164	-5.917	-5.248	-4.866	-4.600	-4.399
0.80	-0.013	-0.064	-0.134	-0.294	-5.026	-4.694	-4.388	-4.191
0.85	-0.11	-0.054	-0.111	-0.239	-4.785	-4.418	-4.166	-3.976
0.90	-0.09	-0.046	-0.094	-0.199	-0.463	-4.145	-3.912	-3.738
0.93	-0.08	-0.042	-0.085	-0.179	-0.408	-0.750	-3.723	-3.569
0.95	-0.08	-0.039	-0.080	-0.168	-0.377	-0.671	-3.556	-3.433
0.97	-0.007	-0.037	-0.075	-0.157	-0.350	-0.607	-1.056	-3.259
0.98	-0.007	-0.036	-0.073	-0.153	-0.337	-0.580	-0.971	-3.142
0.99	-0.007	-0.035	-0.071	-0.148	-0.326	-0.555	-0.903	-2.972
1.00	-0.007	-0.034	-0.069	-0.144	-0.315	-0.532	-0.847	-2.178

Table B.7.4 Values of $(S^R)^1/R$

Tr/Pr	0.01	0.05	0.1	0.2	0.4	0.6	0.8	1.0
0.30	-16.782	-16.774	-16.764	-16.744	-16.705	-16.665	-16.626	-16.586
0.35	-15.413	-15.408	-15.401	-15.387	-15.359	-15.333	-15.305	-15.278
0.40	-13.990	-13.986	-13.981	-13.972	-13.953	-13.934	-13.915	-13.896
0.45	-12.564	-12.561	-12.558	-12.551	-12.537	-12.523	-12.509	-12.496
0.50	-11.202	-11.200	-11.197	-11.092	-11.082	-11.172	-11.162	-11.153
0.55	-0.115	-9.948	-9.946	-9.942	-9.935	-9.928	-9.921	-9.914
0.60	-0.078	-8.828	-8.826	-8.823	-8.817	-8.811	-8.806	-8.799
0.65	-0.055	-0.309	-7.832	-7.829	-7.824	-7.819	-7.815	-7.510
0.70	-0.040	-0.216	-0.491	-6.951	-6.945	-6.941	-6.937	-6.933
0.75	-0.029	-0.156	-0.340	-6.173	-6.167	-6.162	-6.158	-6.155
0.80	-0.022	-0.116	-0.246	-0.578	-5.475	-5.468	-5.462	-5.458
0.85	-0.017	-0.088	-0.183	-0.400	-4.853	-4.841	-4.832	-4.826
0.90	-0.013	-0.068	-0.140	-0.301	-0.744	-4.269	-4.249	-4.238
0.93	-0.011	-0.058	-0.120	-0.254	-0.593	-1.219	-3.914	-3.894
0.95	-0.010	-0.053	-0.109	-0.228	-0.517	-0.961	-3.697	-3.658
0.97	-0.010	-0.048	-0.099	-0.206	-0.456	-0.797	-1.570	-3.406
0.98	-0.009	-0.046	-0.094	-0.196	-0.429	-0.734	-1.270	-3.264
0.99	-0.009	-0.044	-0.090	-0.186	-0.405	-0.680	-1.098	-3.093
1.00	-0.008	-0.042	-0.086	-0.177	-0.382	-0.632	-0.977	-2.399

APPENDIX-C

CALCULATIONS

Problem Under Study

A benzene toluene solution containing 40 wt% benzene at 30°C is to be continuously rectified at 1 std atmosphere pressure at a rate of 5000 kg/hr to provide a distillate containing 95% benzene and a residue containing 1% benzene (by weight). The feed is to be preheated by heat exchange with the residue, which (i.e., residue) will leave the system at 45°C. The distillate is to be totally condensed to a liquid and the reflux returned at the bubble point.

Solution by Ponchon Savarit Method

Molecular weight

Benzene : 78.113 kg/kmole

Toluene : 92.14 kg/kmole

$$F = \frac{5000\ (0.4)}{78.113} + \frac{5000\ (0.6)}{92.14}$$

$$= 25.603933 + 32.559149$$

$$= 58.163082 \text{ kmol/hr}$$

$$x_F = \frac{25.603933}{58.163082} = 0.440209$$

$$M_{av} \text{ for feed} = \frac{5000}{58.163082} = 85.965179 \text{ kg/kmole}$$

$$x_D = \frac{95/78.113}{\dfrac{95}{78.113} + \dfrac{5}{92.14}} = 0.957287$$

$$M_{av} \text{ for distillate} = \frac{100}{\dfrac{95}{78.113} + \dfrac{5}{92.14}} = 78.712143 \text{ kg/kmole}$$

$$X_w = \frac{\dfrac{1}{78.113}}{\dfrac{1}{78.113} + \dfrac{99}{92.14}}$$

$$M_{av} \text{ for residue} = \frac{100}{\frac{1}{78.113} + \frac{99}{92.14}} = 91.974838 \text{ kg/kmole}$$

$$D + W = 58.163082$$

$$D(0.957287) + W(0.011775) = 58.163082(0.440209)$$

Solving both equations simultaneously, we get

$$W = 31.807959 \text{ kmol/hr}$$

$$= 31.807959 \times (91.974838) = 2925.531876 \text{ kg/hr}$$

$$D = 26.355124 \text{ kmol/hr}$$

$$= 26.355124 \times (78.712143) = 2074.468289 \text{ kg/hr}$$

The bubble points at different compositions of the benzene-toluene mixture calculated by Program No. 1, are tabulated below. The corresponding value of y (i.e., mole fraction of benzene vapour in benzene toluene mixture) at that temperature is also given.

Table C.1: Bubble points of benzene-toluene mixture at different compositions

x	y	Bubble point (K)
0.0	0	383.77615
0.1	0.209161	379.28714
0.2	0.376082	375.25345
0.3	0.511123	371.60809
0.4	0.621830	368.29312
0.5	0.713620	365.26309
0.6	0.790513	362.48010
0.7	0.855544	359.91208
0.8	0.911022	357.53207
0.9	0.958711	355.31808
1.0	1.0	353.25208
0.011775 (Residue)	0.027263	383.22104
0.440209 (feed)	0.660752	367.04306
0.957287 (Distillate)	0.983065	354.11725

The dew points for different compositions of vapour of benzene-toluene mixture calculated by Program No. 1 are tabulated below

Table C.2: Dew points of benzene-toluene mixture at different compositions

y	Dew Point (K)
0.0	383.77615
0.1	381.69818
0.2	379.49615
0.3	377.14920
0.4	374.63538
0.5	371.9240
0.6	368.97415
0.7	365.73209
0.8	362.11908
0.9	358.02103
1.0	353.25208
0.011775 (residue)	383.53711
0.44-0209 (feed)	373.57111
0.957287 (distillate)	355.38742

The equation for the calculation of the heat capacity of liquid mixture, C_L in kJ/kmole, is given by

$$C_L = A + BT + CT^2$$

The values of constants A, B and C for both the components (benzene and toluene) is given in Table B.2. Enthalpies of liquid and enthalpies of vapour at different compositions of the mixture calculated by Program No. 1 are tabulated below

Table C.3 : Enthalpies of liquid and vapour for benzene-toluene mixture at different compositions

x	H_L (kJ/kmole)	H_G (kJ/kmole)
0.0	18020.412	51196.633
0.1	16994.512	49297.742
0.2	16072.198	47770.707
0.3	15237.559	46522.566
0.4	14477.225	45486.473
0.5	13780.691	44614.933
0.6	13139.300	43872.988
0.7	12545.826	43234.391
0.8	11994.252	42679.250
0.9	11479.643	42192.445
1.0	10997.930	41762.176
0.011775 (Residue)	17893.563	50948.711
0.440209 (feed)	14190.050	45118.434
0.957287 (Distillate)	11199.863	41939.578

With the use of software POLYMATH, we obtain the equation H_L vs x and H_G vs y as mentioned below

$H_L = 17527.6 - 6920.69x$

$H_G = 51282.2 - 9423.89y$

At x = 0.011775

$H_L = H_W = 17527.6 - 6920.69 \times 0.011775$

$= 17446.10935$ kJ/kmole

At y = 0.957287

$H_{G1} = H_G = 51282.2 - 9423.89 \times (0.957287)$

$= 42260.83261$ kJ/kmole

$H_D = H_{LD} = H_L = 17527.6 - 6920.65\ (0.957287)$

$= 10902.55172$ kJ/kmole

According to the problem given, the feed is preheated by heat exchange with the residue. The temperature of feed (on the feed plate) can be obtained by the enthalpy balance for feed and the residue, between which heat transfer takes place. By hit and trial, the temperature of feed (on the feed plate) can be obtained.

Heat capacities of different components of the feed and feed itself at their bubble point, are given as

$C_{ben\,F} = 138.561661$ kJ/kmole K

$C_{tol\,F} = 161.313004$ kJ/kmole K

$C_{Feed} = 0.440209 \times 138.561661 + (1 - 0.440209) \times 161.313004$

$= 151.297653$ kJ/kmole K

Now, by enthalpy balance

$58.163082 \times (151.297653)\,(T_F - 303.16)$

$= 31.807959 \times (167.160736) \times (383.22104 - 318.16)$

$T_F = 342.47076$ K

Enthalpy of preheated feed at calculated temperature by taking 0°C as reference temperature is

$H_F = 151.297653 \times (342.47076 - 273.16)$

$= 10486.555664$ kJ/kmole

The location of Q_{min} line on the x-y diagram was obtained by program no. 2. Q_{min} line is obtained at isotherm line (at 366.22K). At this isotherm line, the composition and enthalpy of liquid are respectively

$x = 0.467401$ $H_L = 14292.877930$ kJ/kmole

and the composition and enthalpy of vapour mixture are

$y = 0.685513$ $H_G = 44822.00$ kJ/kmole

The equation of Q_{min} line can be written as (as obtained by linear-regression method)

$Q_{min} = 139970.171875x - 51129.382812$

By putting $x = x_D$ and $x = x_W$ separately, in preceding equation, we obtain the enthalpy of distillate and residue

At x = 0.957287

$$Q'_{min} = Q_{min} = 139970.171875 \text{ x } 0.957287 - 51129.382812$$
$$= 82862.243112 \text{ kJ/kmole}$$

At x = 0.011775

$$Q''_{min} = Q_{min} = 139970.171875 \text{ x } 0.011775 - 51129.382812$$
$$= -49481.234038 \text{ kJ/kmole}$$

The minimum reflux ratio (R_{min}) for the benzene-toluene system can be calculated as

$$R_{ex,min} = \frac{Q'_{min} - H_{G1}}{H_{G1} - H_{Lo}}$$

$$= \frac{(82862.243112 - 42260.83261}{(42260.83261 - 10902.55172)}$$

$$= 1.295$$

The optimum reflux ratio is generally taken as 1.2 to 1.5 times of minimum reflux ratio

$$R_{ex} = 1.2 \text{ x } 1.295 = 1.554$$

Taking reflux ratio, $R_{ex} = 1.6$

$$1.6 = \frac{Q' - H_{G1}}{H_{G1} - H_{Lo}}$$

$$Q' = 92434.078125 \text{ kJ/kmole}$$

The value of Q" can be obtained by following enthalpy balance equation

$$FH_F = DQ' + WQ''$$

$$58.163082\ (10486.555664) = 26.355124\ (92434.078) + 31.807959\ Q''$$

$$Q'' = -57412.710938 \text{ kJ/kmole}$$

The condenser duty and reboiler duty are

Condenser Duty

$$Q' = H_D + \frac{Q_c}{D}$$

$$Q_c = D(Q' - H_D)$$

$$Q_c = 26.355124\ (92434.078125 - 10902.55172)$$

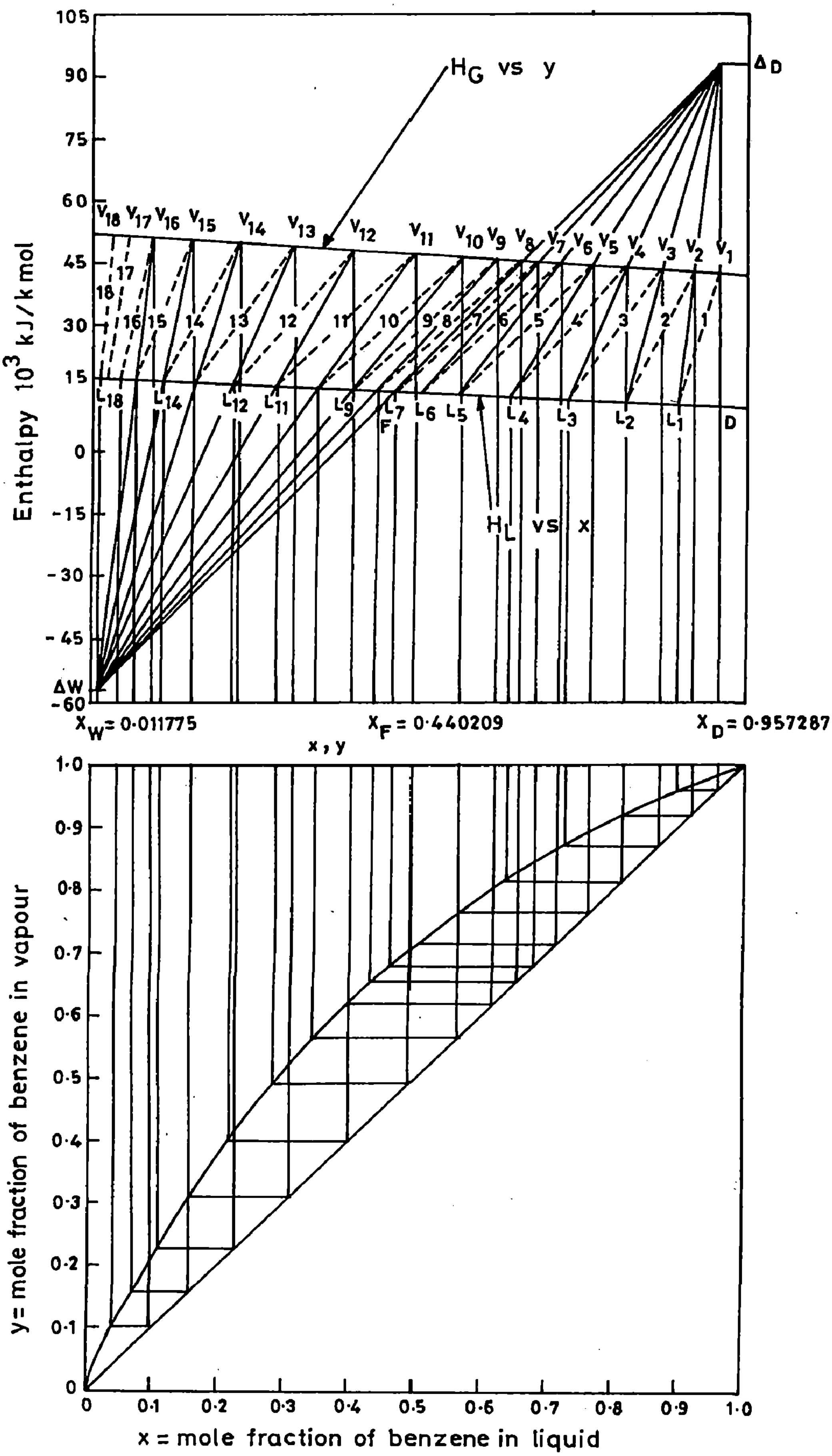

Fig. C·1 H-xy Diagram for Benzene-Toluene System

$= 2148773.5$ kJ/hr $= 596.882$ kW

≈ 597 kW

Reboiler Duty

$$Q' = H_D - \frac{Q_R}{W}$$

$$Q_R = (H_W - Q'')W$$

$= (17446.10935 + 57412.711) \times 31.807959$

$= 2381106.25$ kJ/hr

$= 661.418$ kJ/sec

≈ 661 kW

By program no. 3, we find the number of stages in the distillation column. The values of x and y on each stage is tabulated under

Table : C.4 : Values of x and y on each stage

Stage No.	x	y
1	0.897010	0.957287
2	0.818201	0.920262
3	0.728026	0.872060
4	0.639026	0.817189
5	0.562730	0.763329
6	0.504628	0.717389
7	0.464177	0.682546
8	0.437563	0.658212
9	0.398930	0.620717
10	0.347292	0.566172
11	0.285301	0.493049
12	0.219639	0.404933
13	0.158502	0.311204
14	0.107864	0.223566
15	0.069720	0.150707

16	0.042940	0.095663
17	0.025035	0.056934
18	0.013445	0.031000
19	0.006097	0.014197

$x_W = 0.011775$ $\qquad\qquad$ $y_W = 0.027263$

$W = 31.807959$

$L_{18} = V_w + W$

$$\frac{L_{18}}{V_w} = \frac{y_w - x_w}{x_{18} - x_w}$$

By solving the preceding equations

$L_{18} = V_w + 31.807959$

$$\frac{L_{18}}{V_w} = \frac{(0.027263 - 0.011775)}{(0.013445 - 0.011775)}$$

$L_{18} = 35.652168$ kmole/hr

$V_w = 3.844210$ kmole/hr

Fraction of the bottom product, sent as reflux in stripping section (β) calculated as

$$\beta = \frac{V_w}{V_w + W} = \frac{3.844210}{3.844210 + 31.807999}$$

$$= 0.107825$$

Amount of heat per kmole required by residue product for vaporisation is

$$H_w = \beta * H_{Gw} + (1-\beta) H_{Lw}$$

$$= 0.107825 \text{ x } 50981.953125 + (1 - 0.107825) \text{ x } 17893.558599$$

$$= 21461.328125 \text{ kJ/kmole}$$

Heat rate required by residue product is

$$= 21461.328125 \text{ x } (31.807959) \text{ x } \frac{1}{3600}$$

$$= 189.622513 \text{ kJ/sec}$$

Calculation of Quantity of Coolant and Steam

T_{w1} = 25 + 273.16=298.16 K T_{w2} = 40 + 273.16 = 313.16 K

T_{c1} = 355.38 K T_{c2} = 354.12 K

Properties of water at average temperature (i.e., 32.5°C)

C_{pw} = 4.1795 kJ/kg°C ρ_w = 994.9 kg/m^3

$Q_c = m_{coolant} \cdot C_{pw} (T_{w2} - T_{w1})$

$$m_{coolant} = \frac{Q_c}{C_{pw}(T_{w2} - T_{w1})} = \frac{597}{4.1795 \text{ x } 15}$$

$$= 9.52267 \text{ kg/sec}$$

Volume of cooling water = $\frac{m_{coolant}}{\rho_w}$ = 0.009571 m^3/sec

No. of operating hrs. = 8000 hrs/yr

Volume of cooling water required =.0.009571 x 3600 x 8000

= 275658.75 m^3/yr

Assuming that low pressure steam is available at 387.379, the mass of steam required for heating the bottom products can be calculated

T_{r1} = 383.537 K T_{r2} = 383.221 K T_s = 387.379 K

λ_{steam} at 387.379 K = 2218.54 kJ/kg

m_{steam} = 661/2218.54 = 0.297944 kg/sec

$$m_{steam} = \frac{0.297944 \text{ x } 3600 \text{ x } 8000}{1000} = 8580.77 \text{ tonnes/yr}$$

Heat Pump Assisted Distillation Column

In this heat pump assisted distillation column, an external refrigerant flows in a closed cycle, and does not exchange mass with the distillation column.

Isobutane is selected here as a refrigerant because of the following reasons :

(a) Isobutane has low boiling point and fairly high vapour density at atmospheric pressure

(b) For the required temperature range, its compression ratio is fairly low

(c) It does not affect metals of the equipments

(d) Regarding environmental consideration also, it is a safe refrigerant.

The temperature of evaporating refrigerant is assumed as 340 K, i.e., $T_1 = 340$ K. As evident from the plot in Chapter 6, total costs were found minimum at $\Delta T_r = 4°C$, so the temperature of condensing refrigerant at reboiler is 387.379 K (because bubble point of residue is 383.379 K)

Hence $T_1 = 340$ K $\qquad T_3 = 387.379$ K

$P_1 = 10.21$ bar $\qquad P_2 = 25.682$ bar

$\omega = 0.181$

$$T_{r1} = \frac{T_1}{T_c} = \frac{340}{408.1} = 0.833129$$

$$P_{r1} = \frac{P_1}{P_c} = 10.21/36.55 = 0.279343$$

$$\frac{dB^o}{dT_{r1}} = \frac{0.675}{T_{r1}^{2.6}} = 1.085055$$

$$\frac{dB^1}{dT_{r1}} = \frac{0.722}{T_{r1}^{5.2}} = 1.865663$$

Entropy of refrigerant at real gas state 1

$$\frac{S_1^R}{R} = -P_{r1}\left[\frac{dB^o}{dT_{r1}} + \omega\frac{dB^1}{dT_{r1}}\right]$$

$$\frac{S_1^R}{R} = -0.279343\left[1.085055 + 0.181\times(1.865663)\right]$$

$$S_1^R = -0.397433\times(8.3143)$$

$$= -3.304377 \text{ kJ/kmole K}$$

By hit and trial we get $T_2 = 393.426$

Coefficients of heat capacity equation(for ideal gas state)are given in Table B.3.

$$< C_p^{ig} >_s \ln\left(\frac{T_2}{T_1}\right) = 8.3143\left[1.677\ln\left(\frac{T_2}{T_2}\right) + 37.853\text{x}10^{-3}\right.$$

$$\left.(T_2 - T_1) - \frac{11.945\text{x}10^{-6}}{2}(T_2^2 - T_1^2)\right]$$

$$= 8.3143\left[1.677\ \ln\left(\frac{393.426}{340}\right) + 37.853\text{x}10^{-3}(393.426 - 340)\right.$$

$$\left. - \frac{11.945\text{x}10^{-6}}{2}(393.426^2\ 340^2)\right]$$

$= 16.903484$

Entropy change of refrigerant from ideal gas state 1 to ideal gas state 2

$$\Delta S^{ig} = 16.903484 - 8.3143\ \ln\left(\frac{25.682}{10.21}\right)$$

$= 9.234183$ kJ/kmole K

Reduced temperature and pressure at real gas state 2 are

$$T_{r2} = \frac{T_2}{T_c} = \frac{393.426}{408.1} = 0.964043$$

$$P_{r2} = \frac{P_2}{P_c} = \frac{25.682}{36.55} = 0.702654$$

By interpolating the values obtained from Table B.7.3 and B.7.4, we get

$$\frac{S_2^R}{R} = -1.228925 + 0.181 \times (-1.542699)$$

$$S_2^R = -12.539242 \text{ kJ/kmole K}$$

$$\Delta S = S_2^R - S_1^R + \Delta S^{ig}$$

$= -12.539242 + 3.304377 + 9.234183$

$= -0.000687$

Therefore, the compression of refrigerant is isentropic.

The degree of superheat = $T_2 - T_3$ = 393.426 – 387.329 = 6.097°C can be neglected for practical purposes.

Heat of vaporisation at condenser temperature (354.75K)

Benzene = 30.6325×10^3 kJ/Kmole

Toluene = 34.855×10^3 kJ/Kmole

Amount of heat required to be removed per kg of distillate in the condenser

$= 0.957287 \times (30.6325 \times 10^3) + 0.042713 \times (34.855 \times 10^3)$

$$= 29324.09403 \text{ x } \frac{1}{78.113} \quad 1488.761615 \times \frac{1}{92.14}$$

$$= 391.56367 \text{ kJ/kg}$$

Amount of heat per sec to be removed in condensation

$$= 391.56367 \text{ x } 2074.408289 \text{ x } \frac{1}{3600}$$

$$= 225.635116 \text{ kJ/sec}$$

Latent heat of isobutane (at 340 K) = 273.1 kJ/kg

$$225.635116 = m_{ref} \text{ x } 273.1 \text{ kJ/kg}$$

where m_{ref} is the mass flow rate of refrigerant

$$m_{ref} = 0.8262 \text{ kg/sec}$$

Compressor work

$$\Delta H^{ig} = H_2^{ig} - H_1^{ig} = \int_{T_1}^{T_2} C_p^{ig}\, dT$$

$$\Delta H^{ig} = 8.143\left[1.677(T_2 - T_1) + \frac{37.853\times10^{-3}}{2}(T_2^2 - T_1^2) - \frac{11.945\times10^{-6}}{3}(T_2^3 - T_1^3)\right]$$

$$= 8.3143\ [1.677(393.426 - 340) + \frac{37.853\times10^{-3}}{2}(393.426^2\text{-}340^2)$$

$$- \frac{11.945\times10^{-6}}{3}(393.426^3 - 340^3)]$$

$$= 6196.142579 \text{ kJ/kmole}$$

$$T_{r1} = 0.833129$$

$$B^o = 0.0873 - \frac{0.422}{T_{r1}^{1.6}} = -0.482162$$

$$\frac{dB^o}{dT_r} = \frac{0.675}{T_{r1}^{2.6}} = 1.085055$$

$$B^1 = 0.139 \frac{0.172}{T_{r1}^{4.2}} = -0.231285$$

$$\frac{dB^1}{dT_{r1}} = \frac{0.722}{T_r^{5.2}} = 1.865663$$

Enthalpy of refrigerant for state 1

$$\frac{H_1}{RT_c} = P_{r1}\left[B^o - T_{r1}\frac{dB^o}{dT_{r1}} + \omega\left(B' - T_{r1}\frac{dB'}{dT_{r1}}\right)\right]$$

$$=0.279343\ [-0.482162 - 0.833129\times 1.085055 + 0.181(-0.231285 - 0.833129\times 1.865663)]$$

$$H_1^R = -1620.174438 \text{ kJ/kmole}$$

By interpolating the values obtained from Tables B.7.1 and B.7.2, the enthalpy of refrigerant for state 2

$$\frac{H_2R}{RT_c} = -1.473874 + 0.181\times(-1.583847)$$

$$H_2^R = -5973.663086 \text{ kJ/mole}$$

Isentropic enthalpy change of refrigerant

$$(\Delta H)_s = \Delta H^{ig} + H_2^R - H_1^R$$

$$= 6196.142579 + (-5973.663086) + 1620.174438$$

$$= 1842.653931 \text{ kJ/kmole of refrigerant}$$

Molecular weight of refrigerant = 58.123 kg/kmole

$$W_s = (\Delta H)_s = 1842.653931\times\frac{1}{58.123}$$

$$= 31.70266 \text{ kJ/kg of refrigerant}$$

$$W_s = 31.70266 \text{ x } 0.8262$$

$$= 26.19274 \text{ kJ/sec}$$

Compressor efficiency are usually in the range of 0.7 to 0.8. Assuming the overall compressor efficiency of 0.75

$$W = \frac{26.19274}{0.75} = 34.923693 \approx 35 \text{ kW}$$

Heat of vaporization of Isobutane at 387.379 K = Amount of heat per sec supplied by refrigerant

$$= 0.8262 \text{ x } 164.702$$

$$= 136.076792 \text{ kJ/sec}$$

Heat rate to be supplied by auxiliary reboiler

= (189.622513 – 136.076792)

= 53.545721 kJ/sec

Amount of steam required in auxiliary reboiler

At 387.379K λ_{steam} = 2218.54 kJ/kg of steam

$53.545721 = m_{steam} \times 2218.54$

$m_{steam} = 0.024136$ kg/sec

$$m_{steam} = 0.024136 \times 3600 \times 8000 \times \frac{1}{1000}$$

= 695.10433 tonnes/yr

Cost of Utilities

Rates of

Cooling water = Rs. 1.25 /m^3

Electricity = Rs. 6/kW-hr

Steam(low pressure) = Rs. 250 / tonne

(high pressure)= Rs. 800 / tonne

Conventional Distillation Column

Cooling water requirement = 275658.75 m^3/yr

Cost of cooling water = Rs. 1.25 x 275658.75

= Rs. 3,44,573.44

Steam requirement = 8580.778 tonnes/hr

Cost of steam = Rs. 250 x 8580.778

= Rs 2145194.50

Total utility cost = Rs. 2489768.03

Heat pump with external refrigerant

Steam requirement = 695.104 tonnes/yr

Cost of steam = 695.104 x 250

= Rs. 173776.00

Cost of electricity = 35 kW x 8000 hrs/yr x Rs. 6 per kW-hr

= Rs. 16,80,000.00

Total utility cost = Rs. 18,53,776.00

Calculation of Area of Heat Exchanger

Conventional Distillation Column

$T_{w1} = 298.16\,K$ $\quad$ $T_{w2} = 313.16\,K$

$T_{c1} = 355.38\,K$ $\quad$ $T_{c2} = 354.12\,K$

$\theta_i = T_{c1} - T_{w1} = 57.22$

$\theta_o = T_{c2} - T_{w2} = 40.96$

$\because \quad \frac{\theta_i}{\theta_o} < 2$, we can use AMTD

$U = 600\ W/m^2K$

$Q = U\ A\ (AMTD)$

$$597 \times 10^3 = 600 \times (A_c) \times \left(\frac{57.22 + 40.96}{2}\right)$$

$A_c = 20.268\ m^2$

$\approx 20.3\ m^2$

Reboiler

$T_S = 387.379\ K$ $\quad$ $T_{r1} = 383.537\ K$ $\quad$ $T_{r2} = 383.221\ K$

$\theta_i = T_s - T_{r2} = 4.158$

$\theta_o = T_s - T_{r1} = 3.842$

$\because \quad \frac{\theta_i}{\theta_o} < 2$, we can use AMTD

$U = 900$

$$661 \times 10^3 = 900 \times (A_R) \left(\frac{4.158 + 3.842}{2}\right)$$

$A_R = 183.61\ m^2$

Heat Pump Assisted Distillation Configuration

Condenser

$$\theta_i = T_{c1} - T_{w1} = 355.38 - 340 = 15.38$$

$$\theta_o = T_{c2} - T_{w2} = 354.12 - 340 = 14.12$$

$$\because \quad \frac{\theta_i}{\theta_o} < 2\text{, we can use AMTD}$$

$U = 500\ \mathrm{W/m^2K}$

$$597 \times 10^3 = 500 \times (A_c) \times \left(\frac{15.38 + 14.12}{2}\right)$$

$$A_c = 80.949\ \mathrm{m}^2$$

$$\approx 81\ \mathrm{m}^2$$

Reboiler

$$\theta_i = T_s - T_{r2} = 387.379 - 383.221 = 4.158$$

$$\theta_o = T_s - T_{r1} = 387.379 - 383.537 = 3.842$$

$$\because \quad \frac{\theta_i}{\theta_o} < 2\text{, we can use AMTD}$$

$U = 500\ \mathrm{W/m^2K}$

$$136.076 \times 10^3 = 500 \times (A_R) \left(\frac{4.158 + 3.842}{2}\right)$$

$$A_R = 68.038\mathrm{m}^2$$

Auxiliary Reboiler

$$T_s = 120 + 273.16 = 393.16\ \mathrm{K}$$

$$\theta_i = 393.16 - 383.221 = 9.939$$

$$\theta_o = 393.16 - 383.537 = 9.623$$

$U = 900\ \mathrm{W/m^2K}$

$$53.545 \times 10^3 = 900 \times A_R\ (9.781)$$

$$A_R = 6.08\ \mathrm{m}^2$$

Cost of Equipments

Conventional Distillation Column

Condenser

$A_c = 20.268$

$C_{C,A} = 0.2 \times 78963.5\ A_c^{0.602}$

$= \text{Rs. } 96639.92$

Reboiler

$A_R = 183.61\ m^2$

$C_{R,A} = 0.2 \times 104420\ A_R^{0.602}$

$= \text{Rs. } 4,81,592.01$

Heat Pump Assisted Distillation Column Using External Refrigerant

Condenser

$A_c = 80.95$

$C_{C,A} = 0.2 \times 78963.5\ A_c^{0.602}$

$= \text{Rs. } 222434.90$

Reboiler

$A_R = 34.02\ m^2$

$C_{R,A} = 0.2 \times 104420\ A_R^{0.602}$

$= \text{Rs. } 174549.15$

Auxiliary Reboiler

$A_R = 6.08\ m^2$

$C_{R,A} = 0.2 \times 104420\ A_R^{0.602}$

$= \text{Rs. } 61904.70$

Compressor

$W = 35\ \text{kW}$

$$C_{comp,A} = 0.2 \times 1.4 \times 145221\ W^{0.73}$$

$$= \text{Rs. } 544950.59$$

Economic Feasibility of Heat Pump

From the table 5.2, it is evident that total annual cost for the column coupled with heat pump is less than that for conventional distillation. So, it can be concluded that heat pump assisted distillation column is economically feasible for $\Delta T_r = 4°C$.

APPENDIX-D

TOTAL ANNUAL COST FOR DISTILLATON COLUMN COUPLED WITH HEAT PUMP (IN LAKHS OF RS.)

Table D.1 : For various values of U.C.I. (F.C.I. = 1.0)

ΔT_r	U.C.I.			
	1.0	**1.5**	**2.0**	**3.0**
1	31.69	39.01	46.34	60.99
2	29.98	37.49	44.99	60.01
3	29.54	37.23	44.92	60.29
4	29.48	37.34	45.21	60.93
5	29.59	37.63	45.66	61.74
6	29.8	38	46.21	62.62
7	30.08	38.47	46.85	63.63
8	30.45	39.04	47.63	64.81
9	30.87	39.67	48.47	66.07
10	31.24	40.21	49.19	67.15
11	31.63	40.8	49.96	68.3
12	31.92	41.23	50.54	69.16
13	32.15	41.59	51.02	69.89
14	32.43	42	51.57	70.71
15	32.75	42.47	52.18	71.61
16	33.12	43	52.88	72.64

Table D.2 : For various values of U.C.I. (F.C.I. = 1.5)

ΔT_r	U.C.I.			
	1.0	**1.5**	**2.0**	**3.0**
1	40.20	47.53	54.86	69.51
2	37.46	44.97	52.48	67.49
3	36.63	44.31	52.00	67.38
4	36.36	44.22	52.09	67.81
5	36.36	44.39	52.43	68.50
6	36.49	44.70	52.90	69.32
7	36.73	45.12	53.51	70.28
8	37.09	45.68	54.27	71.45
9	37.51	46.31	55.11	72.71
10	37.88	46.85	55.83	73.79
11	38.28	47.45	56.61	74.95
12	38.57	47.88	57.19	75.81
13	38.80	48.23	57.66	76.53
14	39.08	48.65	58.22	77.35
15	39.41	49.13	58.84	78.27
16	39.80	49.68	59.56	79.32

Table D.3 : For various values of U.C.I. (F.C.I. = 2.0)

ΔT_r	U.C.I.			
	1.0	**1.5**	**2.0**	**3.0**
1	48.72	56.05	63.37	78.03
2	44.94	52.45	59.96	74.97
3	43.71	51.40	59.09	74.46
4	43.24	51.10	58.97	74.69
5	43.12	51.15	59.19	75.26
6	43.18	51.39	59.60	76.01
7	43.39	51.77	60.16	76.93
8	43.73	52.32	60.91	78.09
9	44.15	52.95	61.75	79.35
10	44.51	53.49	62.47	80.43
11	44.93	54.10	63.26	81.60
12	45.22	54.53	63.84	82.46
13	45.44	54.87	64.31	83.17
14	45.73	55.29	64.86	84.00
15	46.07	55.79	65.50	84.93
16	46.48	56.36	66.24	86.00

Table D.4 : For various values of U.C.I. (F.C.I. = 3.0)

ΔT_r	U.C.I.			
	1.0	**1.5**	**2.0**	**3.0**
1	65.75	73.08	80.41	95.06
2	59.91	67.41	74.92	89.94
3	57.88	65.57	73.25	88.63
4	57.00	64.86	72.72	88.45
5	56.64	64.68	72.71	88.78
6	56.57	64.77	72.98	89.39
7	56.69	65.08	73.47	90.24
8	57.00	65.59	74.18	91.36
9	57.43	66.23	75.03	92.62
10	57.79	66.77	75.75	93.71
11	58.23	67.40	76.56	94.90
12	58.51	67.82	77.13	95.75
13	58.73	68.16	77.59	96.46
14	59.02	68.59	78.16	97.29
15	59.39	69.10	78.82	98.25
16	59.84	69.72	79.60	99.36