Thermal Coupling in Non-ideal Multicomponent Distillation

A Thesis Submitted to the College of Engineering of Nahrain University in Partial Fulfillment of the Requirements for the Degree of Master of Science in Chemical Engineering

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ABSTRACT

This study deals with minimizing energy requirement in multicomponent non-ideal distillation processes using thermal coupling technique.

Two ternary (Methanol-Ethanol-Water and Acetone-methanol-Water) with different feed composition of [(0.333,0.333,0.333), (0.8,0.1,0.1), (0.1,0.8,0.1), (0.1,0.1,0.8)], and one quaternary feed systems (n-Hexane – Methyl-cyclo-pentane – Ethanol and Benzene) with different feed composition of [(0.25,0.25,0.25,0.25), (0.7,0.1,0.1,0.1), (0.1,0.7,0.1,0.1), (0.1,0.1,0.7,0.1), (0.1,0.1,0.7,0.1)] were considered.

The feed systems were assumed as liquids at their boiling point, three fractional recoveries of 0.9, 0.925 and 0.95. The operating pressure was assumed to be constant at 1 atm.

Nine different configurations were used to separate the feed systems according to their non-ideality.

The results are compared with the best three configurations of conventional systems and the percentage saving in total reboiler load and total annual cost have been calculated with respect to these three configurations.

The results obtained were compared with previous works using other techniques such as heat pump and heat matching.

A computer programme for multicomponent non-ideal distillation using thermal coupling technique was developed using Mat lab V6.5 language. The optimal configuration for each feed type and feed composition was obtained.

It is found that thermal coupling technique can be used to give saving in total reboiler load from 41.18% to 96.21 and saving in total annual cost from 54.89% to 80.21%. These results show that thermal coupling technique is more efficient than the others.

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Chapter One Introduction

1.1 Introduction

Separations are "big businesses" in chemical processing. It has been variously estimated that the capital investment in separation equipment is 40-50% of the total for a conventional fluid processing unit.

Many forms of energy supplied to separation processes, these forms are electrical, mechanical, chemical or thermal energy, depending upon the type of the processes.

Of the total energy consumption of an average unit, the separation steps accounts for about 70%. And of the separation consumption, the distillation method accounts for about 95%.[1]

Distillation is the most widely used separation technique in the process industry. Its main disadvantage is the high energy consumption and the energy required for the distillation columns often represents most part of the total energy cost of the plant.

The classical design of a multicomponent distillation plant only involves simple columns: each simple column in a multicomponent distillation configuration receives a feed and performs a sharp separation between two components of the feed mixture. In this case, for the separation of n-component mixtures sequences of n-1 simple columns with n-1 condensers and n-1 reboilers are requested. [2]

The principle of the work of distillation process is the equilibrium stage theory, when a liquid containing two or more components is heated to its boiling point, the composition of vapor will normally be different from that of the liquid phase, this difference in composition of the two phases is called equilibrium stage theory.[3] An important requirement of distillation unit is the provision of contact between the vapor and the liquid streams so that the equilibrium is nearly approached by hydrodynamic study of vapor and liquid on the plate.[4]

Distribution coefficient K, the term which is used in the equilibrium relationships for any component in an equilibrium stage. For ideal solution:

$$K_i = \frac{y_i}{x_i} = \frac{p_i}{P} \tag{1.1}$$

For non-ideal solution, activity coefficient γ_i is added, which represents the degree of deviation from ideality.

$$K_i = \frac{\gamma_i y_i}{x_i} = \frac{\gamma_i p_i}{P} \qquad (1.2)$$

An important motivation for studying integrated distillation column arrangements is to reduce the energy consumption of distillation process.[18]

Many techniques are presented in the literature that minimizes energy requirements of the distillation column. Thermal coupling is one of these techniques, which considered in this work.

Thermal coupling between two columns in a sequence can be adopted to reduce the energy consumption of the process; a thermally coupled sequence is obtained by removing condensers and/or reboilers from a simple column configuration.[2]

A distillation system contains thermalcoupling when a heat flux is utilized for more than one fractionation and the heat transfer between fractionation sections occur by a direct contact of vapour and liquid.

Also thermal coupling technique is considered by reduction in the number of columns required, this is proposed by taking one side stream or more from the column.[5]

1.2 The Aim of this Project:-

The purpose of this project is to study the minimization of the energy requirements in multicomponent non-ideal distillation using thermal coupling technique, by studying the effects of changing feed composition, configuration and fractional recovery on two ternary and one quaternary non-ideal feed systems and comparing the results with previous works (heat pump and heat matching) on the same systems but using thermal coupling technique for minimizing the energy requirements.

Chapter Two Literature survey

2.1 Introduction:-

In the chemical industries, the task of separation is a very energy consuming process, where distillation is the process most widely used for separation. Distillation columns are used for about 95% of liquid separations and the energy use from this process accounts for an estimated 3% of the world energy consumption. With rising energy awareness and growing environmental concerns there is a need to reduce the energy use in industry [6].

For the distillation process, because it is such a high-energy consumer, any energy savings should have an impact on the overall plant energy consumption. The use of heat integration combined with complex configurations for distillation columns holds a great promise of energy savings up to about 70%.

In addition to saving energy, accompanied by reduced environmental impact and site utility costs, there is also a possibility for reduction in capital costs.

The separation of multicomponent mixtures into three or more products is mostly performed in a sequence of simple distillation columns. Complex column arrangements with thermal coupling are an attractive alternative promising savings in both energy and capital cost. Thermally coupled distillation column can save significant amounts of energy by reducing thermodynamic losses. In such a setup, a number of columns (typically two) are coupled together through vapor and liquid streams without reboilers or condensers between the columns. One practical application of the thermal coupled column has been known for a long time. However, only a limited number of such columns have been implemented in the field. Part of the reservations towards thermally coupled columns can be attributed to difficulties in controlling these columns. Another main reason is the lack of powerful design methods that allow a rapid economic screening of the different configurations during the early process design phase.[7]

2.2 Energy Saving Method in Multicomponent Distillation for Non-ideal Systems:

There are a number of different methods or designs that can be applied to save energy in distillation, such as integration of distillation columns with the heat pumps, multieffect distillation, and complex arrangements such as thermally coupled columns and other methods.[8]

There are three options for saving energy in distillation[9]:

- 1. Make the process itself more energy-efficient.
- 2. Augment it with advanced processes to form energy-efficient systems.
- 3. Replace it with an alternative separations technology.

2.2.1 Energy Saving through Heat Stream Matching:

Heat matching is possible only between the hot streams and the inlet feed streams (heat economizer) which give more than 6% saving in total energy consumption. The problem of finding the optimal design of heat exchanger networks in multicomponent distillation can be divided into three parts. The first is finding the optimum configuration for least energy without heat interchange, the second, the heat interchange between reboilers and condensers, and the third, the heat interchange between intermediate cooler and heater.

Nakkash [10], studied the optimal design configuration for least energy with energy matching between reboilers and condensers only and with intermediate heat load for nearly ideal four component feedstock. The results show that there is a saving in energy from 7-39%, this increased to 8-43% when intermediate coolers and heaters are proposed.

2.2.2 Multieffect Method:

Multieffect distillation has long been considered **as** one of the methods to reduce energy consumption in distillation columns. Multieffect integration is achieved for two or more distillation columns by running one of the columns at a higher pressure and integrating the condenser of this high-pressure (HP) column with the reboiler of the low pressure (LP) column, that means the column pressures are adjusted such that the cooling (energy removal) in one column can be used as heating (energy input) in another column as shown in figure (2.1).

For the multieffect systems there are two modes of integration: forward integration, where the heat integration is in the direction of the mass flow; and backward integration, where the integration is in the opposite direction of the mass flow.

Engelien and Skogestad [3] are applied in order to screen the three cases based on minimum vapor flow rate criteria, also the required pressure levels for



Figure 2.1 Multiple effect distillation showing limiting effect of temperature drop across column[12]

2.2.3 Split Tower:

Split tower was used to reduce the number of reboilers in the configuration and to reuse the heat from the condenser in the reboiler. The split tower system has a single reboiler and single condenser as shown in the figure (2.2). The temperature difference between the reboiler and condenser will be much greater than that of an ordinary column. This occurs because the two columns each have their own temperature difference to be met from the top to bottom, and the driving force for the condenser-reboiler must be supplied.

The split tower arrangement has a large temperature difference between the reboiler and condenser, thus it will probably be desirable to minimize this by using small delta T's across the reboiler, condenser-reboiler, and condenser. This will mean a large heat exchanger surface being required. Even so, it is likely a higher temperature heat source will be needed for the reboiler. As it is at a higher temperature, the heat will be more expensive, such as a higher pressure steam. This means we are saving energy, but using a more costly source.

The feed to a single tower will be split in two for the two column arrangement. Therefore, the individual columns will be about one-half the size of the single column. However, the relative volatility and the mass flow rate/area through the columns will change with the pressure, resulting in a differently sized tower than just one-half the size. The savings of the split tower arrangement come from the reduced heat requirement. However, the value of the heat used should be higher per Btu used than in the case of a single column.[10],[11]

Hababa[12] studied this method for two ternary and one quaternary nonideal system. His results show that when operating the towers at the same pressure, there is no energy integration thus very low percentage saving in total energy consumption.

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Figure 2.2 Split tower technique[12]

2.2.4 Vapor Recompression or Heat Pump:

Vapor recompression consists of taking the overhead vapors of a column, condensing the vapor to liquid, and using the heat liberated by the condensation to reboil the bottoms liquid from the same column as shown in figure (2.3). The temperature driving force needed to force heat to flow from the cooler overhead vapors to the hotter bottoms product liquid is set up by either compressing the overhead vapor so it condenses at a higher temperature, or lowering the pressure on the reboiler liquid so it boils at a lower temperature, then compressing the bottoms vapor back to the column pressure. A conventional column has a separate condenser and reboiler, each with its own heat transfer fluid such as cooling water and steam. The vapor recompression column has a combined condenser-reboiler, with no external heat transfer fluids.[11]

Nakkash and Al-Ramadhani [13]studied heat pumps in multicomponent distillation of nearly ideal hydrocarbon systems. They found that heat pump system gave a saving in total annual cost from 5% to 77% over a conventional system and the percentage reduction in exergy losses with heat pump was 27% to 97% over the conventional system.

Al-Mo'otasim [10]studied heat pumps in multicomponent distillation of non-ideal hydrocarbon systems. She found that there is reduction in energy requirements was ranging from 12% to 76%, and give a percentage saving in total annual cost ranging from 10% to 77%. The results show that when using heat pump technique there is an average of 20% saving in total energy consumption over that with heat integration.



Figure 2.3b Indirect vapor recompression [12]

2.2.5 Thermal Coupling Method:-

Thermally coupled system of distillation columns serves for separation of one feed stream into three product streams. It consists of two apparatuses connected by liquid and vapor streams and contains only one reboiler and one condenser. Thermally coupled distillation system is a lower cost alternative to the conventional systems and can be designed to be quite flexible in internal distributions of liquid and vapor flows[14].

Thermally coupled distillation column arrangements have been known for over 50 years. It has been established that when thermal coupling can be applied, energy savings of 30% are typical when compared with a conventional arrangement. In addition, the thermally coupled design can save up to 30% of the capital cost compared with a conventional arrangement.

Thermally coupled distillation systems can separate close boiling components with considerable saving of heating and cooling costs.

The thermally coupled distillation sequences outperformed the dynamic behavior of the conventional distillation sequences for set point tracking. This result is important to establish that thermally coupled distillation sequences not only can have significant energy savings but also good dynamic properties.

Because of the internal thermal coupling, a certain amount of heat is transferred from the rectifying section to the stripping section and brings the downward reflux flow for the former and the upward vapor flow for the latter. As a result, the condenser and the reboiler are not required and energy savings are realized.[15]

In the case of ternary mixtures, these thermally coupled arrangements include the side stripper (TCDS-SS) as figure (2.4), the side rectifier (TCDS-SR) as figure (2.5) and the fully thermally (Petlyuk scheme) coupled column as figure (2.6). Among them, the fully thermally coupled (Petlyuk scheme) arrangement provides up to 50% energy saving, when compared to conventional sequences. . In particular, the Petlyuk column is the most energy-efficient option, but its structure poses two interesting features. One, it has the highest number of interconnections, and two, the streams in the vapor phase (and therefore also in the liquid phase) flow in the two directions, back and forth between the columns.

These aspects affect not only the design but also the control properties of the Petlyuk system.

Alternative options can be developed through the correction of each of these two items. Thus, through a reduction on the number of interconnections, or through the use of unidirectional interconnecting flows, one can conceptually generate simpler schemes, in principle easier to control.[16]



Figure 2.4a Side stripper thermal coupling column



Figure 2.4b Side rectifier thermal coupling column



Figure 2.4c Fully thermal coupling column (Pytlek column)

2.2.5.1 Literature Review for Thermal Coupling Method in Distillation:-

Thermal coupling is one of the techniques used to minimize energy consumption by reducing the number of reboilers and/or condensers or both. This idea is not new.

Theoretical studies had been submitted in this work,e.g.,Petlyuk, Platonor [17], have shown that the column coupling configurations are capable of achieving typically 30% of energy savings compared with a conventional sequence.

Stupin [18] showed that the thermally coupled system at minimum reflux requires 27% less vapor boil-up than the conventional scheme.

Tedder and Rudd [5], have considered an economic method for the evaluation of simple serial distillation configurations. Eight configurations are compared economically by a computer design model using short-cut method. In these configurations towers may receive multiple feed streams and produce more than two products.

Tobyia [19] studied the thermal coupling technique for nearly ideal feedstocks, it was found that thermal coupling technique requires less reboilers and condensers and the total energy saving was 1-86%.

Triantafyllou and smith [20] report typically savings in the order of 30% in both energy and capital costs compared to traditional arrangements with two columns in series.

Finn [11] studied the analysis of side stripper, side rectifier and fully thermally (Petlyuk scheme) coupled column and showed that expected savings of minimum internal vapor flows, and therefore of minimum energy requirements, of up to 30% could be obtained with respect to the operation of conventional direct and indirect distillation sequences.

More recent works, Hernández and Jiménez cited in [11], Grossmann et al. [11] have reported the use of optimization strategies for thermal coupling distillation column to detect designs with minimum energy consumption under (finite reflux) conditions.

The research of Liu and Qian [2] has shown that the energy saving could be up to 40-50% compared with conventional distillation column.

Hernández et al.[11] showed that the energy savings of thermal coupling distillation systems sequence can be explained in terms of the internal composition profiles of the intermediate component.

2.3 Vapor-Liquid Equilibrium for Multicomponent Distillation (VLE):-

The equilibrium (theoretical) stage concept figure (2.5) is central in distillation. Here we assume vapor-liquid equilibrium (VLE) on each stage and that the liquid is sent to the stage below and the vapor to the stage above. For some trayed columns this may be a reasonable description of the actual physics,



Figure (2.5) equilibrium stage concept

For practical calculations, the critical step is usually not the modeling of the stages, but to obtain a good description of the VLE.[4]

Modeling and design of multicomponent distillation column requires correlation related liquid and vapor phases compositions. Complexity of this correlation depends on the components number, their nature and the interaction between components.

Antoin [20] suggested a relation that predicted vapor pressure at instant temperature.

$$\ln p^* = A + \frac{B}{T + C}$$
 (2.1)

This relation has three constants, which depend on the nature of components, and it is applicable directly for one component, but for a mixture, modifications were needed.

Application of Antoin on a mixture relation builds on two assumptions, the ideal gas behavior and ideal liquid behavior. Activity coefficient is used to correct the idealization of vapor and liquid.[6]

2.3.1 Thermodynamic of Equilibrium:-

Gibbs [14] introduced the thermodynamic treatment of multicomponent phase equilibrium which based on the concept of chemical potential.

When the temperature and pressure of liquid phase and vapor phase is equal to that of other and when the chemical potential of each specie present is the same in both phases, then the liquid phase and vapor phase are said to be in thermodynamic equilibrium.

Lewis [15] showed that a physically more meaningful quantity equivalent to the chemical potential could be obtained by a simple transformation. The result of this transformation is a quantity called the fugacity which is a "corrected pressure" and has a unit of pressure

For a component in a mixture of ideal gases the fugacity is equal to its partial pressure.

In real mixtures the fugacity can be considered as a partial pressure which is corrected for non-ideal behavior.[14]

2.3.2 Fundamental Equations for the Vapor-Liquid Equilibrium:-

When the vapor phase is in equilibrium with liquid phase, the fugacity of each component in both phases is equal.

 Where

N=components number.

In the case that the vapor phase obeys the laws of an ideal gas, the following equation can be established:

$$f_i^{\nu} = PY_i \qquad \dots \dots (2.3)$$

If the liquid phase can be regarded as an ideal solution, then:

At equilibrium:

Where *P* is the total pressure of the system, P_i is the vapor pressure of the i-th component and X_i and Y_i are the mole fractions of the i-th component in the liquid and vapor phase, respectively.

For non ideal system, the fugacity of the liquid phase is given by:

In this case the vapor-liquid equilibrium can not be calculated unless the activity coefficient is obtained. Therefore the case of non-ideal solutions the prediction of the activity coefficient is most important.[14]

2.3.3 Activity Coefficient Calculation:

Many models are presented, the most important models are:

1.NRTL Model.

2.UNIQUAC Model.

3.UNIFAC Model.

4. Wilson Model.

2.3.3.d.Wilson Model:

Wilson model [16] was the most popular model because Wilson equation has found wide application, both in the correlation of binary data and the prediction of multicomponent vapor-liquid behavior. It's popularity is based upon it's simplicity of expression and accuracy comparable to that obtained by the other new complex models. The success of this model in the correlation of vapor-liquid equilibrium data prompted the development of alternative local-composition models.

Wilson equation contains just two parameters for a binary system and written as follow:

$$\frac{G^{E}}{RT} = x_1 \ln(x_1 + x_2 \Lambda_{12}) - x_2 \ln(x_2 + x_1 \Lambda_{21}) \qquad (2.35)$$

 Λ_{12} and Λ_{21} must be positive numbers.[17]

2.4 Design Methods for Multicomponent Non-ideal Distillation Systems:-

There are two methods used in the design of multicomponent distillation columns:-

1.Short-cut method.

2.Plate-to-plate methods.

2.4.1 Short-cut Method:-

Shortcut models are well established for grassroots design of distillation columns and have been widely applied. Shortcut models are quicker to solve, do not have significant convergence problems and are more robust than rigorous models for column optimization. This shortcut method includes a new approach to locating the feed trays in a complex column.[18]

a shortcut approach to get fast, good estimations of the limiting flows in complex separation systems is proposed *for sharp separations* between the key components (which are not adjacent in volatility if distributed components are present).[19]

This model is primarily based on a modified Underwood method, the Gilliland and Kirkbride correlations, the Fenske equation and the material balances Shortcut procedures can be used to determine the minimum energy demand of a previously specified separation even for azeotropic mixtures.

For distillation of ideal mixtures reliable shortcut methods (e.g. Fenske-Underwood-Gilliland) have been known for quite some time. However such methods are not applicable for strongly nonideal azeotropic mixtures which are encountered in many industrial processes.

This model fixes both the column configurations and the operating conditions, including steam flow rates, and calculate the product flow rates, temperatures and compositions, and the various heat duties. Short-cut methods can be considered as simplifications of the MESH equations. [20]

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Other authors, in particular Stewart et al.[21] use discrete weighted residual methods for the development of short-cut models.

Eckert and Hlavelek modified the Smith –Brinkly method for use in computing non-ideal multicomponent distillation, they tested their procedure for number of strongly non-ideal systems.[22]

2.4.2 Rigorous Methods for Multicomponent Non-ideal Systems:

Rigorous methods (plate to plate calculations) are more accurate and convenient to give the temperature, composition, stream flow rates and heat load at each stage.

Early attempts to solve the material and enthalpy balance equations for stage to stage by calculational procedures of Lewis Matheson, and Thiele-Geddes , based on equation tearing for solving simple fractionators with one feed and two products.

Kinoshita and Hashimoto developed a powerful new simulation procedure for multicomponent distillation column processing non-ideal solutions.

Yeomans and Grossmann presented the **rigorous** synthesis of heat integrated sequences applying disjunctive programming techniques to formulate the problem). Finally, a major challenge that remains is the **rigorous** global optimization.[21]

Chapter Three Theoretical Aspect

3.1 Introduction:

In order to predict the performance of the distillation column and due to the difficulty in using a real process, a computer simulation of the mathematical model of the distillation column is required to aid the selection and design of the suitable system.

The complexity of the modeling of distillation column is due to the large number of variables that have to be considered such as temperature, pressure drops across the plate, tray hydrodynamic ,tray holdup... etc, finally determination of steady state condition variables.

There are two main types of problems encountered when performing distillation column calculations:

- 1. Column design for a given product specification, i.e. determination the number of plates in the column, the location of feeds and the side stream, and the heating and the cooling requirements.
- 2. Analysis of specified column in the steady state case, where the column is specified completely and the data of the flow temperature, pressure, vapor and liquid concentrations... etc will be calculated.

3.2 Method of Analysis:

The analysis emphasizes to investigate the possibility of energy recovery in non-ideal multicomponent distillation using thermal coupling technique to separate two ternary and one quaternary system feed stock mixtures into a relatively pure products, and how the variation of these possibilities was carried out when the feed composition, degrees of recovery will vary.

By using different configurations the separation was carried out for each feed system depending upon its ideality. A modified computer programmes for short-cut method (empirical method). The feed systems are assumed to be liquid at their boiling points and three degree of recoveries of 0.9, 0.925, and 0.95 in which the flow rates, composition and temperature of all process streams within the configuration are determined together with the process design of all columns, heat load for condensers and reboilers, number of plates, actual reflux ratio and feed plate location.

Short-cut method was used to design the distillation column for non-ideal multicomponent system, to get first estimation of the process variables.

3.3 Variable Specifications:

The variables considered for the process system are:

- 1. Feed composition.
- 2. Degree of recovery.
- 3. Type of systems.
- 4. Configurations.

Two ternary and one quaternary non-ideal feed systems table (3.1) have chosen because the physical properties and the binary interaction forces are available in the literature. Also they were studied to compare the present results with the previous works on the same systems.

Different feed compositions of ternary and quaternary feed system were studied table (3.2) according to light and heavy key components and three different recoveries of 0.9, 0.925, and 0.95 for feed system a, b and c. Different configurations for feed system a, b and c for conventional and thermal coupling were considered figures (3.1) to (3.8). All feed systems were assumed to be liquids at their boiling point, total condensation to give a maximum heat removed at the top of the column. The operating pressure of each column in configuration was assumed to be constant at 1 atm. The ratio of actual to minimum reflux ratio was taken constant as a value of 1.25.

component	Ternary feed system		
	a	b	
А	Methanol Ace		
В	Ethanol	Methanol	
С	Water	Vater Water	

Table (3.1) Feed system components [17]

Component	Quaternary feed system	
	С	
D	n-hexane	
E	Methyl-Cyclo-Pentane	
F	Ethanol	
G	Benzene	

Component	Ternary feed composition			
	1	2	3	4
А	0.333	0.8	0.1	0.1
В	0.333	0.1	0.8	0.1
С	0.333	0.1	0.1	0.8

Table (3.2) Ternary and quaternary feed system composition [17]

component	Quaternary feed composition				
	1	2	3	4	5
D	0.25	0.7	0.1	0.1	0.1
Е	0.25	0.1	0.7	0.1	0.1
F	0.25	0.1	0.1	0.7	0.1
G	0.25	0.1	0.1	0.1	0.7



Figure 3.1 Thermal coupling configuration 1, feed systems a and b



Figure 3.2 Thermal coupling configuration 2, feed system b



Figure 3.3 Thermal coupling configuration 3, feed system b

3.4 Prediction of Vapor- Liquid Equilibrium for Non-ideal Systems:

The prediction of multicomponent vapor- liquid equilibrium behavior is very important in industrial application.

Among the models of prediction of vapor-liquid equilibrium for non-ideal systems, Wilson equation has found wide application, both in the correlation of binary data and in the prediction of multicomponent of vapor-liquid equilibrium behavior. In this work, Wilson model was used because of the availability of the data and to compare the results with previous works.

3.4.a Wilson model:

Wilson equation (1964) is derived to solve the equation of excess free energy,

Wilson equation is:

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Where

$$\Lambda_{ij} = \frac{v_j^L}{v_i^L} \exp\left[-\left(\lambda_{ij} - \lambda_{ii}\right)/RT\right] \qquad (3.2)$$

And

$$\Lambda_{ji} = \frac{v_i^L}{v_j^L} \exp\left[-\left(\lambda_{ji} - \lambda_{jj}\right)/RT\right] \qquad (3.3)$$

Although

 $\lambda_{ij} = \lambda_{ji} \tag{3.4}$

$$\Lambda_{ij} = \Lambda_{ji} \tag{3.5}$$

And

$$\Lambda_{ii} = \Lambda_{jj} = 1.0 \tag{3.4}$$

Therefore to apply Wilson's model it is important to determine Λ_{ij} and Λ_{ii} (Wilson's constants).

3.4.b Enthalpy of non-ideal systems:

Because of the excess free energy, the prediction of enthalpy of non-ideal system is important. Where for ideal system the excess free energy equal zero.

$$\Delta G^{E} = \Delta G - \Delta G^{I} \tag{3.5}$$

Where

 ΔG^{E} = Excess free energy.

 ΔG = Real free energy.

 ΔG^{I} =Ideal free energy.

The relationship between excess molal free energy, excess molal enthalpy and entropy is:

$$\Delta G^{E} = \Delta H^{E} - T \Delta S^{E} \qquad (3.6)$$

Wilson (1964) gave an expression to determine excess enthalpy of non-ideal solutions:

$$H^{E} = \sum_{i=1}^{c} x_{i} H_{i}^{-E} = \sum_{i=1}^{c} \left\{ x_{i} \left[\frac{\sum_{i=1}^{c} x_{i} (\delta \Lambda_{ij} / \delta T) R T^{2}}{x_{i} + \sum_{i, j \neq 1} x_{j} \Lambda_{ij}} \right] \right\}$$
(3.7)

Where

$$\left(\delta\Lambda_{ij} / \delta T\right) R T^{2} = \left(\lambda_{ij} - \lambda_{ii}\right) \Lambda_{ij} \qquad (3.8)$$

For binary systems H^E becomes:

For more than two components equation (3.7) becomes:

$$H^{E} = \sum_{i=1}^{c} \left\{ x_{i} \left[\frac{\sum_{i=1}^{c} x_{i} (\lambda_{ij} - \lambda_{ii}) \Lambda_{ij}}{x_{i} + \sum_{i, j \neq 1} x_{j} \Lambda_{ii}} \right] \right\}$$
(3.10)
It is therefore convenient to calculate the excess enthalpy for any solution and then adding this value to the enthalpy value of ideal system to get the actual value of enthalpy for the solution.

Equation (3.10) was used to calculate the excess enthalpy of a nonideal multicomponent system in the liquid phase only.

3.5 Design Models:

The calculations were made by using a short-cut method for both conventional and thermal coupling technique and a computer program developed using matlab appendix (B).

3.5.1 Mathematical Model for the Short-cut Design Calculation:

Empirical correlation is the basic of this model which calculate:

- 1. Minimum reflux ratio.
- 2. Minimum number of plates.
- 3. Actual number of plates.
- 4. Actual reflux ratio.
- 5. Top and bottom temperature.
- 6. Heat load at top and bottom of the column.
- 7. Feed plate location.

Underwood equation is used to determine the minimum reflux ratio:

$$\sum_{i=1}^{N} \frac{\alpha_i x_{i,d}}{\alpha_i - \phi} = R_m + 1 \tag{3.11}$$

 ϕ was calculated from Fenske equations:

$$\sum_{i=1}^{N} \left[\frac{\alpha_i x_{if}}{\alpha_i - \phi} \right] = 1 - q \qquad (3.12)$$

And $\alpha_{LK} \leq \phi \leq \alpha_{HK}$

Where

Heat required to vaporize the feed

q=-----

Latent heat of vaporization

The value of ϕ is calculated from the previous equations by trial and error, then R_m is calculated from equation (3.11).

Operating reflux ratio= $R=R_m*1.25$ (3.13)

Gilliand, Van Winkle and Todd relationships were used to calculate the theoretical number of plates:

a. for $(R-R_m)/(R+1) < 0.125$

$$\frac{N-N_m}{N+1} = 0.5039 + 0.5068 \left(\frac{R-R_m}{R+1}\right) - 0.0908 \log\left(\frac{R-R_m}{R+1}\right) \quad \dots \dots \dots (3.14)$$

b. for $(R-R_m)/(R+1) > 0.125$

$$\frac{N-N_m}{N+1} 0.6257 - 0.9868 \left(\frac{R-R_m}{R+1}\right) + 0.516 \left(\frac{R-R_m}{R+1}\right)^2 - 0.1738 \left(\frac{R-R_m}{R+1}\right)^3 \dots$$
..... (3.15)

For columns with one side stream, equations (3.12) to (3.15) were applied twice, first section from top tom the side stream and second section is from side stream to the bottom, and then the total theoretical plates were considered one less than sum of the two sections.

Vapor-liquid equilibrium was calculated using both Wilson and Antoine equations:

The Antoine coefficients were given in appendix (C).

The ideal enthalpy of vapor and liquid were used in the form of third degree polynomials as a function of temperature. The coefficients of these polynomials were given in appendix (C). The sum of ideal enthalpy and excess is the actual enthalpy of the components in the non-ideal systems.

The details of the short-cut method were explained in appendix (A) and the developed program and its flow charts were given in appendix (B).

3.6 Mathematical Models for Calculations:

3.6.1 Mathematical Models for Material Balance:

Overall and component material balances have been proposed for each column and each configuration.

3.6.1.a Conventional distillation columns:

Conventional column is a column with one feed and two products, distillate and waste.

Moles of distillate= $\sum_{i=1}^{lk-1}$ moles of I component+ moles of lk

component+ moles of hk component.

$$D = \sum (Z_{i,f} \cdot F) + Z_{lk,f} \cdot F \cdot RF_{lk} + Z_{hk,f} \cdot F \cdot (1 - RF_{hk}) \qquad (3.18)$$

$$F=D+W$$
(3.19)

3.6.1.b Thermal coupling distillation columns:

Thermal coupling columns are columns with more than two products and could be more than one feed.

Distillation columns with one side stream divided into two sections, the first from top to the side stream with light and heavy key components, and the second from side stream to the bottom with different light and heavy key components and the heavy key of the first section is equal to the light key of the second section.

If there are two side streams, the column is divided into three sections.

3.6.1.a.1 Columns with two feed and one side stream:

Moles of
$$D = \sum_{i=1}^{k-1} (\text{moles of } i) + \text{moles of } lk + \text{moles of } hk.$$

$$D = \sum_{i=1}^{k-1} (Z_{i,f1}.F1) + Z_{ik,f1}.F1.RF_{ik} + Z_{hk,f1}.F1.(1 - RF_{hk}) \qquad \dots \dots (3.20)$$
Moles of S=moles of lk+ moles of hk+ moles of hk1

 $S = (Z_{lk,f1}.F_1.(1 - RF_{lk}) + Z_{lk,f2}F_2) + (Z_{hk,f1}.F_1 - RF_{hk} + Z_{hk1,f2}.F_2.RF_{lk}) + (Z_{hk1,f1}.F_1 + Z_{hk1}.F_2.(1 - RF_{hk1}))$(3.21)

F1+F2=D+S+W(3.22)

3.6.1.a.2 Special columns:

1. Column 2 in configuration 4 and 5.

The side stream is assumed to be the feed which produce the distillate of column 2 and the bottom product of column 3.

Moles of
$$D = \sum_{i=1}^{lk-1}$$
 moles of i+ moles of lk+ moles of hk.

$$D = \sum_{i=1}^{lk-1} (Z_{i,f} . F) + Z_{lk,f} . F . RF_{lk} + Z_{hk,f} . F . (1 - RF_{hk}) \qquad (3.23)$$

Moles of $S = \sum_{i=1}^{k}$ moles of i+ moles of hk+ moles of hk1

$$S = \sum_{i=1}^{lk} (Z_{i,f} \cdot F) + Z_{hk,f} \cdot F \cdot RF_{hk} + Z_{hk1,f} \cdot F \cdot (1 - RF_{hk1}) \qquad (3.24)$$

Moles of W=moles of hk+ moles of hk1+ $\sum_{j=hk1+1}^{n}$ moles of j

$$W = Z_{hk,f} \cdot F \cdot (1 - RF_{hk}) + Z_{hk1,f} \cdot F \cdot RF_{hk1} + \sum_{j=hk_{1}+1}^{n} (Z_{j,f} \cdot F)$$
 (3.25)

$$F1+Fr=D+S+W$$
(3.26)

2.column 2 of configuration 3.

The side stream is assumed as the feed which produces the bottom product of the column 1 and the distillate of column 2.

Moles of D=
$$\sum_{i=1}^{lk-1}$$
 moles of i+ moles of lk+ moles of hk

$$D = \sum (Z_{i,f} \cdot F) + Z_{lk,f} \cdot F \cdot RF_{lk} + Z_{hk,f} \cdot F \cdot (1 - RF_{hk}) \qquad (3.27)$$

Moles of S=moles of lk+ moles of hk+ $\sum_{j=hk1}^{n}$ moles of j

$$S = Z_{lk,f} \cdot F \cdot (1 - RF_{lk}) + Z_{hk,f} \cdot F \cdot RF_{hk} + \sum_{j=hk1}^{n} (Z_{j,f} \cdot F)$$
 (3.28)

Moles of W=moles of hk+ moles of hk1+ $\sum_{j=hk1+1}^{n}$ moles of j

$$W = Z_{hk,f} \cdot F \cdot (1 - RF_{hk}) + Z_{hk1,f} \cdot F \cdot RFhk1 + \sum_{j=hk1+1}^{n} (Z_{j,f} \cdot F)$$
 (3.29)

F + Fr = D + S + W(3.30)

3.6.2 Cost Estimation:

Equipment cost, operating cost were calculated depend on the equations of Henry method.

Equipment cost= cost of column+ cost of condenser+ cost of reboiler.

Operating cost=28% (total equipment cost)+cost of utilities.

Cost of utilities=cost of steam+ cost of cooling water.

Total annual cost=depreciation+ annual operating cost.

Total annual cost=(equipment cost/service life)+annual operating cost.

The details were given in appendix (A).



Figure 3.6 feed system (a)



Figure 3.7 feed system(b)



Figure 3.8 feed system (c)

Chapter Four

Results and Discussion

4.1 Introduction:-

In this chapter, three types of feed systems were studied by varying the feed compositions, fractional recovery and configuration, by using short-cut model. All results presented in this chapter were taken from short-cut model.

Total reboiler load, percentage saving in total reboiler load and percentage saving in total annual cost using thermal coupling technique for all feed systems at different feed composition, fractional recovery and configurations were reported in tables, and/or represented graphically to ease the comparison.

In this chapter, a comparison for the results of present work of thermal coupling technique and previous works of heat pump and heat matching were reported in tables only.

4.2 Effect of Process Variables on Total Reboiler Load Using Thermal Coupling Technique:-

4.2.1 Effect of Feed Composition:-

Four feed compositions and one operating pressure of 1 atm for ternary feed systems a and b, and five feed compositions and one operating pressure of 1 atm for feed system c were studied. The results obtained were listed in tables (4.1) to (4.2) for feed system a, tables (4.7) to (4.8) for feed system b and tables (4.13) to (4.14) for feed system c. The figures showed these results are (4.1) to (4.2) for feed system a, (4.3) to (4.4) for feed system b and (4.5) to (4.6) for feed system c. For feed system a and b, the results show a maximum reboiler load at feed composition 2 because there is a large mole fraction of light key component in the feed which needs high reboiler load to separate it, this maximum reboiler load decreased as the composition change to 3, 1 and 4 because of the decreasing the value of the mole fraction of light key component in the feed.

For feed system c the results show a maximum reboiler load at feed composition 2 because the high mole fraction of light key component in the feed, this maximum value decreased as the composition changed from 3,4,1 and 5.

4.2.2 Effect of Fractional Recoveries:-

Three fractional recoveries of 0.9, 0.925 and 0.95 were considered. The results are given in tables (4.1) and (4.2) for feed system a, tables (4.7) and (4.8) for feed system b and tables (4.13) and (4.14) for system c. These results also showed the effect of fractional recoveries on reboiler load in figures (4.1) and (4.2) for feed system a, figures (4.3) and (4.4) for feed system b and figures (4.5) and (4.6) for feed system c.

The reboiler load increased as the fractional recovery increased for all feed systems as the fractional recovery increased except in composition 4 for system a and composition 3 for system b because the separation of components of composition more than 50% in the feed as bottom product requires less reboiler load.

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4.2.3 Effect of Configurations:-

Three configurations for feed systems a, b and c were considered. The results are listed in tables (4.1) and (4.2) for feed system a, tables (4.7) and (4.8) for feed system b and tables (4.13) and (4.14) for system c These results also showed the effect of fractional recoveries on reboiler load in figures (4.1) and (4.2) for feed system a, figures (4.3) and (4.4) for feed system b and figures (4.5) and (4.6) for feed system c.

The results show that the optimum (minimum) value of the reboiler load is obtained when using configuration 1 because it has a liquid side stream which is not need high reboiler load for all feed system a, b and c.

4.2.4 Comparison with Previous Works:-

The results of comparison between thermal coupling technique and previous works heat matching and heat pump were obtained under the same conditions of feed systems, feed compositions, fractional recoveries and operating pressure from the following equation:-

% comparison of reboiler load=((REBLA of thermal coupling-REBLA of other techniques)/REBLA of thermal coupling)*100(4.1)

The results were tabulated in tables (4.3) to (4.6) for feed system a, tables (4.9) to (4.12) for feed system b and tables (4.15) to (4.18) for feed system c.

The negative sign appeared in the results means that the thermal coupling technique is more efficient than other techniques according to equation (4.1)

Table (4.1) Effect of change of fractional recovery and feed composition on reboiler load (kcal/hr $*10^{-6}$) for system a and configuration 1at constant pressure of 1 atm.

RO Z	0.9	0.925	0.95
1 (0.333,0.333,0.333)	1.062	1.100	1.136
2 (0.8,0.1,0.1)	1.423	1.530	1.643
3 (0.1,0.8,0.1)	1.432	1.470	1.479
4 (0.1,0.1,0.8)	0.44	0.43	0.42

Table (4.2) Effect of change of fractional recovery and feed composition on reboiler load (kcal/hr $*10^{-6}$) for system a and configuration 2 at constant pressure of 1 atm.

RO Z	0.9	0.925	0.95
1 (0.333,0.333,0.333)	1.363	1.418	1.475
2 (0.8,0.1,0.1)	1.472	1.583	1.698
3 (0.1,0.8,0.1)	1.63	1.62	1.58
4 (0.1,0.1,0.8)	0.959	1.023	1.111

Table (4.3) % comparison of reboiler load between thermal coupling and heat pump techniques for system a and configuration 2 at constant pressure of 1 atm.

Ro		0.9		0.925			0.95		
Z	REBLA	REBLA	% of	REBLA	REBLA	% of	REBLA	REBLA	% of
\backslash	of H.P.	of T.C.	comparison	of H.P.	of T.C.	comparison	of H.P.	of T.C.	comparison
1	1.66	1.06	-56.1	1.69	1.10	-64.23	2.97	1.13	-64.17
2	1.67	1.42	-17.03	1.83	1.53	-19.37	1.97	1.65	-19.68
3	2.95	1.43	-106.3	3.34	1.47	-127.4	2.9	1.48	-96.21
4	1.14	0.959	-18.87	1.17	1.023	-14.37	1.22	1.11	-9.81

Table (4.4) % comparison of reboiler load between thermal coupling and heat pump techniques for system a and configuration 2 at constant pressure of 1 atm.

Ro		0.9			0.925			0.95		
	REBLA of H P	REBLA of T C	% of comparison	REBLA of H P	REBLA of T C	% of comparison	REBLA of H P	REBLA of T C	% of comparison	
1	1.66	1.363	-21.06	1.69	1.418	-26.94	2.97	1.475	-26.1	
2	1.67	1.472	-13.45	1.83	1.583	-15.6	1.97	1.698	-16.02	
3	1.5	0.722	-11.37	1.72	1.023	-12.87	1.93	1.11	-98.11	
4	1.14	0.959	-18.87	1.17	1.023	-14.37	1.22	1.111	-9.811	

Table (4.5) % comparison of reboiler load between thermal coupling and heat matching techniques for system a and configuration 1 at constant pressure of 1 atm.

Ro		0.9			0.925			0.95		
Z	REBLA of H.M.	REBLA of T.C.	% of comparison	REBLA of H.M.	REBLA of T.C.	% of comparison	REBLA of H.M.	REBLA of T.C.	% of comparison	
1	1.66	1.363	-56.31	1.81	1.418	-64.55	1.88	1.475	-65.49	
2	1.69	1.472	-18.76	1.84	1.583	-20.26	1.98	1.698	-20.51	
3	2.97	0.959	-107.4	3.36	1.023	-128.6	2.93	1.111	-98.11	
4	2.97	1.432	-19.92	3.36	1.47	-16.32	2.93	1.479	-11.61	

Table (4.6) % comparison of reboiler load between thermal coupling and heat matching techniques for system a and configuration 2 at constant pressure of 1 atm.

Ro		0.9		0.925			0.95		
	REBLA	REBLA	% of	REBLA	REBLA	% of	REBLA	REBLA	% of
	of H.M.	of T.C.	comparison	of H.M.	of T.C.	comparison	of H.M.	of T.C.	comparison
1	1.66	1.062	-21.79	1.81	1.100	-27.64	1.88	1.136	-27.46
2	1.69	1.423	-14.81	1.84	1.530	-16.23	1.98	1.643	-16.61
3	2.97	0.959	-107.4	3.36	1.023	-128.6	2.93	1.111	-98.11
4	2.97	1.432	-19.92	3.36	1.470	-16.32	2.93	1.479	-11.61



Figure 4.1 The effect of fractional recovery and feed composition on reboiler load for system a configuration 2.



Figure 4.2 The effect of fractional recovery and feed composition on reboiler load for system a configuration 3.

Table (4.6) Effect of change of fractional recovery and feed composition on reboiler load (kcal/hr*10^-6) for system b and configuration 1at constant pressure of 1 atm.

RO Z	0.9	0.925	0.95
1 (0.333,0.333,0.333)	0.774	0.823	0.865
2 (0.8,0.1,0.1)	3.17	2.78	2.35
3 (0.1,0.8,0.1)	0.722	0.799	0.884
4 (0.1,0.1,0.8)	0.190	0.199	0.213

Table (4.7) Effect of change of fractional recovery and feed composition on reboiler load (kcal/hr*10^-6) for system b and configuration 3 at constant pressure of 1 atm.

Z RO	0.9	0.925	0.95
1 (0.333,0.333,0.333)	0.889	0.926	0.950
2 (0.8,0.1,0.1)	3.79	3.13	2.49
3 (0.1,0.8,0.1)	0.732	0.801	0.873
4 (0.1,0.1,0.8)	0.365	0.405	0.452

pre	pressure of 1 atm.										
Ro	0.9				0.925		0.95				
Z	REBLA	REBLA	% of	REBLA	REBLA	% of	REBLA	REBLA	% of		
	of H.P.	of T.C.	comparison	of H.P.	of T.C.	comparison	of H.P.	of T.C.	comparison		
1	0.97	0.774	-25.32	1.02	0.823	-23.94	1.05	0.865	-19.08		

2.78

0.799

0.199

1.35

1.61

0.53

-23.94

43.25

-101.5

-166.3

1.5

1.75

0.57

0.865

2.347

0.884

0.213

-19.08

26.29

-97.96

-167.6

57.07

-114.7

-163.2

2

3

4

1.23

1.55

0.5

3.163

0.722

0.190

Table (4.8) % comparison of reboiler load between thermal coupling and heat pump techniques for system b and configuration 1at constant

Table (4.9) % comparison of reboiler load between thermal coupling and heat pump techniques for system b and configuration 3 at constant pressure of 1 atm.

Ro		0.9		0.925			0.95		
	REBLA	REBLA	% of	REBLA	REBLA	% of	REBLA	REBLA	% of
	of H.P.	of T.C.	comparison	of H.P.	of T.C.	comparison	of H.P.	of T.C.	comparison
1	0.97	0.889	-9.11	1.02	0.926	-10.15	1.05	0.950	-8.42
2	1.23	3.79	64.14	1.35	3.132	49.55	1.5	2.49	30.77
3	1.55	0.732	-111.7	1.61	0.801	-101	1.75	0.873	-100.5
4	0.5	0.365	-36.99	0.53	0.405	-30.86	0.57	0.452	-26.11

Ro		0.9			0.925			0.95		
Z	REBLA	REBLA	% of .	REBLA	REBLA	% of .	REBLA	REBLA	% of .	
	of H.M.	of T.C.	comparison	of H.M.	of T.C.	comparison	of H.M.	of T.C.	comparison	
1	0.99	0.774	-27.91	1.04	0.823	-26.37	1.07	0.865	-23.7	
2	1.2	3.163	56.44	1.4	2.78	42.89	1.6	2.35	25.44	
3	1.56	0.722	-120.2	1.63	0.799	-104	1.77	0.884	-100.2	
4	0.52	0.190	-173.7	0.55	0.199	-176.4	0.58	0.213	-172.3	

Table (4.10) % comparison of reboiler load between thermal coupling and heat matching techniques for system b and configuration 1at constant pressure of 1 atm.

Table (4.11) % comparison of reboiler load between thermal coupling and heat matching techniques for system b and configuration 3 at constant pressure of 1 atm.

Ro		0.9		0.925			0.95		
	REBLA	REBLA	% of .	REBLA	REBLA	% of .	REBLA	REBLA	% of .
\backslash	of H.M.	of T.C.	comparison	of H.M.	of T.C.	comparison	of H.M.	of T.C.	comparison
1	0.99	0.889	-11.36	1.04	0.926	-12.31	1.07	0.950	-12.63
2	1.2	3.79	63.62	1.4	3.13	49.23	1.6	2.35	29.97
3	1.56	0.732	-117.2	1.63	0.801	-103.5	1.77	0.873	-102.7
4	0.52	0.365	-42.47	0.55	0.405	-35.8	0.58	0.452	-28.32



Figure 4.3 The effect of fractional recovery and feed composition change on reboiler load for system b configuration 1.



Figure 4.4 The effect of fractional recovery and feed composition change on reboiler load for system b configuration 3.

Table (4.12) Effect of change of fractional recovery and feed composition on reboiler load (kcal/hr $*10^{-6}$) for system c and configuration 4 at constant pressure of 1 atm.

RO Z	0.9	0.925	0.95
1 (0.25,0.25,0.25,0.25)	14.87	12.79	12.6
2 (0.7,0.1,0.1,0.1)	31.68	22.81	19.03
3 (0.1,0.7,0.1,0.1)	31.45	19.93	17.05
4 (0.1,0.1,0.7,0.1)	30.33	27.59	16.88
5 (0.1,0.1,0.1,0.7)	7.06	8.35	9.81

Table (4.13) Effect of change of fractional recovery and feed composition on reboiler load (kcal/hr $*10^{-6}$) for system c and configuration 5 at constant pressure of 1 atm.

RO Z	0.9	0.925	0.95
1 (0.25,0.25,0.25,0.25)	15.06	12.99	12.8
2 (0.7,0.1,0.1,0.1)	41.39	26.8	20.76
3 (0.1,0.7,0.1,0.1)	31.52	20	17.12
4 (0.1,0.1,0.7,0.1)	30.67	27.95	17.25
5 (0.1,0.1,0.7)	7.31	8.57	10

Table (4.14) comparison of reboiler load between thermal coupling and heat pump for system c configuration 4.

Ro	0.9									
Z	REBLA of H.P.	REBLA of T.C.	% of comparison							
1	6.01	14.87	59.66							
2	10.99	31.68	65.28							
3	8.8	31.45	72.81							
4	8.5	30.33	90.49							
5	4.55	7.06	35.28							

Table (4.15) comparison of reboiler load between thermal coupling and heat pump for system c configuration 5.

Ro	0.9									
Z	REBLA of H.P.	REBLA of T.C.	% of comparison							
1	6.01	15.06	60.17							
2	10.99	41.39	73.42							
3	8.8	31.52	72.87							
4	8.5	30.67	90.52							
5	4.55	7.31	37.76							

Ro	0.9									
Z	REBLA of H.M.	% of comparison								
1	6.76	14.87	54.89							
2	11.85	31.68	62.56							
3	8.76	31.45	72.24							
4	8.65	30.33	90.37							
5	4.5	7.06	36.26							

Table (4.16) comparison of reboiler load between thermal coupling and heat matching for system c configuration 4.

Table (4.17) comparison of reboiler load between thermal coupling and heat matching for system c configuration 5.

Ro	0.9									
Z	REBLA of H.M.	REBLA of T.C.	% of comparison							
1	6.76	15.06	55.48							
2	11.85	41.39	71.35							
3	8.76	31.52	72.30							
4	8.65	30.67	90.41							
5	4.5	7.31	38.44							



Figure 4.5 The effect of fractional recovery and feed composition change on reboiler load for system c configuration 4.



Figure 4.6 The effect of fractional recovery and feed composition change on reboiler load for system c configuration 5.

4.3 Effect of Process Variables on the Percentage Saving in Total Reboiler Load with Thermal Coupling Technique:-

Percentage saving in total reboiler load obtained from the following equation:

% saving in total energy consumption= $\frac{Q_c - Q_t}{Q_c}$ (4.2)

Where

Qc=total reboiler load for conventional system.

Qt=total reboiler load using thermal coupling technique.

The increasing and decreasing in the saving in total reboiler load depends on the reboiler load results of thermal coupling and conventional systems.

4.3.1 Effect of Feed Composition:-

The results of percentage saving in total reboiler load were listed in tables (4.18) and (4.19) for feed system a, tables (4.24) and (4.25) for feed system b and tables (4.30) and (4.31) for feed system c.

These results were presented in figures (4.10) to (4.12) for feed system a, figures (4.13) to (4.15) for feed system b and figures (4.16) to (4.18) for feed system c.

4.3.2 Effect of Fractional Recoveries:

The results of percentage saving in total reboiler load were listed in tables (4.18) and (4.19) for feed system a, tables (4.24) and (4.25) for feed system b and tables (4.30) and (4.31) for feed system c.

The results were presented in figures (4.7) and (4.8) for feed system a, figures (4.9) and (4.10) for feed system b and figures (4.11) and (4.12) for feed system c.

4.3.3 Effect of Configurations:-

The results of percentage saving in total reboiler load were listed in tables (4.18) and (4.19) for feed system a, tables (4.24) and (4.25) for feed system b and tables (4.30) and (4.31) for feed system c.

The results were presented in figures (4.7) and (4.8) for feed system a, figures (4.9) and (4.10) for feed system b and figures (4.11) and (4.12) for feed system c.

4.3.4 Comparison with Previous Works:-

The results of the present work using thermal coupling techniques are compared with the previous work on heat pump and energy matching for non-ideal systems.

The tables of these results are (4.20) to (4.21) for feed system a show that thermal coupling technique is the more efficient than heat pump except at feed composition 2 where heat pump gives better results. Tables (4.22) to (4.23) show that thermal coupling is more efficient than heat matching at all cases.

This efficiency is because of the increasing of percentage saving in total reboiler load of thermal coupling than others.

For feed system b, thermal coupling technique is more efficient than heat pump and heat matching in all conditions tables (4.26) to (4.29).

For feed system c, tables (4.32) to (4.33) show that heat pump and heat matching give best results.

Table (4.18) Effect of change of fractional recovery and feed composition on % saving in total reboiler load for system a and configuration 1 at constant

pressure of 1 atm.

RO Z	0.9	0.925	0.95
1 (0.333,0.333,0.333)	42.965	42.044	41.534
2 (0.8,0.1,0.1)	40.109	38.530	37.050
3 (0.1,0.8,0.1)	64.607	60.054	54.926
4 (0.1,0.1,0.8)	42.11	44.20	46.93

Table (4.19) Effect of change of fractional recovery and feed composition on % saving in total reboiler load for system a and configuration 2 at constant pressure of 1 atm.

RO Z	0.9	0.925	0.95
1 (0.333,0.333,0.333)	26.799	25.290	24.087
2 (0.8,0.1,0.1)	38.047	36.400	34.943
3 (0.1,0.8,0.1)	59.74	55.87	51.88
4 (0.1,0.1,0.8)	-26.184	-31.830	-40.384

Table (4.20) % comparison of percentage saving total reboiler load between thermal coupling and heat pumps techniques for system a and configuration 1 at constant pressure of 1 atm.

Ro		0.9			0.925	5	0.95			
Z	%S.R.I of H.P.	0 %S.R.L of T.C.	% of comparison	%S.R.L of H.P.	% S.R.L of T.C.	% of comparison	%S.R.L of H.P.	% S.R.L of T.C.	% of comparison	
1	33.69	42.965	21.59	32.36	42.044	23.03	30.36	41.534	26.90	
2	53.02	40.109	-32.19	47.85	38.530	-24.19	45.69	37.050	-23.32	
3	25.74	64.607	60.16	25.36	60.054	57.77	23.7	54.926	56.85	
4	25.48	42.11	38.27	25.37	44.20	42.63	23.9	46.93	49.09	

Table (4.21) % comparison of percentage saving total reboiler load between thermal coupling and heat pumps techniques for system a and configuration 2 at constant pressure of 1 atm.

Ro		0.9			0.92	5		0.95			
Z	%S.R.I of H.P.	L %S.R.L of T.C.	% of comparisor	%S.R.I of H.P.	S.R.L of T.C.	% of comparison	%S.R.L of H.P.	% S.R.L of T.C.	% of comparison		
1	33.69	42.965	21.59	32.36	42.044	23.03	30.36	41.534	26.90		
2	53.02	40.109	-32.19	47.85	38.530	-24.19	45.69	37.050	-23.32		
3	25.75	59.74	56.91	25.38	55.87	54.61	23.78	51.87	54.32		
4	25.94	-26.18	199.2	25.36	-31.83	179.6	23.89	-40.38	159.1		

Table (4.22) % comparison of percentage saving total reboiler load between thermal coupling and heat matching techniques for system a and configuration 1 at constant pressure of 1 atm.

-													
Rc)		0.9				0.92	25		0.95			
Z	%S.R.	L. %	6S.R.L	% of	%S.R	l.L	%S.R.I	2 % of	%S.R.I	S.R.L	% of		
	of H.M	1. of	of T.C.	comparis	on of H.	М.	of T.C.	compariso	on of	of T.C.	comparison		
	N								H.M.				
1	8.10	42.9	65	81.15	7.19	42	2.044	82.89	7.0	41.534	83.15		
2	6.1	40.1	09	84.79	5.9	38	3.530	84.69	5.8	37.050	84.35		
3	5.8	64.6	07	91.02	4.4	60).054	92.67	5.6	54.926	89.81		
4	11.97	42.1	11	71.74	12.15	4	4.20	72.63	10.6	46.93	77.41		

Table (4.23) % comparison of percentage saving total reboiler load between thermal coupling and heat matching techniques for system a and configuration 2 at constant pressure of 1 atm.

Rc)	0.9					0.925					0.95		
Ż	%S. of H	R.L. .M.	%S.R.L of T.C.	% of compari	son	%S.R.L of H.M.		%S.R. of T.C	L L	% of comparison		%S.R.I of H.M.	2 %S.R.L of T.C.	% of comparison
1	8.10	42.9	965	81.15	7.1	19 42.		.044	82.89			7.0	41.534	83.15
2	6.1	40.1	109	84.79	5.	.9 38		.530	84.69			5.8	37.050	84.35
3	5.8	59.	.74	90.29	4.2	25	55	5.87	(92.13		5.5	51.879	89.21
4	11.9	-26	.18 1	45.45	12	.1	-3	1.83	1	38.01		10.6	-40.38	126.25



Figure 4.6 The effect of fractional recovery and feed composition on % saving in total reboiler load for system a configuration 1.



Figure 4.7 The effect of fractional recovery and feed composition on % saving in total reboiler load for system a configuration 2.

Table (4.24) Effect of change of fractional recovery and feed composition on % saving in total reboiler load for system b and configuration 1 at constant pressure of 1 atm.

RO-Z	0.9	0.925	0.95
1 (0.333,0.333,0.333)	92.19	92.07	91.99
2 (0.8,0.1,0.1)	82.47	83.31	84.66
3 (0.1,0.8,0.1)	95.3	95.15	94.95
4 (0.1,0.1,0.8)	96.14	96.21	96.19

Table (4.25) Effect of change of fractional recovery and feed composition on % saving in total reboiler load for system b and configuration 3 at constant pressure of 1 atm.

RO-Z	0.9	0.925	0.95
1 (0.333,0.333,0.333)	91.03	91.08	91.20
2 (0.8,0.1,0.1)	79.01	81.23	83.67
3 (0.1,0.8,0.1)	95.24	95.14	95.01
4 (0.1,0.1,0.8)	92.58	92.29	91.92

Table (4.26) % comparison of percentage saving total reboiler load between thermal coupling and heat pumps techniques for system b and configuration 1 at constant pressure of 1 atm.

Ro)	0.9			0.925			0.95		
Z`	\ %S.R	.L %S.R.	L % of	%S.R.	L % S.R.	L % of	%S.R.L	% S.R.L	% of	
	of H.	P. of T.C	comparis	on of H.F	P. of T.C	. compariso	on of H.P.	of T.C.	comparison	
1	24.56	92.19	73.36	24.02	92.07	73.91	24.00	91.99	73.91	
2	18.5	82.47	77.7	16.95	83.31	79.77	16.33	84.66	80.68	
3	53.69	95.3	43.66	45.58	95.15	52.09	45.51	94.95	52.07	
4	35.04	96.14	63.55	34.10	96.21	64.56	34.00	96.19	64.65	

Table (4.27) % comparison of percentage saving total reboiler load between thermal coupling and heat pumps techniques for system b and configuration 3 at constant pressure of 1 atm.

Ra)		0.	9				0.92	25				0.95		
Z	\ %S.F	R.L	%S.R.	L % of		%S.R.	.L	% S.R.	L	% of		%S.R.L	% S.R.L	% of	
	of H.	P.	of T.C	. compar	ison	of H.F	<u>.</u>	of T.C.		compariso	on	of H.P.	of T.C.	compari	ison
1	24.56	91	1.03	73.02	2	4.02	9	1.08		73.63	4	24.00	91.20	73.6	58
2	18.5	79	9.01	76.72	1	6.95	8	1.23		79.26		16.33	83.67	80.4	5
3	53.69	95	5.24	43.63	4	5.58	9	5.14		52.09	4	45.51	95.01	52.	1
4	35.04	92	2.58	62.15	3	4.10	9	2.29		63.05		34.00	91.92	63.0)1

Table (4.28) % comparison of percentage saving total reboiler load between thermal coupling and heat matching techniques for system b and configuration 1 at constant pressure of 1 atm.

Ro)	0.9			0.92	25		0.95	
Z	%S.F of H.	R.L. %S.R M. of T.C	.L % of C. comparis	%S.R. on of H.M	L %S.R. A. of T.C	L % of . comparise	%S.R.L on of H.M.	%S.R.L of T.C.	% of comparison
1	9.7	92.19	89.478	9.3	92.07	89.899	9.8	91.99	90.216
2	5.06	82.47	93.82	5.59	83.31	93.38	6.53	83.67	92.20
3	6.8	95.3	93.704	5.6	95.15	94.115	5.3	94.95	94.418
4	19.8	96.14	79.405	17.9	96.21	81.395	17.4	96.19	81.91

Table (4.29) % comparison of percentage saving total reboiler load between thermal coupling and heat matching techniques for system b and configuration 3 at constant pressure of 1 atm.

Ro		0.9			0.92	25	5 0.95		
Z	%S.I	R.L. %S.R	.L % of	%S.R.	L %S.R.I	L % of	%S.R.L	%S.R.L	% of
	∖ of H	M. of T.C	 comparise 	on of H.N	<i>I</i> . of T.C.	compariso	on of H.M.	of T.C.	comparison
1	9.7	91.03	89.34	9.3	91.08	89.79	9.8	91.20	90.13
2	5.09	79.01	93.55	5.59	81.23	93.11	6.53	83.67	92.11
3	6.8	95.24	93.7	5.6	95.14	94.11	5.3	95.01	94.42
4	19.8	92.58	78.61	17.9	92.29	80.61	17.4	91.92	81.07



Figure 4.8 The effect of fractional recovery and feed composition on % saving in total reboiler load for system b configuration 1.



Figure 4.9 The effect of fractional recovery and feed composition on % saving in total reboiler load for system b configuration 3.

Table (4.30) Effect of change of fractional recovery and feed composition on % saving in reboiler load for system c and configuration 2 at constant pressure of 1 atm.

RO Z	0.9	0.925	0.95
1 (0.25,0.25,0.25,0.25,0.25)	8.88	9.93	9.68
2 (0.7,0.1,0.1,0.1)	6.74	32.03	15.42
3 (0.1,0.7,0.1,0.1)	5.49	8.54	9.45
4 (0.1,0.1,0.7,0.1)	1.15	3.42	5.33
5 (0.1,0.1,0.1,0.7)	6.6138	5.8625	5.6731

Table (4.31) Effect of change of fractional recovery and feed composition on % saving in reboiler load for system c and configuration 3 at constant pressure of 1 atm.

RO Z	0.9	0.925	0.95
1 (0.25,0.25,0.25,0.25,0.25)	7.72	8.52	8.24
2 (0.7,0.1,0.1,0.1)	30.77	20.14	7.73
3 (0.1,0.7,0.1,0.1)	5.29	8.22	9.08
4 (0.1,0.1,0.7,0.1)	0.78	2.16	3.25
5 (0.1,0.1,0.1,0.7)	3.31	3.38	3.85

Ro		0.9					
Z	% S.R.L. of H.P.	% S.R.L of T.C.	% of comparison				
1	9.89	8.88	-11.39				
2	9.68	6.74	-43.62				
3	6.91	5.49	-26.43				
4	1.33	1.15	-15.81				
5	11.69	6.6138	-7.77				

Table (4.33) comparison of % saving in total reboiler between thermal coupling and heat pump for system c configuration 4.

Table (4.34) comparison of % saving in total reboiler between thermal coupling and heat pump for system c configuration 5.

Ro		0.9	
Z	% S.R.L. of H.P.	% S.R.L of T.C.	% of comparison
1	9.89	7.72	-28.12
2	9.68	30.77	68.54
3	6.91	5.29	-30.62
4	1.33	0.78	-70.51
5	58	3.31	-1654

Table (4.35) comparison of % saving in total reboiler between thermal coupling and heat matching for system c configuration 4.

Ro		0.9	
Z	% S.R.L. of H.M.	% S.R.L of T.C.	% of comparison
1	13.06	8.88	-47.09
2	8.44	6.74	-25.26
3	6.73	5.49	-22.45
4	2.29	1.15	-99.66
5	7.2	6.61	-8.86

Table (4.36) comparison of % saving in total reboiler between thermal coupling and heat matching for system c configuration 5.

Ro		0.9	
Z	% S.R.L. of H.M.	% S.R.L of T.C.	% of comparison
1	13.06	7.72	-69.17
2	8.44	30.77	75.57
3	6.73	5.29	-27.22
4	2.29	0.78	-196.9
5	7.2	3.31	-117



Figure (4.10) The effect of fractional recovery and feed composition on % saving in total reboiler load for system c configuration 4.



Figure (4.11) The effect of fractional recovery and feed composition on % saving in total reboiler load for system c configuration 5.
4.4 Percentage Saving in Annual Cost:-

The total annual cost increases with the increase of the total reboiler load, the total annual cost is proportional to the total reboiler load. This proportionality is due to the cost of steam which constituting the major portion of the total annual cost but the percentage saving in total annual cost is not proportional with reboiler load which may increase or decrease depending on the annual cost of the conventional systems according to the equation of percentage saving in annual cost is:-Percentage saving in annual cost=((SANNc-SANNt)/SANNc)*100(4.3)

Where

SANNc=annual cost of conventional system.

SANNt=annual cost using thermal coupling.

The increasing and decreasing in the saving in total reboiler load depends on the reboiler load results of thermal coupling and conventional systems.

The negative sign appears in the results means that there is no saving in total annual cost.

4.5 Effect of Process Variables on the Percentage Saving in Total Annual Cost With Thermal Coupling Technique:-4.5.1 Effect of Feed Composition:-

The results are tabulated in tables (4.37) to (4.38) for feed system a, tables (4.41) to (4.42) for feed system b and tables (4.43) to (4.44) for feed system c, and shown in figures (4.12) to (4.13) for feed system a, figures (4.14) to (4.15) for feed system b and figures (4.16) to (4.17) for feed system c.

4.5.2 Effect of Fractional Recoveries:-

The results are tabulated in tables (4.37) to (4.38) for feed system a, tables (4.41) to (4.42) for feed system b and tables (4.43) to (4.44) for feed system c, and shown in figures (4.12) to (4.13) for feed system a, figures (4.14) to (4.15) for feed system b and figures (4.16) to (4.17) for feed system c.

4.5.3 Effect of Configurations:-

The results are tabulated in tables (4.37) to (4.38) for feed system a, tables (4.41) to (4.42) for feed system b and tables (4.43) to (4.44) for feed system c, and shown in figures (4.12) to (4.13) for feed system a, figures (4.14) to (4.15) for feed system b and figures (4.16) to (4.17) for feed system c.

4.5.4 Comparison with Previous Works:-

The results of comparison were tabulated in tables (4.40) to (4.41) for feed system a, tables (4.43) to (4.44) for feed system b and tables (4.47) to (4.48) for feed system c.

For feed system a, the results showed that thermal coupling is more efficient than heat pump technique.

For feed systems b and c, all the negative sign appeared in the results means that heat pump is more efficient than thermal coupling.

Table (4.37) Effect of change of fractional recovery and feed composition on % saving in annual cost for system a and configuration 1 at constant pressure of 1 atm.

RO Z	0.9	0.925	0.95
1	36.724	36.204	35.725
2	34.523	33.171	31.911
3	55.874	51.936	47.517
4	36.08	37.94	40.27

Table (4.38) Effect of change of fractional recovery and feed composition on % saving in annual cost for system a and configuration 2 at constant pressure of 1 atm.

RO Z	0.9	0.9 0.925	
1	20.997	19.857	18.565
2	36.213	34.874	33.594
3	53.96	48.99	43.59
4	-32.505	-37.646	-45.611

Table (4.40) % comparison of percentage saving in annual cost between thermal coupling and heat pump techniques for system a and configuration 1 at constant pressure of 1 atm.

Ra)	0.	9		0.92	.5		0.95	
Z`	%S.A of H.	A.C. %S.A. P. of T.C	C. % of . compariso	%S.A. on of H.P	C. %S.A.C . of T.C.	C. % of comparison	%S.A.C. of H.P.	%S.A.C. of T.C.	% of comparison
1	62.48	36.724	41.22	58.01	36.204	37.59	59.25	35.725	39.70
2	57.46	34.523	39.92	53.12	33.171	37.55	48.63	31.911	34.38
3	72.15	55.874	22.56	71.46	51.936	27.32	69.85	47.517	31.97
4	25.91	36.08	28.21	29.7	37.94	21.71	30.5	40.27	24.26

Table (4.41) % comparison of percentage saving in annual cost between thermal coupling and heat pump techniques for system a and configuration 2 at constant pressure of 1 atm.

Ro	D	0.9			0.925			0.95		
	%S.A of H.	A.C. %S.A. P. of T.C	C. % of . compariso	%S.A.C on of H.P.	C. %S.A.C. of T.C.	. % of comparison	%S.A.C. of H.P.	%S.A.C. of T.C.	% of comparison	
1	62.48	20.997	66.39	58.01	19.857	37.59	59.25	18.565	39.70	
2	57.46	36.213	36.98	53.12	34.874	37.55	48.63	33.594	34.38	
3	40.36	53.96	25.21	33.58	48.99	31.44	27.20	43.59	37.60	
4	50.26	-32.50	164.67	48.46	-37.65	177.68	45.23	-45.611	200.84	



Figure 4.12 The effect of fractional recovery and feed composition on % saving in total annual cost for system a configuration 2.



Figure 4.13 The effect of fractional recovery and feed composition on % saving in total annual cost for system a configuration 3.

Table (4.42) Effect of change of fractional recovery and feed composition on % saving in annual cost for system b and configuration 1 at constant pressure of 1 atm.

RO Z	0.9	0.925	0.95
1	14.93	13.88	12.99
2	-78.89	-70.93	-58.04
3	44.78	43.55	41.83
4	54.15	54.89	54.47

Table (4.43) Effect of change of fractional recovery and feed composition on % saving in annual cost for system b and configuration 3 at constant pressure of 1 atm.

RO Z	0.9	0.925	0.95
1	4.87	5.38	6.57
2	95.61	88.59	64.46
3	-391.38	42.86	41.39
4	22.31	19.59	16.13

Table (4.44) % comparison of percentage saving in annual cost between thermal coupling and heat pump techniques for system b and configuration 1 at constant pressure of 1 atm.

Ra)	0.9)		0.925			0.95	
Z	%S.A	A.C. %S.A.C	C. % of	%S.A.C.	%S.A.C.	% of	%S.A.C.	%S.A.C.	% of
1	56.26		comparison	54.02	01 1.C.	comparison	50.49	011.0.	-
1	30.30	14.93	-277.5	54.25	13.88	-290.7	50.48	12.99	288.6
2	65.84	78.89	16.54	58.79	70.93	16.85	47.59	58.04	17.99
3	48.23	44.78	-7.70	46.25	43.55	-6.2	41.28	41.83	1.315
4	40.14	54.15	25.87	37.85	54.89	31.04	36.25	54.47	33.45

Table (4.45) % comparison of percentage saving in annual cost between thermal coupling and heat pump techniques for system b and configuration 3 at constant pressure of 1 atm.

Ra)	0.9)		0.925			0.95		
Z`	%S.A of H.	A.C. %S.A.C P. of T.C.	C. % of comparison	%S.A.C. of H.P.	. %S.A.C. of T.C.	% of comparison	%S.A.C. of H.P.	%S.A.C. of T.C.	% o com	f parison
1	56.36	4.87	-1057	54.23	5.38	-908	50.48	6.	57	- 668.3
2	65.84	95.61	31.14	58.97	88.59	33.43	47.59	64	.46	26.17
3	48.23	-391.38	112.32	46.25	42.86	-7.91	41.28	41	.39	0.27
4	40.14	22.31	-79.92	37.85	19.59	-93.21	36.25	16	.13	- 124.7



Figure 4.14 The effect of fractional recovery and feed composition on % saving in total annual cost for system b configuration 1.



Figure 4.15 The effect of fractional recovery and feed composition on % saving in total annual cost for system b configuration 3.

Table (4.46) Effect of change of fractional recovery and feed composition on % saving in annual cost for system c and configuration 4 at constant pressure of 1 atm.

RO Z	0.9	0.925	0.95
1	7.77	8.72	8.51
2	76.59	31.52	14.66
3	4.76	7.43	8.21
4	1.00	3.01	4.68
5	5.70	5.37	4.89

Table (4.47) Effect of change of fractional recovery and feed composition on % saving in annual cost for system c and configuration 5 at constant pressure of 1 atm.

RO Z	0.9	0.925	0.95
1	7.46	8.31	7.93
2	69.55	20.03	7.54
3	5.15	8.02	8.77
4	0.75	2.13	3.18
5	2.89	3.39	3.64

Table (4.48) comparison of % saving in annual cost between thermal coupling and heat pump for system c configuration 4.

Ro	0.9							
Z	% S.A.C. of H.P.	% S.A.C. of T.C.	% of comparison					
1	14.69	7.77	-89.12					
2	61.96	76.59	19.06					
3	5.32	4.76	-11.67					
4	1.5	1.00	-49.98					
5	5.87	5.70	-95.4					

Table (4.49) comparison of % saving in annual cost between thermal coupling and heat pump for system c configuration 5.

Ro		0.9							
Z	% S.A.C. of H.P.	% S.A.C. of T.C.	% of comparison						
1	14.69	7.46	-96.91						
2	61.96	69.55	10.91						
3	5.32	5.15	-3.30						
4	1.5	0.75	-46.98						
5	5.87	2.89	-99.99						



Figure 4.16 The effect of fractional recovery and feed composition on % saving in total annual cost for system c configuration 2.



Figure 4.17 The effect of fractional recovery and feed composition on % saving in total annual cost for system c configuration 3.

Chapter Five

Conclusions and suggestions

5.1 Conclusions:-

1. Optimum (minimum) reboiler load can be obtained when using system b at feed composition 4 [0.1,0.1,0.8] and fractional recovery of 0.9 and using configuration 1 of $0.19*10^{6}$ kcal/hr.

2. It is favoured to separate the component with high portion in the feed as a bottom product or side stream except the lightest one.

3. Separation of the more volatile components take place first leaving the least volatile component till the end in the configuration, if the difference in boiling points for all components in the feed are nearly the same, or if the two components are close in boiling point and are more volatile than the rest.

4. It is economical to separate the side stream in the configuration as a liquid than it as a vapor in the same sequence of the columns, due to the reduction in reboiler load in than former case.

5. On increasing the fractional recovery the total annual cost increasing for all cases, because the distillate increases increasing the reboiler load for all the same columns.

5.2 Suggestions and Future Work:-

1. It is suggested to extend this work to a variable pressure for each column with same configurations.

2. Applying thermal coupling system on the separation of systems more complicated mixtures (azeotropic).

3. The prediction of vapor-liquid equilibrium can be extended to use other models rather than Wilson model such as UNIFAC and UNIQUAC. In addition, the calculation of fugacity coefficient can be added in order to measure the deviation in vapor phase.

4. The same work may be done using exact equilibrium data.

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Appendix A

A.1 Mathematical models for short – cut calculations:

1. Minimum reflux ratio:

Underwood has determined minimum reflux ratio ^[50] relations:

$$\sum_{i=1}^{N} \frac{\alpha_i x_{i,d}}{\alpha_i - \phi} = R_m + 1 \qquad \dots (A.1.1)$$

For ternary mixture

$$\frac{\alpha_A x_{A,d}}{\alpha_A - \phi} + \frac{\alpha_B x_{B,d}}{\alpha_B - \phi} + \frac{\alpha_C x_{C,d}}{\alpha_C - \phi} = R_m + 1 \qquad \dots (A.1.2)$$

For quaternary mixture

$$\frac{\alpha_A x_{A,d}}{\alpha_A - \phi} + \frac{\alpha_B x_{B,d}}{\alpha_B - \phi} + \frac{\alpha_C x_{C,d}}{\alpha_C - \phi} + \frac{\alpha_D x_{D,d}}{\alpha_D - \phi} = R_m + 1 \qquad \dots (A.1.3)$$

 ϕ was calculated from the relation :

$$\sum_{i=1}^{N} \left(\frac{\alpha_{i} x_{if}}{\alpha_{i} - \phi} \right) = 1 - q \qquad \dots (A.1.4)$$

And $\alpha_{LK} \leq \phi \leq \alpha_{HK}$

For ternary component mixture:

$$\frac{\alpha_A x_{A,f}}{\alpha_A - \phi} + \frac{\alpha_B x_{B,f}}{\alpha_B - \phi} + \frac{\alpha_C x_{C,f}}{\alpha_C - \phi} = 1 - q \qquad \dots (A.1.5)$$

For quaternary component mixture:

$$\frac{\alpha_A x_{A,f}}{\alpha_A - \phi} + \frac{\alpha_B x_{B,f}}{\alpha_B - \phi} + \frac{\alpha_C x_{C,f}}{\alpha_C - \phi} + \frac{\alpha_D x_{D,f}}{\alpha_D - \phi} = 1 - q \qquad \dots (A.1.6)$$

The value of ϕ is calculated from previous equations by trial and error, and then R_m is calculated from equation (A.1.1).

Liquid flow rate = L = R * D ... (A.1.7)

Vapor flow rate = V = L + D = (D (R + 1)) ... (A.1.8)

Theoretical number of plates

Gilliand ^[29], Van Winkle and Todd ^[31] relationships were used to calculate the theoretical number of plates:

a. for
$$(R - R_m)/(R + 1) < 0.125$$

$$\frac{N - N_m}{N + 1} = 0.5039 + 0.5068 \left(\frac{R - R_m}{R + 1}\right) - 0.0908 \log \left(\frac{R - R_m}{R + 1}\right)$$
... (A.1.9)
b. for $(R - R_m)/(R + 1) > 0.125$

$$\frac{N - N_m}{N + 1} = 0.6257 - 0.9868 \left(\frac{R - R_m}{R + 1}\right) + 0.516 \left(\frac{R - R_m}{R + 1}\right)^2 - 0.1738 \left(\frac{R - R_m}{R + 1}\right)^3$$
... (A.1.10)

Number of plates above and below feed

Feed plate location was found by using Underwood ^[50], Robinson and Gilliand ^[54] correlations:

$$\frac{x_{D1}}{x_{D2}} = \left(\frac{\Phi_1}{\Phi_2}\right) N_T \frac{x_{F1}}{x_{F2}} \qquad \dots (A.1.11)$$

 N_T is the number of plates above the feed.

$$x_{D1} = \sum_{i=1}^{N} \frac{\alpha_{i} x_{i,d}}{\alpha_{i} - \Phi_{1}} \qquad \dots (A.1.12)$$

$$x_{D2} = \sum_{i=1}^{N} \frac{\alpha_{i} x_{i,d}}{\alpha_{i} - \Phi_{2}} \qquad \dots (A.1.13)$$

 $_{\Phi_1}$ and $_{\Phi_2}$ were calculated by trial and error from the following equation:

$$\sum_{i=1}^{N} \frac{\alpha_i x_{i,d}}{\alpha_i - \Phi} \cdot \frac{D}{V} = 1.0 \qquad \dots (A.1.14)$$

$$x_{F1} = \sum_{i=1}^{N} \frac{\alpha_i x_{i,F}}{\alpha_i - \Phi_1} \qquad \dots (A.1.15)$$
$$x_{F2} = \sum_{i=1}^{N} \frac{\alpha_i x_{i,F}}{\alpha_i - \Phi_2} \qquad \dots (A.1.16)$$

Condenser and Reboiler load

$$Q_{c} = V \left(H_{V} - h_{L} - h_{D} \right) \qquad \dots (A.1.17)$$

$$Q_{R} = D h_{D} + S_{1} h_{S1} + W h_{W} - Q_{c} - F_{1} h_{F1} - F_{2} h_{F2} \qquad \dots (A.1.18)$$

A.2 Mathematical models for cost calculation:

Equipment cost, operating cost and total annual cost were calculated depend on the equations of Henry ^[20] method.

The assumptions made for cost estimation was:

- 1. Tray efficiency was assumed to be 60%.
- 2. Tray spacing was (1.5 ft) 0.457 m.
- 3. Tray area is 85% of the column cross sectional area.
- 4. All the equipments are assumed to be carbon steel.
- 5. The equipment operation time is whole of the year.
- 6. Economical service life is 10 years.

7. The steam used in the reboiler is saturated steam at 250 psia.

8. The rise in temperature of the cooling water in condensers is $(20F^{\circ})$, $11.1C^{\circ}$.

9. The space from the top of the column to first plate is 1.83 m (6 ft) and from the final plate to the bottom is (12 ft) 3.66 m.

A.2.1 Equipment cost

1. Cost of distillation column

 V_T = dimension parameter of the column

$$V_T = DC * HT \qquad \dots (A.2.1.1)$$

 $C_A = \text{cross sectional area of the column} = \pi \cdot Dc^2/4 \qquad \dots (A.2.1.2)$ And the tray area = $T_A = 0.85 * C_A \qquad \dots (A.2.1.3)$

Cost of the column
$$= C_T = C_1 \cdot \left(\frac{V_T}{100}\right)^{E_1} + C_2 \cdot \left(\frac{T_A}{100}\right)^{E_2} \cdot N$$
 ... (A.2.1.4)

Where

 $C_1 = \text{cost}$ of distillation column with dimension parameter of 100 = ID900000

 $C_2 = \text{cost of tray within } (9.29m^2)(100 \text{ ft}^2) = \text{ID } 202500.$

 E_1 = slope of the column diameter parameter versus cost curve.

 E_2 = slope of the tray area versus cost curve.

N = factor used to calculate the height of the column.

2. Cost of condenser

$$A_c$$
 = area of condenser = $Q_c/(U_c * T_{LM})$... (A.2.1.2)

Where, U_c is the overall heat transfer coefficient and is taken as $567.8W/m^2 \cdot K^{\circ} (100Btu/hr ft^2 \cdot f^{\circ})$.

 T_{LM} is the logmean temperature difference, and calculated by:

$$T_{LM} = (T_t - 80) - (T_t - 100) / [(T_t - 80) / (T_t - 100)] \text{ (If } T_t > 100 F^\circ) \dots \text{ (A.2.1.3)}$$
$$T_{LM} = (T_t - 40) - (T_t - 45) / [(T_t - 40) / (T_t - 45)] \text{ (If } T_t < 100 F^\circ) \dots \text{ (A.2.1.4)}$$

$$C_c = \text{cost of condenser} = C_3 \cdot \left(\frac{A_C}{1000}\right)^{E_3} \dots (A.2.1.5)$$

 $C_3 = \text{cost of heat exchanger with surface area of } 92.9m^2$

 E_3 = slope of heat transfer area versus cost curve.

If the surface area of the condenser is greater than $92.9m^2$ the area was divided by two and the cost was calculated for two units of equal size.

3. Cost of reboiler

 A_R = surface area of reboiler = $Q_R/(U_R * T_R)$... (A.2.1.6)

 U_R is the overall heat transfer coefficient for steam and was taken at 710 $W/m^2 K^{\circ}(125 Btu/hr ft^2 F^{\circ})$.

 T_R = is the logarithm mean temperature difference T_R = 401 – T_b ... (A.4.1.10)

$$C_R = \text{cost of reboiler} = C_3 \cdot \left(\frac{A_R}{1000}\right)^{E_3} \dots (A.2.1.7)$$

Equipment cost= $C_{EQ} = C_T + C_C + C_R$ (A.2.1.8)

A.2.2 annual operating cost

 $C_s = \text{cost of steam} = 24 * 365 * C_5 * Q_R * 3.9/1000 * H_{VAP} \qquad \dots (A.2.2.1)$

Where C_s is the cost of 453.6 Kg (1000 lb) of steam =ID 4059.15.

 H_{VAP} is the latent heat of steam =825.0 Btu / lb.

 $C_W = \text{cost of cooling water} = (24 * 365 * C_4 * Q_c * 3.79)/(1000 * 20 * 8.33)$

... (A.2.2.2)

Where C_4 is the cost of 4546 liter (1000 gallon) of cooling water = ID 124.95

Working capital = 18% of equipment cost.

Taxes = 4% of equipment cost.

Insurance = 1% of total equipment cost.

Maintenance = 5% of total equipment cost, the total equal 28% of the total equipment cost.

A.2.3 Total annual cost:

Total annual cost = depreciation + annual operating cost

Total annual cost= CAN = (equipment cost / service life) +annual operating

<u>Appendix B</u>

B.1 Short-cut method program:-

clear; clc: % SHORTCUT CALCULATION PROGRAM RELZ(10)=0; RELY(10)=0; RELX(10)=0; RELX1(10)=0; RELR(10)=0; DL1(10)=0;DL2(10)=0;DL3(10)=0;DL4(10)=0;DL(10)=0;WM(10)=0;WM1(10)=0;COMP(1:10)=0;COMP(1:3)=0;COST(1:50)=0;COST(1:25);KU(25)=0;VM(10)=0;VM1(10)=0:Z(10)=0; X(10)=0; Y(10)=0; R(10)=0; RO(10)=0; ZF(10)=0; BF(10)=0; O3(10)=0; A(10)=0; B(10)=0; C(10)=0; Q(10)=0; VK(10)=0; SK(10)=0;AF(10)=0;Q2(10)=0;U(10)=0;D(10)=0; E(10)=0; F(10)=0; A1(10)=0; A2(10)=0; B1(10)=0; B2(10)=0; C1(10)=0; C2(10)=0; D1(10)=0; D2(10)=0;RELV(10)=0; RELS(10)=0; RELZF(10)=0;PH(10)=0; SUMVAP(10)=0; YY(10)=0; XX(10)=0; SPEC(1:25)=0; SPEC(1:10)=0; PHY1(10)=0;PHY2(10)=0;AY(10)=0;AX(10)=0;XF(10)=0;WY(10)=0;WX(10)=0; XFD(10)=0; XF1(10)=0; XW(10)=0; XW1(10)=0; XD(10)=0; XD1(10)=0;SUMPH1(10)=0;SUMPH2(10)=0;PH1(10)=0;PH2(10)=0; WF(10)=0;WFX(10)=0;W(10)=0;RELW(10)=0;PHY3(10)=0; CV1(3)=0; CV2(3)=0; CV3(3)=0; ETA(6)=0; *** NCOL=2 N=3NOCO=1 KCOST=1;ICOMP=1;GR=0.25; PRET=[1,1]; for MJ=1:NOCO Methanol=1; Ethanol=2: Water=3: RST=[0.99,0.99];NR=1;ROT=[0.9,0.9]; for JJ=1:NR RO(JJ)=0.9; end D(1:N)=[11.67470, 11.28410,11.58040]: E(1:N)=[-3460.90750, -3261.37628, -3754.17459]; F(1:N)=[231.32812, 210.31250, 224.27734]; DEF=[D; E; F]; DEF; CV1(1:N)=[64.51000, 53.86600, 22.88000]; CV2(1:N)=[-0.19720, -0.03111, -0.03642]; CV3(1:N)=[0.00039, 0.00016, 0.00007];

```
CV = [CV1; CV2; CV3]; CV;
 A1(1:N)=[0.00002, -0.19696, 0.00000];
 B1(1:N)=[18.09900, 26.35200, 18.00000];
 C1(1:N) = [0.00001, -0.00011, 0];
D1(1:N)=[0.000, 0.000, 0.000];
 ABCD1=[A1; B1; C1;D1]; ABCD1;
 A2(1:N)=[8464.59998, 11312.90002, 10749.90002];
 B2(1:N)=[3.36319, -1.59611, 7.85602];
 C2(1:N)=[0.10760, 0.02433, -0.00064];
 D2(1:N) = [0.000, 0.000, 0.000];
 ABCD2=[A2; B2; C2;D2]; ABCD2;
  if (KCOST~=0)
   WM(1:N)=[32,46,18];
   FF=0.7;SF=0.1;FC1=0.46;FC2=0.015;FC5=0.60809;FC6=0.06182;
   UC=100;UR=125;C1=600;C2=135;C3=1400;C4=0.0833;C5=2.7061;
   E1=0.5;E2=0.5;E3=0.5;
  end
for IJ=1:ICOMP
 for JJ=1:NR
 FD=100; TF=77; GC=1.987;
 Z(1:N)=[0.333, 0.333, 0.333];
NA=(N^{*}(N-1));
ETA(1:NA)=[-175, 280, 216, 435, 442, 901];
NLT=[1,1]; NHT=[2,2]; NL2T=[2,0]; NH2T=[3,0];
ICOLT=[2,3];NOSST=[1,0];NOLSST=[0,0];NOVSST=[1,0];
NSST=[1,0];TCFT=[1,1];LOSST=[2,0];NOFDT=[1,1];
for IL=1:NCOL
  NOSS=NOSST(IL)
  NOLSS=NOLSST(IL)
  NOVSS=NOVSST(IL)
  if (NOSS \sim = 0)
    if NOSS == 1
      disp('THERE IS ONE SIDE STREAM IN THIS COLOUM');
    end
     NL=NLT(IL)
     NH=NHT(IL)
     NL2=NL2T(IL)
     NH2=NH2T(IL)
    if NOLSS \sim = 1
       if NOVSS ==1
         disp ('THE SIDE STREAM IS VAP.');
       end
     else
       disp ('THE SIDE STREAM IS LIQ.');
    end
   else
```

```
NL=NLT(IL)
  NH=NHT(IL)
 disp ('THERE IS NO SIDE STREAM IN THIS COLOUM');
end
ICOL=ICOLT(IL);NOFD=NOFDT(IL);
RO=ROT(IL);RS=RST(IL);PRE=PRET(IL);
NSS=NSST(IL);TCF=TCFT(IL);LOSS=LOSST(IL);
if (ICOL == 0)
  disp ('BOTTOM PROD. IS FED TO THE LATER COLOUMN');
elseif (ICOL == 1)
  disp('TOP PROD. IS FED TO THE LATER COLOUM');
elseif (ICOL == 2)
  disp('SIDE STREAM IS FED TO THE LATER COLOUM');
elseif (ICOL == 3)
  disp('THIS COULMN IS THE LAST ONE');
elseif (ICOL==4)
  disp ('top and bottom fed to the last column');
end
if (NSS == 0)
  disp ('THE SIDESTREAM NOT FED TO THE NEXT COLUMN');
elseif(NSS==1)
  disp ('THE SIDESTREAM FED TO THE NEXT COLUMN');
end
if(TCF==1)
  disp ('THE FEED IS SATURATED LIQUID');
elseif(TCF==2)
  disp ('THE FEED IS SATURATED VAPOUR');
end
if(LOSS==1)
  disp ('SIDESTREAM BELOW THE FEED');
elseif(LOSS==2)
  disp ('SIDESTREAM ABOVE THE FEED');
elseif(LOSS==0)
  disp ('FOR SPECIAL CASES');
end
for I=1:N
  A(I)=FD*Z(I);
end
А
  T=TF:
[VK,YY,T] = BPT (Z,T,PRE,N,D,E,F,GC,CV,ETA);
for I=1:N
  RELZ(I)=VK(I)/VK(NH);
end
RELZ;
TR=273.2;
```

```
[SUMHL] = HLE(T,Z,TR,N,A1,B1,C1,D1,GC,CV,ETA);
HLFD=SUMHL*FD;
if(NOFD~=1)
  for I=1:N
   AF(I)=FDF*ZF(I);
  end
AF
[VK,YY,T] = BPT (ZF,TF1,PRE,N,D,E,F,GC,CV,ETA);
  for I=1:N
   RELZF(I)=VK(I)/VK(NH2);
  end
RELZF;
[SUMHL]=HLE(TF1,ZF,TR,N,A1,B1,C1,D1,GC,CV,ETA);
HLFDF=FD*SUMHL;
end
NLO=NL-1;
NLE=NL+1;
NHO=NH+1;
NDEL=NH-NL;
NHE=NH-1;
if NOSS ~=0
  NH3=NH2+1;
  for I=1:NLO
    B(I)=A(I);
  end
  B(NL)=A(NL)*RO(JJ);
    B(NH) = A(NH)*(1.0-RO(JJ))*RS;
  for I=NHO:N
    B(I)=0;
  end
else
  %C-----
  %C
        MATERIAL BALANCE CALCULATION
  %C-----
  for I=1:NLO
    B(I)=A(I);
  end
  B(NL)=A(NL)*RO(JJ);
  B(NH) = A(NH)*(1.0-RO(JJ));
  for I=NHO:N
    B(I)=0.0;
  end
  NDEL=NH-NL:
  if (NDEL~=1)
    SUMB1=0.0;
    for I=1:N
```

```
SUMB1=SUMB1+B(I);
    end
    SUMB1=SUMB1+B(NH);
    for I=1:NL
      BF(I)=B(I)/SUMB1;
    end
     BF(NH)=B(NH)/SUMB1;
     GMIN=SUMB1/FD;
    for I=1:NLO
      Q2(I)=0.0;
      Q2(NL) = (1.0-RO(JJ))*A(NL);
      Q2(NH)=A(NH)*RO(JJ);
    end
    for I=NHO:N
      Q2(I)=A(I);
    end
    SUMQ2=0.0;
    for I=1:NL
      SUMQ2=SUMQ2+Q2(I);
    end
    SUMQ2=SUMQ2+Q2(NH);
    for I=NHO:N
      SUMQ2=SUMQ2+Q2(I);
    end
    for I=1:NL
      Q3(I)=Q2(I)/SUMQ2;
    end
    for I=NH:N
      Q3(I)=Q2(I)/SUMQ2;
    end
    GMAX=(FD-SUMQ2)/FD;
    DELG=GMAX-GMIN;
    GOPR=GMIN+GR*DELG;
    SUMB=GOPR*FD;
    B(NLE)=SUMB-SUMB1;
  end
 end
disp('DISTILLATE COMPONENT AMOUNT')
В
SUMB=0.0;
for I=1:N
  SUMB=SUMB+B(I);
end
SUMB;
```

```
for I=1:N
  Y(I)=B(I)/SUMB;
end
Y
T1=TF-3;
T2=TF-3;
[VK, YY, T1] = BPT (Y, T1, PRE, N, D, E, F, GC, CV, ETA);
for I=1:N
  RELY(I)=VK(I)/VK(NH);
end
RELY;
[SUMHL] = HLE (T1,Y,TR,N,A1,B1,C1,D1,GC,CV,ETA);
[SK,T2]=DEW (Y,T2,PRE,N,D,E,F,GC,CV,ETA);
[SUMHV] = HVE (T2,Y,TR,N,A2,B2,C2,D2,GC,CV,ETA);
CONDL=SUMHV-SUMHL;
[SUMHL] = HLE (T1,Y,TR,N,A1,B1,C1,D1,GC,CV,ETA);
  HLD=SUMHL*SUMB;
if (NOSS \sim = 0.0)
  NH3=NH2+1:
  C(1:NLO)=0.0;
if(NOFD~=1)
  C(NL)=A(NL)*(1.0-RO(JJ))+AF(NL);
  C(NH)=A(NH)*RO(JJ)+AF(NL2)*RO(JJ);
  C(NH2)=A(NH2)+AF(NH2)*(1.0-RO(JJ));
else
  C(NL) = A(NL) * (1.0 - RO(JJ));
 C(NH) = A(NH) * RO(JJ);
  C(NL2)=A(NL2)*RO(JJ);
 C(NH2)=A(NH2)*(1.0-RO(JJ));
end
С
C(NH3:N)=0.0;
SUMS=0.0;
for I=1:N
  SUMS=SUMS+C(I);
end
SUMS;
for I=1:N
  X(I)=C(I)/SUMS;
end
Х
TS=TF+10.0;
if (NOVSS \sim = 0.0)
    [SK,TS]=DEW (X,TS,PRE,N,D,E,F,GC,CV,ETA);
    for I=1:N
      RELX(I)=SK(I)/SK(NH);
```

```
RELX1(I)=SK(I)/SK(NH2);
    end
    [SUMHV] = HVE (TS,X,TR,N,A1,B1,C1,D1,GC,CV,ETA);
         HLC=SUMHV*SUMS;
  else
     [VK,YY,TS] = BPT (X,TS,PRE,N,D,E,F,GC,CV,ETA);
    for I=1:N
       RELX(I)=VK(I)/VK(NH);
    end
    for I=1:N
       RELX1(I)=VK(I)/VK(NH2);
    end
         [SUMHL] = HLE (TS,X,TR,N,A1,B1,C1,D1,GC,CV,ETA);
         HLC=SUMHL*SUMS;
  end
   Q(1:NL)=0.0;
if(NOFD \sim = 1)
   Q(NL2)=AF(NL2)*(1.0-RO(JJ));
   Q(NH2)=AF(NH2)*RO(JJ);
   for I=NH3:N
     Q(I)=AF(I);
  end
else
  if(NOSS~=1)
  Q(NL2)=A(NL2)*(1.0-RO(JJ))*(1.0-RS);
  else
  Q(NL2) = A(NL2) * (1.0 - RO(JJ));
  end
end
Q(NH2)=A(NH2)*RO(JJ);
  for I=NH3:N
     Q(I)=A(I);
  end
else
  Q(1:NLO)=0.0;
   Q(NL) = A(NL)*(1.0-RO(JJ));
  Q(NH)=A(NH)*RO(JJ);
  for I=NHO:N
     Q(I)=A(I);
  end
if (NDEL~=1)
  SUMW1=0.0;
  for I=NH:N
    SUMW1=SUMW1+Q(I);
    SUMW1=SUMW1+Q(NL);
    SUMW=FD-SUMB;
```

```
Q(NHE)=SUMW-SUMW1;
  end
end
end
Q
SUMW=0.0;
for I=1:N
  SUMW=SUMW+Q(I);
end
SUMW;
for I=1:N
  R(I)=Q(I)/SUMW;
end
R
T=TF+40;
[VK, YY, T] = BPT (R, T, PRE, N, D, E, F, GC, CV, ETA);
if NOSS \sim = 0.0
   for I=1:N
    RELR(I)=VK(I)/VK(NH2);
   end
else
   for I=1:N
    RELR(I)=VK(I)/VK(NH);
  end
end
RELR;
[SUMHL] = HLE(T,R,TR,N,A1,B1,C1,D1,GC,CV,ETA);
  HLW=SUMHL*SUMW;
if NOSS \sim = 0.0
  for I=1:N
    RELV(I) = (RELY(I) + RELX(I))/2.0;
    RELS(I) = (RELR(I) + RELX1(I))/2.0;
  end
else
  for I=1:N
    RELV(I) = (RELY(I) + RELR(I))/2.0;
  end
end
RELV;
if (NDEL~=1)
  NLM=NL+1;
  PHY=(RELV(NLM)+RELV(NH))/2.0;
  ERR=(RELV(NLM)-RELV(NH))/2.0;
else
  PHY=(RELV(NH)+RELV(NL))/2.0;
  ERR=(RELV(NL)-RELV(NH))/2.0;
```

```
end
 for IK=1:5000
   SUMPH=0.0;
   for I=1:N
     if (RELV(I)-PHY) = 0.0
       PHY=PHY+ERR;
       continue
      end
     PH(I)=Z(I)*RELV(I)/(RELV(I)-PHY);
     SUMPH=SUMPH+PH(I);
    end
    ERR=ERR/2.0;
    if SUMPH > 0.0001
     PHY=PHY-ERR;
    end
    if SUMPH < -0.0001
     PHY=PHY+ERR;
    end
  end
  %C---*-----**
   %C **MINIMUM REFLUX RATIO IS CALCULATED USING TRIAL AND
ERROR
  %C **METHOD TO CALCULATE THE COMMON ROOT VALUE OF
UNDERWOOD EQUATION*
   %C---*-----**
   VMIN=0.0;
  for I=1:N
    SUMVAP(I)=(B(I)*RELV(I)/(RELV(I)-PHY));
    VMIN=VMIN+SUMVAP(I):
  end
   VMIN
  SLMIN=VMIN-SUMB
  RFLXM=SLMIN/SUMB
    REFOP=1.25*RFLXM
   %C-----
   %C * RFLXM IS THE MINIMUM REFLUX RATIO
   %C * REFOP IS THE OPERATING REFLUX RATIO
   %C-----
    SLOP=REFOP*SUMB
    VOPR=SUMB+SLOP
  CONDLA=CONDL*VOPR
  if (NOSS \sim = 0.0)
    REBLA=HLW+HLD+HLC+CONDLA-HLFD;
  if (NOFD~=1)
    REBLA=HLW+HLD+HLC+CONDLA-HLFD-HLFDF;
  else
```

```
REBLA=HLW+HLD+CONDLA-HLFD;
 end
else
 REBLA=HLW+HLD+CONDLA-HLFD;
end
REBLA
 if (NOSS \sim = 0.0)
   F1=(Y(NL)/Y(NH))*(X(NH)/X(NL));
 else
   F1=(Y(NL)/Y(NH))*R(NH)/R(NL);
 end
 F2=(RELV(NL)/RELV(NH));
 BN=\log(F1)/\log(F2);
 E3=(REFOP-RFLXM)/(REFOP+1.0);
 if E3 < 0.125
   E4=0.5039-0.5968*E3-0.039427*log(E3);
 else
   E4=0.6257-0.9868*E3+0.516*E3^2.0-0.1738*E3^3.0;
 end
 ACTP=(E4+BN)/(1.0-E4);
 if NOSS \sim = 0.0
   F3=(X(NL2)/X(NH2))*(R(NH2)/R(NL2));
   F4=RELS(NL2)/RELS(NH2);
   BM = \log(F3)/\log(F4);
   %C-----
   %C *FENS EQUATION IS USED TO CALCULATE
   %C *THE MINIMUM NUMBER OF STAGE
   %C-----
   ACTP1=(E4+BM)/(1.0-E4);
   ACT=ACTP+ACTP1-1.0
 end
 if (NOSS == 0.0)
   XW(NL) = (1.0 - RO(JJ)) * (RELV(NL)/RELV(NH))^BN;
   XFD(NL)=Z(NL)*XW(NL)/(RO(JJ)+XW(NL));
   XFD(NH)=Z(NH)*(1.0-RO(JJ));
   C10=XFD(NL)*Z(NH)/(XFD(NH)*Z(NL));
   C11=RELV(NL)/RELV(NH);
   C12 = \log(C10) / \log(C11);
   ANN=(C12/BN)*ACTP;
   ANW1=ACTP-ANN-1.0;
 else
   if (TS < TF)
     XW(NL2)=(1.0-RO(JJ))*(RELS(NL2)/RELS(NH2))^BM;
     XFD(NL2)=Z(NL2)*XW(NL2)/(RO(JJ)+XW(NL2));
         XFD(NH2)=Z(NH2)*(1.0-RO(JJ));
     C10=XFD(NL2)*Z(NH2)/(XFD(NH2)*Z(NL2));
```

```
C11=RELS(NL2)/RELS(NH2);
   C12 = \log(C10) / \log(C11);
    ANN=(C12/BM)*ACTP1;
   ANW1=ACTP1-ANN;
  end
end
 if (NOFD~=1)
 if(TS <TF1)
 XW(NL2)=(1.0-RO(JJ))*(RELS(NL2)/RELS(NH2))^BM;
 XFD(NL2)=ZF(NL2)*XW(NL2)/(RO(JJ)+XW(NL2));
 XFD(NH2)=ZF(NH2)*(1.0-RO(JJ));
 C10=XFD(NL2)*ZF(NH2)/(XFD(NH2)*ZF(NL2));
 C11=RELS(NL2)/RELS(NH2);
 C12=log(C10)/log(C11);
 ANN1=(C12/BM)*ACTP1;
 ANW2=ACTP1-ANN1;
 end
end
if (KCOST~=0)
 AVMW=0.0;
 [VK,YY,T] = BPT (R,T,PRE,N,D,E,F,GC,CV,ETA);
 for I=1:N
   AVMW=YY(I)*WM(I)+AVMW;
 end
   T6=T*1.8+32.0:
   TB=T6+460.0;
 DVAP=(AVMW*PRE*492.0)/(1.0*359.0*TB);
 DLIO=0.0;
 VT=0.0;
 for I=1:N
   DL1(I)=WM(I)/CV1(I);
   DL2(I)=WM(I)/CV2(I);
   DL3(I)=WM(I)/CV3(I);
   DL(I)=DL1(I)+DL2(I)*T6+DL3(I)*T6^{2}+DL4(I)*T6^{3}.0;
   WM1(I)=YY(I)*WM(I);
   VM1(I)=WM1(I)/DL(I);
   VT=VM1(I)+VT;
 end
 for I=1:N
   VFRAC=VM1(I)/VT;
   DLIQ=DL(I)*VFRAC+DLIQ;
 end
   VR=SUMB*(1.0+REFOP)*2.2045*AVMW/(3600.0*DVAP);
   VL=VR*sqrt(DVAP/(DLIQ-DVAP));
  TT=T1*1.8+32.0;
   WN=VL*((1.0/TT)-(1.0/T6));
```

```
CAF=FC1+FC2*DVAP;
    CAF1=FC5+FC6*DVAP;
 if(DVAP<0.17)
    CAF2=((24.0^0.65)*(DVAP^0.1667))/12.0;
 else
    CAF2=100.0;
 end
 if(CAF>CAF1)
    if(CAF<CAF2)
      CAF=CAF1;
 else
      CAF=CAF2;
 end
end
CAF=CAF*SF:
  ATM=VL/(0.78*CAF*FF);
    DCOL=sqrt(ATM/0.7854);
  if (NOSS~=0)
      HEI=ACT/0.6;
  else
    HEI=ACTP/0.6;
  end
    NHEI=fix(HEI)+1;
    HEIGH=(NHEI*1.5)+18.0;
    VCOL=DCOL*HEIGH;
    CA=3.1416*(DCOL^2)/4.0;
    TRAR=0.85*CA;
    CT(IL)=C1*((VCOL/100.0)^E1)+(C2*((TRAR/100.0)^E2))*NHEI
    if (TT>100.0)
      TLM=((TT-80.0)-(TT-100.0))/log((TT-80.0)/(TT-100.0));
    else
     TLM = ((TT-40.0) - (TT-45.0)) / log((TT-40.0) / (TT-45.0));
    end
    HEATC(IL)=CONDLA*4.187;
    AC=HEATC(IL)*0.94783/(TLM*UC);
    if (AC<1000.0)
      COCOND(IL)=C3*((AC/1000.0)^E3)
    else
      AC = AC/2.0;
     CC(IL)=2.0*(C3*((AC/1000.0)^E3))
    end
     TB1=401.0-T6;
     HEATR(IL)=REBLA*4.187;
     AR=HEATR(IL)*0.94783/(TB1*UR);
     CR(IL)=C3*((AR/1000)^E3)
     CW(IL)=(24.0*365.0*C4*HEATC(IL)*0.94783)/(1000.0*20.0*8.33)
```

```
CS(IL)=(24.0*365.0*C5*HEATR(IL)*0.94783)/(1000.0*825.0)
    CEQ(IL)=CT(IL)+CC(IL)+CR(IL)
    COP(IL)=0.28*CEQ(IL)+CW(IL)+CS(IL)
    CAN(IL) = (CEQ(IL)/10.0) + COP(IL)
    S=0.0;
    for T=1:IL
       S=S+CAN(T);
    end
    S
end
KU(1)=1;
   for J=2:NCOL
      KU(J)=KU(J-1)+1;
   end
if (ICOL == 0)
  for I=1:N
    Z(I)=R(I);
  end
  FD=SUMW;
  disp('The TF for Second column');
  TF=T
elseif (ICOL == 1)
  for I=1:N
     Z(I)=Y(I);
  end
  FD=SUMB;
  TF=T1;
elseif (ICOL == 2)
  for I=1:N
    Z(I)=X(I);
  end
  FD=SUMS;
  TF=T:
elseif(ICOL==4)
  FD=SUMB;
  TF=T1;
  for I=1:N
    Z(I)=Y(I);
  end
  FDF=SUMW;
  TF1=T:
  for I=1:N
    ZF(I)=R(I);
  end
end
 end
```

end end end
B.2 Subroutine programs:-

B.2.1 Bubble point program:-

```
###
%C#
     SUBROUTINE BUBBLE POINT CALCULATION
###
function [VK,YY,T] = BPT (XX,T,PRE,MX,D,E,F,GC,CV,ETA)
SUMT=.1;
for nnn=1:200
 for I=1:MX
   U(I)=D(I)+E(I)/(T+F(I));
    P(I)=exp(U(I));
 end
 NCOMP=MX;
 [XLAMDA,GAMMA,VOL] = WILSON (T, NCOMP, GC, XX, CV, ETA);
 TKA=T+273.15;
 SUMYY=0.0;
 for J=1:MX
   AA=(VOL(J)*(PRE-P(J)))/(GC*TKA);
    FREF(J)=P(J)*exp(AA);
   VK(J)=GAMMA(J)*FREF(J)/PRE;
    YY(J)=XX(J)*VK(J);
    SUMYY=SUMYY+YY(J);
 end
 SUMT=1.0-SUMYY;
    if SUMT > 0.01
   T=T+0.5;
 elseif SUMT <-0.01
   T=T-0.5;
 else
   T:
 end
end
disp ('EQUILIBRIAM KVALUE');VK
disp ('BUBBLE POINT TEMP.'); T
SUMYY
```

B.2.2 Dew point program:-

```
####
%C # SUBROUTIN DEW POINT TEMPERATURE
####
function [SK,T1]=DEW (ZZ,T1,PRE,MZ,D,E,F,GC,CV,ETA)
SUMRR=1;
while abs (SUMRR)>0.01
 for I=1:MZ
   U(I)=D(I)+E(I)/(T1+F(I));
      P1(I)=exp(U(I));
 end
 NCOMP=MZ;
 [XLAMDA,GAMMA,VOL] = WILSON (T1, NCOMP, GC, ZZ, CV, ETA);
 TKA=T1+273.15;
 SUMR=0.0:
 for J=1:MZ
   AA=(VOL(J)*(PRE-P1(J)))/(GC*TKA);
    FREF(J)=P1(J)*exp(AA);
    SK(J)=GAMMA(J)*FREF(J)/PRE;
    RR(J)=ZZ(J)/SK(J);
    SUMR=SUMR+RR(J);
 end
 SUMRR=1.0-SUMR;
 if SUMRR > 0.01
   T1=T1-0.5;
 elseif SUMRR <-0.01
   T1=T1+0.5;
 end
end
disp('EQUILIBRIAM KVALUE');SK'
disp('DEW POINT TEMP.');T1
disp('SUMMATION OF');SUMR
```

B.2.3 Enthalpy of liquid streams program:-

```
####
%C #SUBROUTINE LIQUID ENTHALPY
####
function [SUMHL] = HLE (T2,Q1,TR,ML,A1,B1,C1,D1,GC,CV,ETA)
CV1=CV(1,:); CV2=CV(2,:); CV3=CV(3,:);
for I=1:ML
 HL1(I)=A1(I)+B1(I)*T2+C1(I)*T2^{2}+D1(I)*T2^{3};
end
HL1
SUMHLI=0.0;
for I=1:ML
 HL(I) = HL1(I) * Q1(I);
 SUMHLI=SUMHLI+HL(I);
end
NCOMP=ML:
SUM3=0.0;
K=0;
%C-----
    ALCULATION OF EXCESS ENTHALPY
%C
%C-----
[XLAMDA,GAMMA,VOL] = WILSON (T2, NCOMP,GC,Q1,CV,ETA);
for I=1:ML
 SUM1=0.0:
    SUM2=0.0;
 for M=1:ML
  if I==M
    ETAA=1;
  else
    K=K+1;
    SUM1=SUM1+Q1(M)*XLAMDA(I,M);
    ETAA=ETA(K);
  end
   SUM2=SUM2+(Q1(M)*ETAA*XLAMDA(I,M));
 end
 XSUM1=SUM1+O1(I):
    XSUM2=SUM2/XSUM1;
    SUM3=SUM3+Q1(I)*XSUM2;
end
disp ('SUM3 OUT OF CONTINUE=');SUM3
SUMHL=SUMHLI+SUM3;
disp ('ENTHALPY OF LIQ. COMPONENTS'); HL
disp ('TOTAL ENTHALPY OF LIQ.=');SUMHL
```

B.2.4 Enthalpy of vapor streams program:-

```
##
%C # SUBROUTINE VAPOUR ENTHALPY
##
%C-----
   SUBROUTINE HVE(T3,E1,MV,A2,B2,C2,D2,SUMHV)
%
function [SUMHV] = HVE (T3,E1,TR,MV,A2,B2,C2,D2,GC,CV,ETA)
%DIMENSION A2(10),B2(10),C2(10),D2(10)
%DIMENSION HV1(10),HV(10),E1(10)
%COMMON/ONE/CV1(10),CV2(10),CV3(10),ETA(40)
CV1=CV(1,:); CV2=CV(2,:); CV3=CV(3,:);
%DO 36 I=1,MV
%HV1(I)=A2(I)+B2(I)*T3+C2(I)*T3**2.0+D2(I)*T3**3.0
%36 CONTINUE
for I=1:MV
 HV1(I)=A2(I)+B2(I)*T3+C2(I)*T3^2.0+D2(I)*T3^3.0;
end
SUMHV=0.0;
%DO 37 I=1,MV
HV(I)=HV1(I)*E1(I)
%SUMHV=SUMHV+HV(I)
%37 CONTINUE
for I=1:MV
 HV(I)=HV1(I)*E1(I);
 SUMHV=SUMHV+HV(I);
end
% write(*,45)
%45 format(///3X,31HTOTAL ENTHALPY OF
VAP.COMPONENTS/1H,14X,31(1H-))
%WRITE(*,46)(HV(I),I=1,MV)
%46 FORMAT(4F18.4)
%WRITE(*,47)SUMHV
%47 FORMAT(///3X,23HTOTAL ENTHALPY OF VAP.=,F25.8,14H KCAL PER
MOLE)
%RETURN
%END
disp ('TOTAL ENTHALPY OF VAP.COMPONENTS'); HV
disp ('TOTAL ENTHALPY OF VAP.='); SUMHV
```

B.2.5 Wilson model program:-

```
#####
%C # SUBROUTINE WILSON
#####
%C-----
%C
    @ THIS SUBROUTINE IS USED TO CALCULATE THE ACTIVITY
COEFFICIENT
%C @ OF MULTICOMPONENT MIXTURES ALSO IT CAN CALCULATE THE
WILSON
%C @ PARAMETERS AT ANY TEMPERATURE
%C-----
function [XLAMDA,GAMMA,VOL] = WILSON (T, NCOMP,GC,X,CV,ETA)
CV1=CV(1,:); CV2=CV(2,:); CV3=CV(3,:);
TKA=T+273.15;
for M=1:NCOMP
 VOL(M)=CV1(M)+CV2(M)*TKA+CV3(M)*TKA^2;
end
 K=0;
for I=1:NCOMP
 for J=1:NCOMP
  if I~=J
    K=K+1:
    XLAMDA(I,J)=(VOL(J)/VOL(I))*exp(-ETA(K)/(GC*TKA));
  else
    XLAMDA(I,J)=1.0;
  end
 end
end
for I=1:NCOMP
    XLSUM=0.0;
    XSUM1=0.0;
 for J=1:NCOMP
  XLSUM=XLSUM+X(J)*XLAMDA(I,J);
     XSUM2=0.0:
  for M=1:NCOMP
    XSUM2=XSUM2+X(M)*XLAMDA(J,M);
  end
  XSUM1=XSUM1+X(J)*XLAMDA(J,I)/XSUM2;
 end
 GAMMA(I)=exp(1.0-XSUM1)/XLSUM;
end
```

B.3 Flow chart of short-cut program:











Table C.1 physical properties of feed system one

Component	Antoine coefficients		
1	9.80800	-2804.77188	229.14050
2	11.67470	-3460.90750	231.32812
3	11.58040	-3754.17459	224.27734

Component		Molal volume	
1	56.86600	0.00843	0.00017
2	64.51000	-0.19720	0.00039
3	22.88000	-0.03642	0.0007

Component	Enthalpy coefficient of liquid		
1	0.0002	31.12990	0.00001
2	0.0002	18.09900	0.00001
3	0.0000	18.0000	0.0000

Component	Enthalpy coefficient of vapor		
1	7392.85999	-1.69420	0.02375
2	8464.59998	3.36319	0.1076
3	10749.90002	7.85602	-0.00036

Binary interaction forces
$\lambda_{12} - \lambda_{11} = 25$
$\lambda_{13} - \lambda_{11} = 383$
$\lambda_{21} - \lambda_{22} = 390$
$\lambda_{23} - \lambda_{22} = 216$
$\lambda_{31} - \lambda_{33} = 1474$
$\lambda_{32} - \lambda_{33} = 453$

Component	Antoine coefficients		
1	11.67470	-3460.90750	231.32812
2	11.28410	-3261.37628	210.3125
3	11.58040	-3754.17459	224.27734

Table C.2 physical properties of feed system two

Component		Molal volume	
1	64.51000	-0.19720	0.00039
2	53.86600	-0.03111	0.00016
3	22.89000	-0.03642	0.00007

Component	Enthalpy coefficient of liquid		
1	0.00002	18.09900	0.00001
2	-0.19696	26.35200	-0.00011
3	0.00000	1800000	0.00000

Component	Enthalpy coefficient of vapor		
1	8464.59998	3.36319	0.10760
2	11312.90002	-1.59611	0.02433
3	10749.90002	7.85602	-0.00064

Binary interaction forces
$\lambda_{12} - \lambda_{11} = -175$
$\lambda_{13} - \lambda_{11} = 280$
$\lambda_{21} - \lambda_{22} = 216$
$\lambda_{23} - \lambda_{22} = 435$
$\lambda_{31} - \lambda_{33} = 442$
$\lambda_{32} - \lambda_{33} = 901$

Component	Antoine coefficients		
1	9.04530	-2613.02252	220.15625
2	9.28170	-2789.43430	228.75000
3	12.042110	-3847.62738	231.25000
4	9.24230	-2773.57233	220.00000

Table C.3 physical properties of feed system three

Component		Molal volume	
1	125.96000	-0.14456	0.00055
2	104.27000	-0.08676	0.00039
3	53.70000	0.03110	0.00016
4	70.86000	0.01490	0.00016

Component	Enthalpy coefficient of liquid		
1	-0.00105	51.70000	0.00001
2	-0.10636	38.80230	0.03725
3	-0.19696	26.35200	-0.00011
4	-0.00002	27.94500	-0.00001

Component	Enthalpy coefficient of vapor		
1	9463.23242	26.09780	0.04898
2	8353.41797	18.44516	0.04340
3	11312.90002	-1.59611	0.02433
4	10539.90002	-16.25300	0.04270

Binary interaction forces				
$\lambda_{12} - \lambda_{11} = 425$	$\lambda_{13} - \lambda_{11} = 310$			
$\lambda_{14} - \lambda_{11} = 320$	$\lambda_{21} - \lambda_{22} = -225$			
$\lambda_{23} - \lambda_{22} = 220$	$\lambda_{24} - \lambda_{22} = 197$			
$\lambda_{31} - \lambda_{33} = 2205$	$\lambda_{32} - \lambda_{33} = 2240$			
$\lambda_{34} - \lambda_{33} = 2435$	$\lambda_{41} - \lambda_{44} = 100$			
$\lambda_{42} - \lambda_{44} = 192$	$\lambda_{43} - \lambda_{44} = 70$			

الخلاصة

هذه الدراسة تهتم بتقليل متطلبات الطاقة في عملية التقطير اللامثالي متعدد المكونات بأستخدام تقنية الأزدواج الحراري.

تم الأخذ بنظر الأعتبار نظامان ثلاًثيان للتغذية (ميثانول-ايثانول-ماء اسيتون-ميثانول-ماء) و نظام رباعی واحد (ن-هکسان-م س ب-ايثانول-بنزين).

هذه الأنظمة فرضت بأنها سائلة في درجة غليانها, ثلاّث نسب مختلفة للأزالة هي 0.925,0.9 و 0.95 و تركيبات مختلفة للتغذية تم دراستها. الضغط التشغيلي تم فرضه بانه ثابت عند 1 جو.

تسع أشكال مختلفة تم دراستها لفصل مكونات انظمة التغذية وفقا للامثاليتها. تم مقارنة النتائج مع افضل ثلاث اشكال لأنظمة التقطير الأعتيادية ونسبة حفظ الطاقة في المغلي و نسبة الحفظ في الكلفة اليومية قد حسبت بالنسبة لهذه الأشكال.

كذلك فأن النتائج تم مقارنتها مع الدر اسات السابقة ولكن بتقنيات مختلفة مثل المضخة الحرارية. تم الحصول على افضل شكل لكل نظام تغذية و لكل تركيب.

و قد وخد بان تقنية الأزدواج الحراري التي أستخدمت قد اعطت حفظا في طاقة المغلي بنسبة 64.18% الى 80.21% هذه النتائج بينت بأن الأزدواج الحراري هو أكفأ من التقنيات الأخرى.

شکر و تقدیر

أقدم فائق الشكر والتقدير والأمتنان الى استاذتي و مشرفتي الدكتورة ندى بهجت النقاش لتقديمها يد العون و المساعدة لأكمال متطلبات هذا البحث على أتم وجه. كذلك اشكر كادر رئاسة قسم الهندسة الكيمياوية من أساتذة و منتسبين لمساعدتي في اتمام البحث. أود ان اشكر و أقر بالعرفان لو الدي الغالي و امي الحنون عمي و عمتى لما لهم الفضل الأكبر في اتمام در استي وكافة افر اد عائلتي و كل من ساندني. شكر خاص لزوجي العزيز لتشجيعه لي وتعاونه الكبير.

الأزدواج الحراري في التقطير اللامثالي متعدد المكونات

رسالة مقدمة الى كلية الهندسةفي جامعة النهرين و هي جزء من متطلبات نيل درجة ماجستير علوم في الهندسة الكيمياوية

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جمادى الأولى آيار