

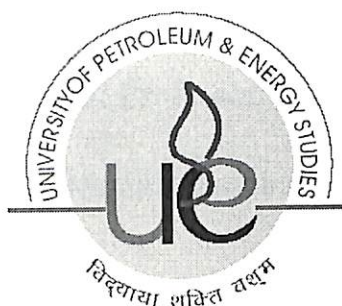
**PERFORMANCE RATING IN
A REACTIVE DISTILLATION COLUMN
THESIS**

Submitted in Partial Fulfilment of the requirements for the Award of the Degree of

**MASTER OF TECHNOLOGY
(REFINING AND PETROCHEMICAL ENGINEERING)**

Submitted By

SANJEEV KUMAR AWARI



**COLLEGE OF ENGINEERING
UNIVERSITY OF PETROLEUM & ENERGY STUDIES
DEHRADUN**

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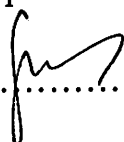
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CERTIFICATE

This is to certify that the work contained in this thesis titled “PERFORMANCE RATING IN A REACTIVE DISTILLATION COLUMN” has been carried out by SANJEEV KUMAR AWARI, under my supervision and has not been submitted elsewhere for a degree.


(Signature of Supervisor)

G. Sanjay Kumar,

Assistant Professor,

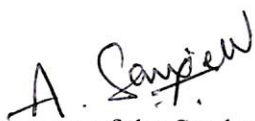
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UPES, Dehradun.

Date:

DECLARATION

I hereby declare that the work which is being presented in the thesis entitled “PERFORMANCE RATING IN A REACTIVE DISTILLATION COLUMN” by “Mr. SANJEEV KUMAR AWARI” in partial fulfilment of requirements for the award of degree of M. Tech. (Refining & Petrochemical Engineering) submitted in the Department of Chemical Engineering at UNIVERSITY OF PETROLEUM & ENERGY STUDIES, DEHRADUN is an authentic record of my own work carried out during a period from 1ST NOV, 2010 to 31ST APR, 2010 under the supervision of G. Sanjay Kumar. The matter presented in this thesis has not been submitted by me in any other University / Institute for the award of M. Tech Degree. *Due to the confidentiality of data, the original name, location and identity of the data has been changed.*



Signature of the Student

This is to certify that the above statement made by the candidate is correct to the best of
My /our knowledge



Signature of Supervisor(s)

ACKNOWLEDGEMENT

There are many people to acknowledge when a report like this is completed. My sincere thanks goes to all those who are directly or indirectly involved in this project and took time out of their busy schedules to pour insights into my report.

My sincere thanks are due to G. Sanjay Kumar for his insightful guidance and feedback without which I would not have succeeded in my endeavour.

The University of Petroleum & Energy Studies must be credited for letting me do a project of my area of interest, keeping faith in me and letting it happen. Last and most assuredly not least, I am deeply indebted to many people including my present class-mates, who have helped and extended their support to me directly and indirectly in this project.

Date: 3rd May 2010

Place : Dehradun.

SANJEEV KUMAR AWARI

ABSTRACT

Reactive Distillation is one of the major steps in the distillation history. It has been giving special attention from past two decades. Presently more than 150 reactive distillation columns in operation worldwide. Reactive distillation process couple the physical separation as well as chemical reactions in a single unit operation. Process synthesis for reactive distillation includes design and optimisation of the column. Because of the interactions between reaction and distillation in the combined unit, the modelling, design and performance evaluation of reactive distillation is complex. The reaction influences the composition on each tray in reactive zone, and thus mass transfer and vapour and liquid loads; for homogeneously catalysed reactions, the liquid hold-up is another important design parameter, because the reaction extent is not only a function of tray compositions and temperature. Thus, many critical parameters dictate the performance of the reactive distillation column. An alternative approach, which is adopted in this work, is to assume that the reaction equilibrium is achieved in each stage.

In the current work, the performance rating of a reactive distillation column is calculated by using WILSON activity coefficient model for methyl acetate and water system which is reversible reaction. An attempt has been made to compare the predicted performance results in the present work with the results of HYSYS simulation tool.

CONTENTS

LIST OF FIGURES	viii
LIST OF TABLES	ix
NOMENCLATURE	x
1. INTRODUCTION	1
1.1. METHODS USED FOR SEPARATING AZEOTROPIC MIXTURES	3
1.2. REACTIVE DISTILLATION	4
1.3. PRESENT STUDY	9
2. LITERATURE SURVEY	10
3. METHODOLOGY	12
4. CALCULATIONS	16
5. RESULTS	27
6. APPENDIX	33
7. REFERENCES	37
8.	

LIST OF FIGURES

1. FIG 1. EXPERIMENTAL SETUP OF CONTINUOUS REACTIVE DISTILLATION COLUMN	08
2. FIG 2. TEMPERATURE PROFILE	29
3. FIG 3. LIQUID COMPOSITION PROFILE	29
4. FIG 4. TEMPERATURE PROFILE	32
5. FIG 5. LIQUID COMPOSITION PROFILE	32

LIST OF TABLES

1. TABLE 1. LIQUID COMPOSITION DATA	12
2. TABLE 2. MOLECULAR WEIGHT DATA OF COMPONENTS	15
3. TABLE 3. VAPOUR COMPOSITION ON 1 ST TRAY	16
4. TABLE 4. LIQUID COMPOSITION ON 1 ST TRAY	16
5. TABLE 5. VAPOUR COMPOSITION ON 2 ND TRAY	17
6. TABLE 6. LIQUID COMPOSITION ON 2 ND TRAY	17
7. TABLE 7. WILSON PARAMETERS FOR COMPONENTS	18
8. TABLE 8. LIQUID COMPOSITION IN 1 ST ITERATION	25
9. TABLE 9. CONVERGED LIQUID COMPOSITION	26
10. TABLE 10. LIQUID AND VAPOUR COMPOSITION ON 5 TH TRAY	26
11. TABLE 11. LIQUID COMPOSITION RESULTS FROM CALCULATIONS	27
12. TABLE 12. TEMPERATURE AND PRESSURE RESULTS FROM CALCULATIONS	28
13. TABLE 13. LIQUID COMPOSITION RESULTS FROM HYSYS	30
14. TABLE 14. TEMPERATURE AND PRESSURE RESULTS FROM HYSYS	31

NOMENCLATURE

L	Rectifying section liquid flow rate
V	Rectifying section vapour flow rate
\bar{L}	Stripping section liquid flow rate
\bar{V}	Stripping section vapour flow rate
y_{n+1}	Vapour composition on n+1th tray
x_n	Liquid composition on n th tray
x_D	Distillate composition
x_B	Bottom composition
v_i	Molar volume of i th component
A_{ij}	Wilson constant
R	Gas constant
a_i	Activity
a'_i	Transformed activity
M_i	Molecular weight of i th component
D	Distillate flow rate
B	Bottom product flow rate
Re	Reflux ratio
MeOH	Methanol
HAc	Acetic acid
MeAC	Methyl acetate
H_2O	Water

Greek letters

γ_i activity coefficient

Λ Wilson parameter

1. INTRODUCTION

Distillation is the oldest separation process in the chemical process industries for separating the mixtures on the basis of relative volatility and boiling point difference. It has been around 4000 BC, and it was discovered by Babylonians. First it was used for beverage purpose by Jabir Ibn Hayyan in 721 AD. In 19th century modern techniques were added to the distillation column like pre-heating and reflux. First patent came into picture in 1830 by British Patent and issued to Aenas Coffey for a whiskey distillation column. In every chemical plant, distillation column and support facilities can account for about one third of the total capital cost and more than half of the energy consumption. So, the design and optimization of the distillation column have a critical impact on the economics of the entire process and Industry.

In general, at phase equilibrium, the compositions of the coexisting vapor and liquid phases are different. Distillation exploits this difference in the relative volatilities of the individual components in the mixture to achieve the desired separation. For many mixtures, the order of the components' relative volatilities does not change over the entire range of mixture compositions. However, some mixtures exhibit one or more azeotropes, or points at which the compositions of the coexisting liquid and vapor phases are the same. As a result, it is not possible to separate these mixtures into their pure constituents via distillation alone.

An azeotrope can be either homogeneous, containing one liquid phase, or heterogeneous, consisting of two liquid phases. Heterogeneous azeotropes can be easily separated using a decanter coupled with one or more distillation columns, which exploits both vapor-liquid and liquid-liquid equilibrium driving forces. Homogeneous azeotropic compositions that are pressure-sensitive can be separated using pressure-swing distillation, which utilizes two or more distillation columns operating at different pressures together with appropriate recycle strategies to achieve the desired separation. However, if the change in azeotrope composition is small, the pressure-swing distillation sequence will have very large recycle flow rates, resulting in an uneconomical process.

In all other cases, the only way to separate homogeneous azeotropic mixtures via distillation is by adding an extraneous component, referred to as an entrainer or mass-separating agent, to facilitate the separation. Entrainers are also used to enable the separation of non-azeotropic mixtures where the direct separation is either not feasible due to process constraints (e.g., maximum operating temperature) or highly uneconomical (e.g., due to the presence of a severe tangent pinch, as in the case of acetic acid and water).

1.1. METHODS USED FOR SEPARATING AZEOTROPIC MIXTURES

1. **Extractive distillation:** In this process the separating agent (third component) may be a higher-boiling point liquid or solvent that is miscible with both of the key components but is chemically more similar to one of them. The key component that is more like the solvent will have a lower activity coefficient in the solution than the other component, so the separation is enhanced.
2. **Salt distillation:** Salt-effect distillation is a method of extractive distillation in which a salt is dissolved in the mixture of liquids to be distilled. The salt acts as a separating agent by raising the relative volatility of the mixture. One advantage of salt-effect distillation over other types of distillation is the potential for reduced costs associated with energy usage. In addition, the salt ions have a greater effect on the volatility of the mixture to be distilled than other liquid separating agents.
3. **Heterogeneous azeotropic distillation:** If the constituents of a mixture are not completely miscible an azeotrope can be found inside the miscibility gap. Heterogeneous entrainers cause liquid-liquid phase separation to occur in such a way that the composition of each phase lies on either side of a distillation boundary. In this way, the entrainer allows the separation to “jump” over a boundary that would otherwise be impassable.
4. **Homogeneous azeotropic distillation :** If the azeotropic composition is outside the miscibility gap or the constituents of a mixture are completely miscible an azeotrope cannot be found inside the miscibility gap
5. **Pressure-swing distillation:** Some mixtures lose azeotropic behavior when the system pressure is changed. In this case, separation can be achieved without using an additional entrainer. So pressure-swing distillation is a method for separating a **pressure-sensitive azeotrope** that utilizes two columns operated in sequence at different pressures.
6. **Reactive distillation:** In this process the separating agent reacts preferentially and reversibly with one of the azeotropic constituents. The reaction product is then distilled from the non reacting components and the reaction is reversed to recover the initial component.

1.2. REACTIVE DISTILLATION

Reactive Distillation is one of the major steps in the distillation history. It has been giving special attention from past two decades. Reactive distillation process couple the physical separation as well as chemical reactions in a single unit operation. Initially it was dealt with homogeneous catalyzed reactions such as hydrolysis and esterifications. Heterogeneous catalyzed reactive distillation is the recent development. First implementation of reactive distillation column took place in 1980s.

Reactive distillation may be advantageous for liquid-phase reaction systems when the reaction must be carried out with a large excess of one or more of the reactants, when a reaction can be driven to completion by removal of one or more of the products as they are formed, or when the product recovery or by-product recycle scheme is complicated or made infeasible by azeotrope formation. For consecutive reactions in which the desired product is formed in an intermediate step, excess reactant can be used to suppress additional series reactions by keeping the intermediate-species concentration low. A reactive distillation can achieve the same end by removing the desired intermediate from the reaction zone as it is formed.

Similarly, if the equilibrium constant of a reversible reaction is small, high conversions can be achieved by use of a large excess of reactant. Alternatively, by Le Chatelier's principle, the reaction can be driven to completion by removal of one or more of the products as they are formed. Typically, reactants can be kept much closer to stoichiometric proportions in a reactive distillation. When a reaction mixture exhibits azeotropism, the recovery of products and recycle of excess reagents can be quite complicated and expensive. Reactive distillation can provide a means of breaking azeotropes by altering or eliminating the condition for azeotrope formation in the reaction zone through the combined effects of vaporization-condensation and consumption production of the species in the mixture.

Alternatively, a reaction may be used to convert the species into components that are more easily distilled. In each of these situations, the conversion and selectivity often can be improved markedly, with much lower-reactant inventories and recycle rates, and much simpler recovery schemes. The capital savings can be quite dramatic.

Although reactive distillation has many potential applications, it is not appropriate for all situations. Since it is in essence a distillation process, it has the same range of applicability as other distillation operations. Distillation-based equipment is not designed to effectively handle solids, supercritical components (where no separate vapour and liquid phases exist), gas-phase reactions, or high-temperature or high pressure reactions such as hydrogenation, steam reforming, gasification, and hydro - dealkylation.

Conditions for the use of a Reactor and Distillation Column Sequencing:

1. The chemical reaction must occur in the liquid phase irrespective of the occurrence of a homogeneous catalyst, or at the interface of a liquid and a solid catalyst.
2. Distillation parameters along with the reaction parameters are the same.
3. The reaction is not affected by the removal of any product which means that the reaction is equilibrium-limited which thereby helps in a critical situation which refers to the recovery of the excess reagent thereby avoiding the formation of azeotropes.
4. In case of an irreversible reaction this helps a lot by giving a better yield of the product where in later case the products are separated by the use of distillation column.

In case of the distillation columns used after reactors certain factors play major role:

1. Feed entry.
2. Product Removal stages.
3. In case the **heat of the reaction is appreciable** then the use of interchangers and intercoolers is a must.

Since reaction and separation phenomena are closely coupled in a reactive distillation process, simulation and design is significantly more complex than that of sequential reaction and separation processes. In spite of the complexity, however, most commercial computer process modelling packages offer reliable and flexible routines for simulating steady state reactive distillation columns, with either equilibrium or kinetically controlled reaction models.

As with other enhanced distillation processes, the results are very sensitive to the thermodynamics model chosen and the accuracy of the VLE data used to generate model parameters. Of equal, if not more significance is the accuracy of data on reaction rate as a function of temperature. Very different conclusions can be drawn about the feasibility of a reactive distillation if the reaction is assumed to reach chemical equilibrium on each stage of the column or if the reaction is assumed to be kinetically controlled. Tray holdup and stage requirements are two important variables directly affected by the form of the reaction model chosen.

When an equilibrium reaction occurs in a vapour-liquid system, the phase compositions depend not only on the relative volatility of the components in the mixture, but also on the consumption (and production) of species. At a reactive azeotrope the mass exchange between the vapour and liquid phase and the generation (or consumption) of each species is balanced such that the composition of neither phase changes. Reactive azeotropes show the same distillation properties as ordinary azeotropes and therefore affect what products are achievable. Reactive azeotropes are not easily visualized in conventional y - x coordinates but become apparent upon a transformation of coordinates which depends on the number of reactions, the order of each reaction (e.g., $A + B \leftrightarrow C$ or $A + B \leftrightarrow C + D$), presence of non-reacting components, and the extent of reaction.

The situation becomes more complicated when the reaction is kinetically controlled and does not come to complete-chemical equilibrium under the conditions of temperature, liquid holdup, and rate of vaporization in the column reactor.

Multiple Steady States problem and Reactive Distillation:

Due to the interaction between chemical reaction and distillation, reactive distillation can exhibit highly nonlinear behaviour and multiple steady state solutions are often possible. By multiple steady states MSS in a distillation column we refer to output multiplicities. That is, that a column of a given design exhibits different column profiles and, therefore, different product compositions at steady state for the same set of inputs feed composition, flow rate and quality and the same values of the operating parameters.

Non-linear behaviour and solution multiplicity of mathematical model are well known in chemical reactors, e.g. the continuous stirred tank reactor (CSTR) as well as in a few non-reactive azeotropic distillations. In reactors, the multiplicity can be caused either by heat effects or by kinetic instabilities. For non-reactive distillation columns, multiple steady states can occur due to singularities in the mass–molar relationships, the dependence of the heat vaporization on composition for special choices of the input variables, or the presence of certain azeotropic behaviour in mixtures. In principle, any of these sources, or their combinations and interactions of reaction and fractionation can cause multiple steady states in reactive distillation columns.

As reactive distillation involves the combined effects of reaction and distillation, it is important to know in which operating region (reaction controlled or fractionation controlled) a reactive distillation column is operating, to understand how the column will respond to changes in operating variables.

Commercial Applications:

1. The Esterification of acetic acid with ethanol to produce ethyl acetate and water.
2. The reaction of formaldehyde and methanol to produce methylal and water, using a solid acid catalyst.
3. The Esterification of acetic acid with methanol to produce methyl acetate and water using sulfuric acid as catalyst.
4. The reaction of isobutene with methanol to produce methyl-*tert*-butyl ether (MTBE), using a solid strong-acid ion-exchange resin catalyst.

Lab Analysis of Continuous Reactive Distillation Column:

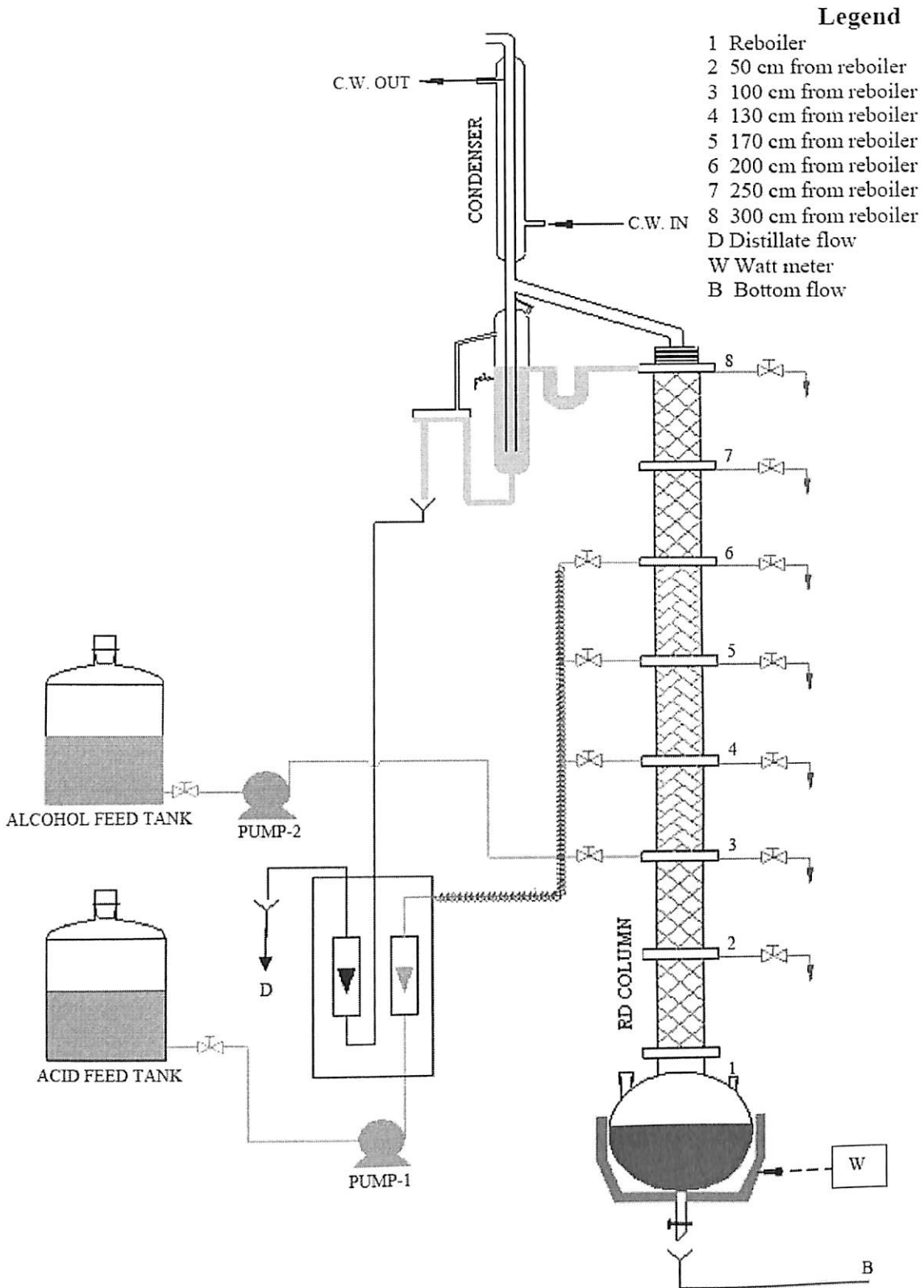


Fig 1. Experimental setup of continuous reactive distillation column

Reactive Distillation Column favours to following types of reactions:

1. Acetylation
2. Aldol condensation
3. Alkylation
4. Amination
5. Dehydration
6. Esterification
7. Etherification
8. Hydrolysis
9. Isomerisation
10. Oligomerization
11. Transesterification

1.3. **PRESENT STUDY:**

In the present study to design a reactive distillation column, WILSON activity coefficient model was used. For calculating Wilson parameters, liquid composition and vapour composition, developed a C++ programme. After calculating liquid and vapour compositions on each tray, compared with the results calculated by using Aspen HYSYS simulation tool. Results are displayed in “RESULTS AND DISCUSSIONS”.

2. LITERATURE SURVEY

In literature, a large number of models (designing and modelling) are available for reactive distillation column.

1. In 1987 by Domingos Barbosa, Michael F. Doherty, proposed a new set of transformed composition variables are introduced to simplify the design of reactive distillation column for single feed and multi component reactive distillation columns. The new transformed composition variables are used to derive the relationships between design variables easily.
2. In 2000 J. W. Lee, S. Hauan, K. M. Lien and A. W. Westerberg proposed a design for reactive distillation column by using Ponchon – Savarit method for a binary reactive distillation column. This method is specifically for isomerization and decomposition reactions.
3. In 2000 J. W. Lee, S. Hauan, K. M. Lien and A. W. Westerberg published a paper of reactive distillation column design using Mc – Cabe Thiele method for binary system.
4. In 2003 Robert S. Huss, Fengrong Chen, Michael F. Malone, Michael F. Doherty proposed hierarchy of methods, models and calculation techniques which supports reactive distillation column design.
5. Suman Thotla, Sanjay M. Mahajani published a paper for reactive distillation design and proposed design guidelines for multiple reactant systems like esterification, cross aldol condensation reactions and also some cases which are associated with non – ideality through formation of azeotropes. The parametric studies for the representative hypothetical reaction system, involving both reversible and irreversible reactions, form the basis of these guidelines.
6. Michael F. Doherty and George Buzad presented a design procedure for kinetically controlled reactive distillation columns and also showed that the amount of liquid holdup per stage has a significant effect on the design.
7. G. Jan Harmsen published a full review of commercial applications of reactive distillation, present research work on reactive distillation, design and operation procedures about reactive distillation column.
8. Q. Smejkal, M. Soos published a paper and compared the results using Aspen Plus and HYSYS simulation tools for acetic acid and i – butanol system.

9. A. Tuchlenski, A. Beckmann, D. Reusch, R. Dussel, U. Weidlich, R. Janowsky were discussed about the benefits of the reactive distillation column and also studied about the higher conversions due to shifting the equilibrium to the product side, selectivities due to removal of products from the reaction zone.
10. Jian Xiao, Jiaqi Liu, Juntao Li, Xinghua Jiang, Zhibing Zhang were studied about changes in purity of products by changing reflux ratio, feed mole ratio and volumetric ratio for hydrolyzing methyl acetate in polyvinyl alcohol process in reactive distillation column

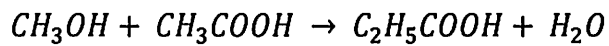
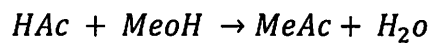
3. METHODOLOGY

Reactive distillation couples the physical separation and chemical reaction in one unit operation. The reaction will occur in reaction zone. Mostly the purity of the products depends on the reactive zone, reflux ratio and type of catalyst used in the reactive zone.

Data available:

1. Distillation composition
2. Distillate flow rate
3. Reflux ratio
4. Bottoms composition
5. Bottoms flow rate
6. Reboiler ratio

The system which we are using here is:



$$\text{Rate of reaction} = \frac{k_f a'_{MeAc} a'_{H_2O} - k_r a'_{HAc} a'_{MeOH}}{(a'_{MeAc} + a'_{H_2O} + a'_{HAc} + a'_{MeOH})^2}$$

Component	Distillate composition	Bottoms composition	Feed Composition
Methanol	0.7749	0.1001	0.4
Acetic Acid	0.0002	0.7199	0.4
Methyl Acetate	0.2249	0.0001	0.1
Water	0.0001	0.1799	0.1

Table 1. Liquid composition data

Distillate Flow Rate = 20 kmol/hr

Bottoms Flow Rate = 25 kmol/hr

Reflux rate = 5.0

Distillate Temperature = 355.28 K

Reboiler Temperature = 402.71 K

Feed Temperature = 348.15

Feed Pressure = 253.6 KPa

Feed Tray = 10

No. Of Plates = 15 + Condenser + Reboiler

In normal distillation column, if we know distillate composition, distillate flow rate and reflux ratio, we are able to find out the compositions in every tray in rectifying section by using rectifying section operating line equation. Stripping section operating line equation is using for calculating the compositions in stripping section.

Same as distillation column, there is a procedure to find out the compositions on each tray in reactive distillation column.

Assumptions to design reactive distillation column are:

1. Assume vapor phase hold up is negligible compare to the liquid hold up on each phase.
2. Reaction will occur in liquid phase and reaction in vapor phase is negligible or not occurs.
3. The liquid volumetric holdups on the plates will be assumed to be constant and it is $1m^3$
4. Plate efficiencies and pressure drops are constant during the operation.
5. Constant molar flow rate during the operation throughout the column.
6. Assume the system is in ideal condition.

Steps to follow for reactive distillation column design:

1. Here we are using total condenser (0th tray). So distillate composition x_D equals to vapor composition on next tray.
2. By dew point calculations, we can find the liquid composition on the tray (1st tray).
3. By using rectifying section operating line equation we can find the vapor composition on next successive tray.

$$y_{n+1} = \frac{L}{V}x_n + \frac{D}{V}x_D$$

4. Stripping operating line equation is using for find the composition in stripping section.

$$y_{n+1} = \frac{\bar{L}}{\bar{V}}x_n - \frac{B}{\bar{V}}x_B$$

5. Operating line equation which is using for find the compositions in reactive zone, if it is in rectifying section is

$$y_{n+1} = \frac{L}{V}x_n + \frac{D}{V}x_D - \frac{(\text{Rate of Reaction} * \text{liquid hold up})}{V}$$

6. After getting vapor composition on the tray, calculate the liquid composition by using dew point calculations.
7. Do the calculations up to last tray in reactive zone.
8. Operating line equation which is using for the compositions in reactive zone, if it is in stripping section is

$$y_n = \frac{\bar{L}}{\bar{V}}x_n - \frac{B}{\bar{V}}x_B + \frac{(\text{Rate of Reaction} * \text{liquid hold up})}{V}$$

9. Wilson activity coefficient model is using for find the rate of reaction.

$$\ln \gamma_i = 1 - \ln \left(\sum_{j=1}^C x_j \Lambda_{ij} \right) - \sum_{k=1}^C \left(\frac{x_k \Lambda_{ki}}{\sum_{j=1}^C x_j \Lambda_{kj}} \right)$$

$$\Lambda_{ij} = \frac{v_j}{v_i} \exp \left(\frac{-A_{ij}}{RT} \right)$$

10. For methyl acetate and water system, rate of reaction is

$$\text{Rate of reaction} = \frac{k_f a'_{MeAc} a'_{H_2O} - k_r a'_{HAc} a'_{MeOH}}{(a'_{MeAc} + a'_{H_2O} + a'_{HAc} + a'_{MeOH})^2}$$

$$\text{Here } k_f = 6.127 * 10^5 \exp\left(-\frac{63730}{R * T}\right)$$

$$k_r = 8.498 * 10^6 \exp\left(-\frac{60470}{R * T}\right)$$

$$a'_i = \frac{K_i a_i}{M_i}$$

$$a_i = x_i \gamma_i$$

Component	K	M
Methanol	5.64	32.04
Acetic acid	3.15	60.05
Methyl acetate	4.15	74.08
Water	5.24	18.02

Table 2. Molecular Weight data of components

4. CALCULATIONS

Here we are using total condenser. So distillate composition equals to vapour compositions on 1st tray. ($x_D = y_2$)

Component	Vapour composition
Methanol	0.7749
Acetic acid	0.0002
Methyl acetate	0.2249
Water	0.0001

Table 3. Vapour Composition on 1st tray

By dew point calculations we will get liquid composition on tray 1.

Component	Liquid Composition
Methanol	0.89465
Acetic acid	0.00049
Methyl acetate	0.10445
Water	0.00017

Table 4. Liquid Composition on 1st tray

To find the vapour composition on 2nd tray, use the rectifying section operating line equation.

Reflux ratio = 5, $D = 20$ kmol/Hr

Iteration 1:

$$y_2 = \frac{L}{V}x_1 + \frac{D}{V}x_D$$

$$\text{Here } Re = \frac{L}{D} = 5$$

$$L = 5 * 20 = 100$$

$$V = L + D = 100 + 20 = 120 \text{ kmol/Hr}$$

Component	Calculations	Vapour Composition
Methanol	$y_2 = \frac{100}{120} * 0.89465 + \frac{20}{120} * 0.7749$	0.87469
Acetic acid	$y_2 = \frac{100}{120} * 0.00049 + \frac{20}{120} * 0.0002$	0.00043
Methyl acetate	$y_2 = \frac{100}{120} * 0.10445 + \frac{20}{120} * 0.2249$	0.12452
Water	$y_2 = \frac{100}{120} * 0.00017 + \frac{20}{120} * 0.0001$	0.00015

Table 5. Vapour composition on 2nd tray

Repeat the same procedure till reactive zone starts (4th tray). Reactive zone starts from 5th tray. Operating line equation to find the compositions in reactive zone is:

$$y_5 = \frac{L}{V}x_4 + \frac{D}{V}x_D - \frac{(\text{Rate of Reaction} * \text{liquid hold up})}{V}$$

To find the rate of reaction, we have to know the liquid composition on 5th tray. So assume liquid composition as successive before tray i.e. 4th tray liquid composition.

Component	Liquid Composition
Methanol	0.97452
Acetic acid	0.00162
Methyl acetate	0.02240
Water	0.00116

Table 6. Liquid composition on 2nd tray

$$\text{Rate of reaction} = \frac{k_f a'_{MeAc} a'_{H_2O} - k_r a'_{HAc} a'_{MeOH}}{(a'_{MeAc} + a'_{H_2O} + a'_{HAc} + a'_{MeOH})^2}$$

Here a_i is activity coefficient. To find out activity coefficient, we are using "WILSON" activity coefficient model.

$$\ln \gamma_i = 1 - \ln \left(\sum_{j=1}^C x_j \Lambda_{ij} \right) - \sum_{k=1}^C \left(\frac{x_k \Lambda_{ki}}{\sum_{j=1}^C x_j \Lambda_{kj}} \right)$$

$$\Lambda_{ij} = \frac{v_j}{v_i} \exp \left(\frac{-A_{ij}}{RT} \right)$$

	Methanol (1)	Acetic Acid (2)	Methyl Acetate (3)	Water (4)	v_i
Methanol (1)	0	2535.197021	9.117197037	620.6314087	0.040762166
Acetic Acid (2)	-547.526001	0	-696.5031128	813.0971069	0.056641104
Methyl Acetate (3)	776.5662231	1123.144043	0	1966.71106	0.08026038
Water (4)	-52.60549164	-180.8370056	887.3704224	0	0.017883383

Table 7. Wilson parameters for components

$$\Lambda_{11} = \frac{0.040762166}{0.040762166} \exp\left(-\frac{0}{1.98721 * 361.799}\right) = 1$$

$$\Lambda_{12} = \frac{0.056641104}{0.040762166} \exp\left(-\frac{-547.526001}{1.98721 * 361.799}\right) = 2.951692736$$

$$\Lambda_{13} = \frac{0.08026038}{0.040762166} \exp\left(-\frac{776.5662231}{1.98721 * 361.799}\right) = 0.676355252$$

$$\Lambda_{14} = \frac{0.017883383}{0.040762166} \exp\left(-\frac{-52.60549164}{1.98721 * 361.799}\right) = 0.471659942$$

$$\Lambda_{21} = \frac{0.040762166}{0.056641104} \exp\left(\frac{2535.197021}{1.98721 * 361.799}\right) = 0.0219847382$$

$$\Lambda_{22} = \frac{0.056641104}{0.056641104} \exp\left(-\frac{0}{1.98721 * 361.799}\right) = 1$$

$$\Lambda_{23} = \frac{0.08026038}{0.056641104} \exp\left(-\frac{1123.144043}{1.98721 * 361.799}\right) = 0.302126329$$

$$\Lambda_{24} = \frac{0.017883383}{0.056641104} \exp\left(-\frac{-180.8370056}{1.98721 * 361.799}\right) = 0.404934287$$

$$\Lambda_{31} = \frac{0.040762166}{0.08026038} \exp\left(-\frac{9.117197037}{1.98721 * 361.799}\right) = 0.501542432$$

$$\Lambda_{32} = \frac{0.056641104}{0.08026038} \exp\left(-\frac{-696.5031128}{1.98721 * 361.799}\right) = 1.840155765$$

$$\Lambda_{33} = \frac{0.08026038}{0.08026038} \exp\left(-\frac{0}{1.98721 * 361.799}\right) = 1$$

$$\Lambda_{34} = \frac{0.017883383}{0.08026038} \exp\left(-\frac{887.3704224}{1.98721 * 361.799}\right) = 0.065714885$$

$$\Lambda_{41} = \frac{0.040762166}{0.017883383} \exp\left(-\frac{620.6314087}{1.98721 * 361.799}\right) = 0.97033959$$

$$\Lambda_{42} = \frac{0.056641104}{0.017883383} \exp\left(-\frac{813.0971069}{1.98721 * 361.799}\right) = 1.034623679$$

$$\Lambda_{43} = \frac{0.08026038}{0.017883383} \exp\left(-\frac{1966.71106}{1.98721 * 361.799}\right) = 0.299752241$$

$$\Lambda_{44} = \frac{0.017883383}{0.017883383} \exp\left(-\frac{0}{1.98721 * 361.799}\right) = 1$$

$$\ln \gamma_1 = 1 - \ln(x_1\Lambda_{11} + x_2\Lambda_{12} + x_3\Lambda_{13} + x_4\Lambda_{14}) - \left(\frac{x_1\Lambda_{11}}{x_1\Lambda_{11} + x_2\Lambda_{12} + x_3\Lambda_{13} + x_4\Lambda_{14}} + \frac{x_2\Lambda_{21}}{x_1\Lambda_{21} + x_2\Lambda_{22} + x_3\Lambda_{23} + x_4\Lambda_{24}} + \frac{x_1\Lambda_{31}}{x_1\Lambda_{31} + x_2\Lambda_{32} + x_3\Lambda_{33} + x_4\Lambda_{34}} + \frac{x_1\Lambda_{41}}{x_1\Lambda_{41} + x_2\Lambda_{42} + x_3\Lambda_{43} + x_4\Lambda_{44}} \right)$$

$$\ln \gamma_1 = 1 - \ln(0.9745 * 1 + 0.0016 * 2.951692736 + 0.0224 * 0.676355252 + 0.0012 * 0.471659942) - \left(\frac{0.9745 * 1}{0.9745 * 1 + 0.0016 * 2.951692736 + 0.0224 * 0.676355252 + 0.0012 * 0.471659942} + \frac{0.0016 * 0.021984382}{0.9745 * 0.021984382 + 0.0016 * 1 + 0.0224 * 0.302126329 + 0.0012 * 0.404934287} + \frac{0.0224 * 0.501542432}{0.9745 * 0.501542432 + 0.0016 * 1.840155765 + 0.0224 * 1 + 0.0012 * 0.065714885} + \frac{0.0012 * 0.97033959}{0.9745 * 0.97033959 + 0.0016 * 1.034623679 + 0.0224 * 0.299752241 + 0.0012 * 1} \right)$$

$$\ln \gamma_1 = 1 - \ln(0.030281573) - 1.003620127$$

$$\ln \gamma_1 = 0.001393193$$

$$\gamma_1 = \exp(0.001393193)$$

$$\gamma_1 = 1.001394164$$

$$\ln \gamma_2 = 1 - \ln(x_1\Lambda_{21} + x_2\Lambda_{22} + x_3\Lambda_{23} + x_4\Lambda_{24}) - \left(\frac{x_1\Lambda_{12}}{x_1\Lambda_{11} + x_2\Lambda_{12} + x_3\Lambda_{13} + x_4\Lambda_{14}} + \frac{x_2\Lambda_{22}}{x_1\Lambda_{21} + x_2\Lambda_{22} + x_3\Lambda_{23} + x_4\Lambda_{24}} + \frac{x_1\Lambda_{32}}{x_1\Lambda_{31} + x_2\Lambda_{32} + x_3\Lambda_{33} + x_4\Lambda_{34}} + \frac{x_1\Lambda_{42}}{x_1\Lambda_{41} + x_2\Lambda_{42} + x_3\Lambda_{43} + x_4\Lambda_{44}} \right)$$

$$\ln \gamma_2 = 1 - \ln(0.9745 * 1 + 0.021984382 + 0.0016 * 1 + 0.0224 * 0.302126329 + 0.0012 * 0.404934287) - \left(\frac{0.9745 * 1 + 0.0016 * 2.951692736 + 0.0224 * 0.676355252 + 0.0012 * 0.471659942}{0.0016 * 1} + \frac{0.9745 * 0.021984382 + 0.0016 * 1 + 0.0224 * 0.302126329 + 0.0012 * 0.404934287}{0.0224 * 1.840155765} + \frac{0.9745 * 0.501542432 + 0.0016 * 1.840155765 + 0.0224 * 1 + 0.0012 * 0.065714885}{0.0012 * 1.034623679} + \frac{0.9745 * 0.97033959 + 0.0016 * 1.034623679 + 0.0224 * 0.299752241 + 0.0012 * 1}{0.0012 * 1} \right)$$

$$\ln \gamma_2 = 1 - \ln(0.030281573) - 3.02585411$$

$$\ln \gamma_2 = 1.471361779$$

$$\gamma_2 = \exp(1.471361779)$$

$$\gamma_2 = 4.355161873$$

$$\ln \gamma_3 = 1 - \ln(x_1\Lambda_{31} + x_2\Lambda_{32} + x_3\Lambda_{33} + x_4\Lambda_{34}) - \left(\frac{x_1\Lambda_{13}}{x_1\Lambda_{11} + x_2\Lambda_{12} + x_3\Lambda_{13} + x_4\Lambda_{14}} + \frac{x_2\Lambda_{23}}{x_1\Lambda_{21} + x_2\Lambda_{22} + x_3\Lambda_{23} + x_4\Lambda_{24}} + \frac{x_3\Lambda_{33}}{x_1\Lambda_{31} + x_2\Lambda_{32} + x_3\Lambda_{33} + x_4\Lambda_{34}} \right) + \frac{x_4\Lambda_{43}}{x_1\Lambda_{41} + x_2\Lambda_{42} + x_3\Lambda_{43} + x_4\Lambda_{44}}$$

$$\ln \gamma_3 = 1 - \ln(0.9745 * 0.501542432 + 0.0016 * 1.840155765 + 0.0224 * 1 + 0.0012 * 0.065714885) - \left(\frac{0.9745 * 0.676355252}{0.9745 * 1 + 0.0016 * 2.951692736 + 0.0224 * 0.676355252 + 0.0012 * 0.471659942} + \frac{0.0016 * 0.302126329}{0.9745 * 0.021984382 + 0.0016 * 1 + 0.0224 * 0.302126329 + 0.0012 * 0.404934287} + \frac{0.0224 * 1}{0.9745 * 0.501542432 + 0.0016 * 1.840155765 + 0.0224 * 1 + 0.0012 * 0.065714885} + \frac{0.0012 * 0.299752241}{0.9745 * 0.97033959 + 0.0016 * 1.034623679 + 0.0224 * 0.299752241 + 0.0012 * 1} \right)$$

$$\ln \gamma_3 = 1 - \ln(0.514220412) - 0.722522644$$

$$\ln \gamma_3 = 0.942580643$$

$$\gamma_3 = \exp(0.942580643)$$

$$\gamma_3 = 2.566596348$$

$$\ln \gamma_4 = 1 - \ln(x_1\Lambda_{41} + x_2\Lambda_{42} + x_3\Lambda_{43} + x_4\Lambda_{44}) - \left(\frac{x_1\Lambda_{14}}{x_1\Lambda_{11} + x_2\Lambda_{12} + x_3\Lambda_{13} + x_4\Lambda_{14}} + \frac{x_2\Lambda_{24}}{x_1\Lambda_{21} + x_2\Lambda_{22} + x_3\Lambda_{23} + x_4\Lambda_{24}} + \frac{x_3\Lambda_{34}}{x_1\Lambda_{31} + x_2\Lambda_{32} + x_3\Lambda_{33} + x_4\Lambda_{34}} + \frac{x_4\Lambda_{44}}{x_1\Lambda_{41} + x_2\Lambda_{42} + x_3\Lambda_{43} + x_4\Lambda_{44}} \right)$$

$$\ln \gamma_4 = 1 - \ln(0.9745 * 1 + 0.0016 * 1.034623679 + 0.0224 * 0.299752241 + 0.0012 * 1) - \left(\frac{0.9745 * 0.471659942}{0.9745 * 1 + 0.0016 * 2.951692736 + 0.0224 * 0.676355252 + 0.0012 * 0.471659942} + \frac{0.0016 * 0.404934287}{0.9745 * 0.021984382 + 0.0016 * 1 + 0.0224 * 0.302126329 + 0.0012 * 0.404934287} + \frac{0.0224 * 0.065714885}{0.9745 * 0.501542432 + 0.0016 * 1.840155765 + 0.0224 * 1 + 0.0012 * 0.065714885} + \frac{0.0012 * 1}{0.9745 * 0.97033959 + 0.0016 * 1.034623679 + 0.0224 * 0.299752241 + 0.0012 * 1} \right)$$

$$\ln \gamma_4 = 1 - \ln(0.955165878) - 0.487692352$$

$$\ln \gamma_4 = 0.558177908$$

$$\gamma_4 = \exp(0.558177908)$$

$$\gamma_4 = 1.747485518$$

$$k_f = 6.127 * 10^5 \exp\left(-\frac{63730}{R * T}\right)$$

$$k_f = 6.127 * 10^5 \exp\left(-\frac{63730}{8.314 * 361.799}\right)$$

$$k_f = 0.000483398$$

$$k_r = 8.498 * 10^6 \exp\left(-\frac{60470}{R * T}\right)$$

$$k_r = 8.498 * 10^6 \exp\left(-\frac{60470}{8.314 * 361.799}\right)$$

$$k_r = 0.019589328$$

$$a'_{MeOH} = \frac{K_1 x_1 \gamma_1}{M_1} = \frac{5.64 * 0.9745 * 1.001394164}{32.04} = 0.171783881$$

$$a'_{HAc} = \frac{K_2 x_2 \gamma_2}{M_2} = \frac{3.15 * 0.0016 * 4.355161873}{60.05} = 0.000370098$$

$$a'_{MeAc} = \frac{K_3 x_3 \gamma_3}{M_3} = \frac{4.15 * 0.0224 * 2.566596348}{74.08} = 0.003220718$$

$$a'_{H_2O} = \frac{K_4 x_4 \gamma_4}{M_4} = \frac{5.24 * 0.0012 * 1.747485518}{18.02} = 0.000589451$$

$$\text{Rate of reaction} = \frac{k_f a'_{MeAc} a'_{H_2O} - k_r a'_{HAc} a'_{MeOH}}{(a'_{MeAc} + a'_{H_2O} + a'_{HAc} + a'_{MeOH})^2}$$

Rate of reaction

$$= \frac{(0.000483398 * 0.171783881 * 0.000370098) - (0.019589328 * 0.003220718 * 0.000589451)}{(0.171783881 + 0.000370098 + 0.003220718 + 0.000589451)^2}$$

$$\text{Rate of reaction} = -4.0193 * 10^{-5}$$

Now find out vapour composition using rectifying operating line equation i.e.

$$y_{5,i} = \frac{L}{V}x_{4,i} + \frac{D}{V}x_{D,i} - \frac{(\text{Rate of Reaction} * \text{liquid hold up})}{V}$$

Methanol:

$$y_{MeOH} = \frac{100}{120} * 0.9745 + \frac{20}{120} * 0.7749 - \frac{(-4.0193 * 10^{-5})}{120}$$

$$y_{MeOH} = 0.941233668$$

Acetic Acid:

$$y_{HAc} = \frac{100}{120} * 0.0016 + \frac{20}{120} * 0.0002 - \frac{(-4.0193 * 10^{-5})}{120}$$

$$y_{HAc} = 0.001367001$$

Methyl Acetate:

$$y_{MeAc} = \frac{100}{120} * 0.0224 + \frac{20}{120} * 0.2249 - \frac{(-4.0193 * 10^{-5})}{120}$$

$$y_{MeAc} = 0.056150334$$

Water:

$$y_{H_2O} = \frac{100}{120} * 0.0012 + \frac{20}{120} * 0.0001 - \frac{(-4.0193 * 10^{-5})}{120}$$

$$y_{H_2O} = 0.001017001$$

By using dew point calculations, we will get liquid composition and Temperature is 361.95°C

Component	Liquid Composition
Methanol	0.9756
Acetic Acid	0.0021
Methyl Acetate	0.0203
Water	0.0021

Table 8. Liquid composition in 1st iteration

Similarly preceding with the iterations the liquid composition on 5th tray converged at

Component	Liquid Composition
Methanol	0.97535
Acetic Acid	0.00215
Methyl Acetate	0.02027
Water	0.00215

Table 9. Converged Liquid composition

Now, Liquid composition and vapour composition on the 5th tray is:

Component	Liquid composition	Vapour composition
Methanol	0.97535	0.94125
Acetic Acid	0.00215	0.00138
Methyl Acetate	0.02027	0.05615
Water	0.00215	0.00098

Table 10. Liquid and Vapour composition on 5th tray

$$\text{Rate of reaction on 5}^{\text{th}} \text{ tray} = -4.0193 \times 10^{-5}$$

$$\text{Temperature} = 361.991^{\circ}\text{C}$$

Repeat the procedure up to reactive zone ends. Here feed line at last tray of the reactive zone i.e. 10th tray. Therefore, use rectifying section operating line equation to find the liquid and vapour compositions in reactive zone. After reactive zone, we have to use stripping section operating line equation line.

5. RESULTS

Calculations are done from designing procedure to design a reactive distillation column which is mentioned above, as follows:

TRAYS	Liquid composition			
	METHNAOL	ACETIC ACID	M-ACETATE	WATER
CONDENSER	0.77488	0.00016	0.22489	0.00007
1	0.89465	0.00049	0.10445	0.00017
2	0.94891	0.00086	0.04924	0.00033
3	0.96886	0.00123	0.02916	0.00063
4	0.97452	0.00162	0.02240	0.00116
5	0.97535	0.00215	0.02027	0.00215
6	0.97334	0.00297	0.01964	0.00396
7	0.96848	0.00448	0.01955	0.00735
8	0.95848	0.00790	0.01969	0.01386
9	0.92991	0.02189	0.02065	0.02757
10	0.78979	0.13245	0.02314	0.05453
11	0.73556	0.18794	0.01192	0.06409
12	0.55761	0.37103	0.00576	0.06551
13	0.25351	0.51011	0.00221	0.24925
14	0.18223	0.55559	0.00062	0.26067
15	0.15430	0.68837	0.00016	0.15769
REBOILER	0.10010	0.71988	0.00009	0.17994

Table 11. Liquid composition results from calculations.

TRAYS	TEMP (K)	PRE (KPa)
CONDENSER	355.272	250
1	357.883	250
2	360.421	253.933
3	361.397	254.2393
4	361.799	254.5439
5	361.991	254.8475
6	362.068	255.1506
7	362.182	255.4537
8	362.353	255.7582
9	362.769	256.0674
10	364.783	256.3958
11	365.710	256.7238
12	374.807	257.0536
13	393.705	257.3909
14	407.269	257.7467
15	412.960	258
REBOILER		

Table 12. Temperature and Pressure results from calculations.

Graphs drawn between temperature and trays and also between liquid composition on each tray and trays, as follows:

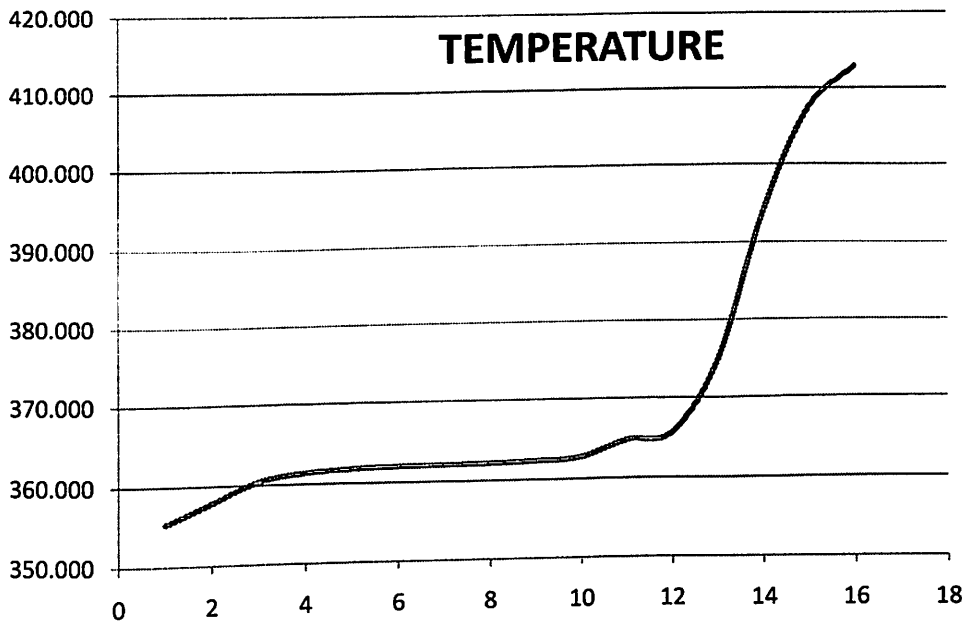


Fig 2. Temperature Profile

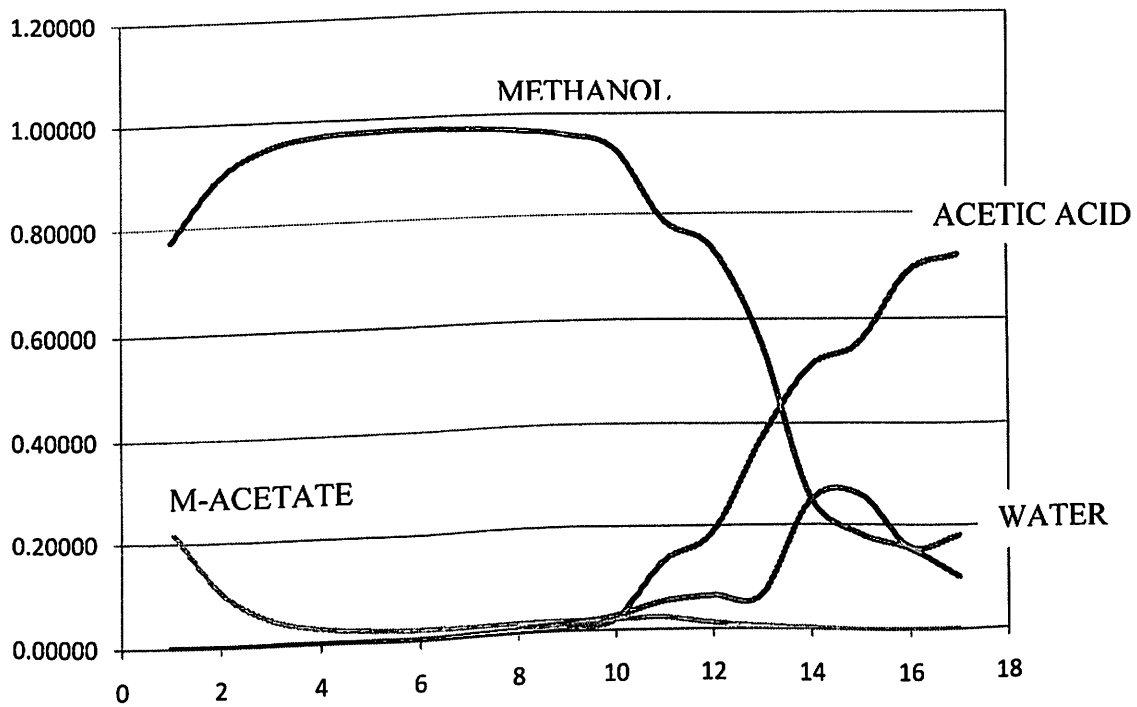


Fig 3. Liquid Composition Profile

Results are tabulated from HYSYS simulation tool, to design a reactive distillation column for methyl acetate and water system is:

TRAYS	LIQUID COMPOSITION			
	METHNAOL	ACETIC ACID	M-ACETATE	WATER
Condenser	0.7749	0.0002	0.2249	0.0001
1	0.8939	0.0005	0.1054	0.0002
2	0.9490	0.0009	0.0497	0.0003
3	0.9688	0.0012	0.0293	0.0006
4	0.9746	0.0016	0.0226	0.0012
5	0.9753	0.0021	0.0205	0.0021
6	0.9732	0.0030	0.0199	0.0039
7	0.9683	0.0046	0.0199	0.0072
8	0.9572	0.0088	0.0203	0.0138
9	0.9235	0.0273	0.0215	0.0277
10	0.7800	0.1428	0.0241	0.0530
11	0.7821	0.1445	0.0121	0.0613
12	0.7621	0.1499	0.0057	0.0822
13	0.6938	0.1730	0.0025	0.1307
14	0.5276	0.2592	0.0010	0.2123
15	0.2852	0.4611	0.0003	0.2534
Reboiler	0.1001	0.7199	0.0001	0.1799

Table 13. Liquid composition results from HYSYS

TRAYS	TEMP (K)	PRE (KPa)
Condenser	355.2772	250
1	357.8877	250
2	360.402	253.933
3	361.3953	254.2393
4	361.788	254.5439
5	361.9568	254.8475
6	362.0623	255.1506
7	362.1737	255.4537
8	362.3523	255.7582
9	362.8043	256.0674
10	365.471	256.3958
11	366.2026	256.7238
12	367.1192	257.0536
13	369.1474	257.3909
14	374.8231	257.7467
15	386.8431	255
Reboiler	402.7085	255

Table 14. Temperature and pressure results from HYSYS

Graphs are drawn between temperature on each tray and tray, and also between liquid composition and tray as follows:

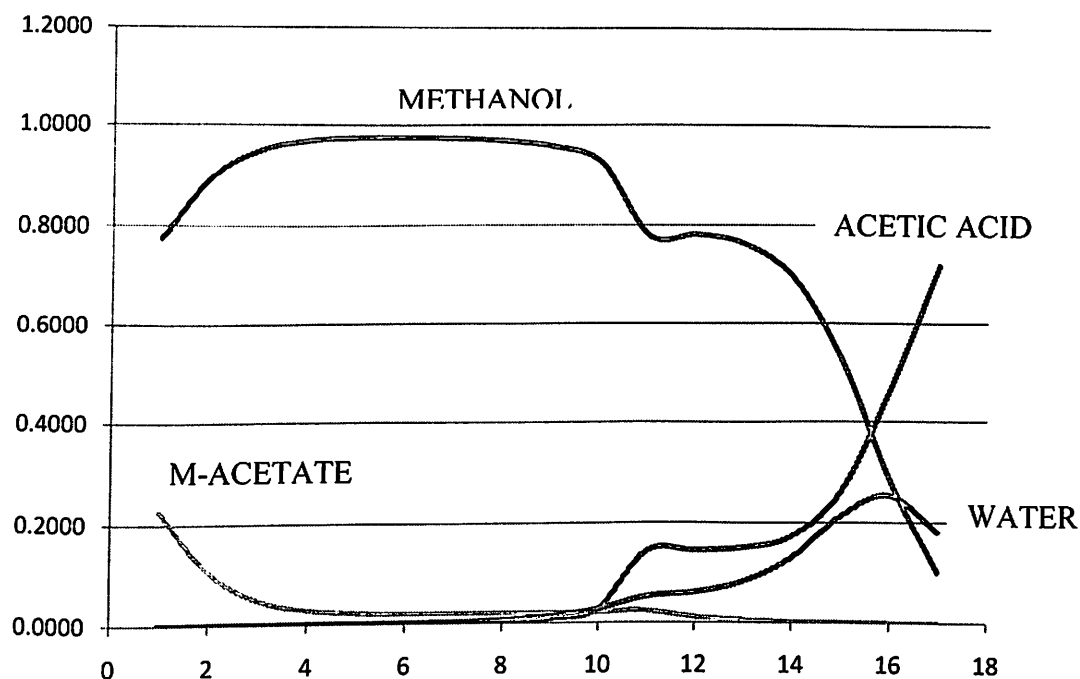


Fig 4. Temperature Profile

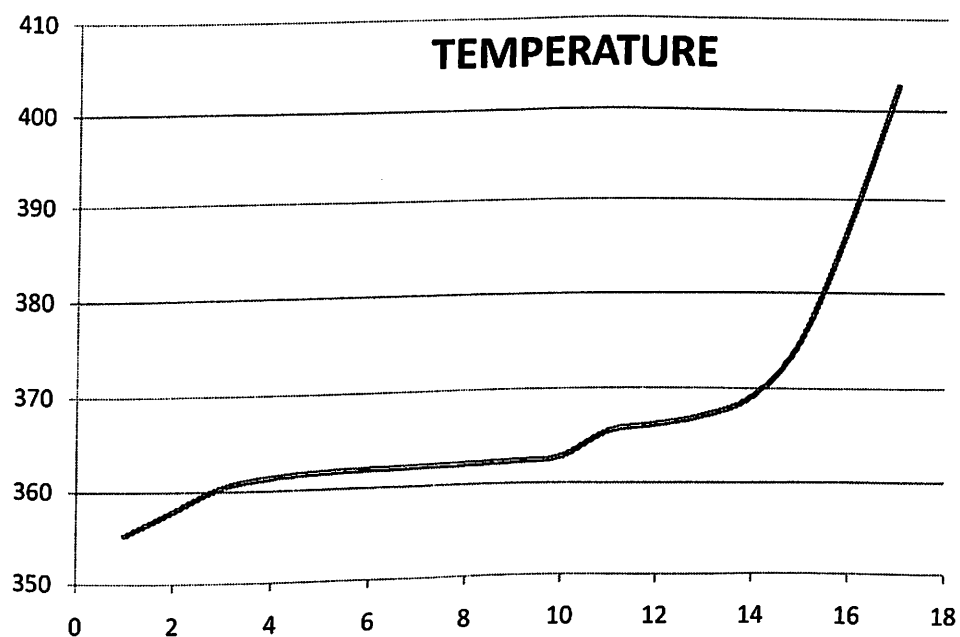


Fig 5. Liquid Composition

6. APPENDIX

C++ programme for Wilson parameters, liquid composition, vapour composition calculations.

WILSON parameters programme:

```
#include<iostream.h>
#include<iomanip.h>
#include<math.h>
#include<conio.h>
#include<fstream.h>
int main()
{
    int i,j,k,NC=4;
    float A[20][20],X[20],G[20],IV[20][20],V[20],R=1.98721,T=366.958;
    float M[20],MSUM[20],LTB[20],LTBS[20],LT[20],sanj[20],LNGAMA[20],GAMA[20];
    cout.precision(5);
    ofstream sanju("gama values.txt");
    A[1][1]=0; A[1][2]=-547.526001; A[1][3]=776.5662231; A[1][4]=-52.60549764;
    A[2][1]=2535.197021; A[2][2]=0; A[2][3]=1123.144043; A[2][4]=-180.8370056;
    A[3][1]=9.117197037; A[3][2]=-696.5031128; A[3][3]=0; A[3][4]=887.3704224;
    A[4][1]=620.6314087; A[4][2]=813.0971069; A[4][3]=1966.71106; A[4][4]=0;
    V[1]=0.040762166; V[2]=0.056641104; V[3]=0.08026038; V[4]=0.017883383;
    X[1]=0.6727; X[2]=0.1706; X[3]=0.1483; X[4]=0.0083;
    for(i=1;i<=4;i++)
    {
        for(j=1;j<=4;j++)
        {
            IV[i][j]=(V[j]/V[i])*exp(-A[i][j]/(R*T));
            M[j]=X[j]*IV[i][j];
            MSUM[i]+=M[j];
        }
    }
}
```

```

for(i=1;i<=4;i++)
{
    sanj[i]=0;
    for(k=1;k<=4;k++)
    {
        LTBS[k]=0;
        for(j=1;j<=4;j++)
        {
            LTB[j]=X[j]*IV[k][j];
            LTBS[k]=LTBS[k]+LTB[j];
        }
        LT[k]=(X[k]*IV[k][i])/LTBS[k];
        sanj[i]=sanj[i]+LT[k];
    }
}
for(i=1;i<=4;i++)
{
    LNGAMA[i]=1-log(MSUM[i])-sanj[i];
    GAMA[i]=exp(LNGAMA[i]);
}
sanju<<"Gama Values are = "<<endl;
for(i=1;i<=NC;i++)
{
    sanju<<GAMA[i]<<endl;;
}
sanju.close();
}

```

Output file:

Gama Values are =

1.11554

0.839864

1.58004

1.74653

Dew point calculations programme:

```
#include<iostream.h>
#include<iomanip.h>
#include<math.h>
#include<conio.h>
#include<fstream.h>

int main()
{
int i,NC=4;
float SUMX,DIFFX,P=1876.354,T=366.958,K[10],a[10],b[10],c[10],X[10],Y[10],G[10];

cout.precision(5);
ofstream sanju("dew temp.txt");
Y[1]=0.6897;Y[2]=0.1422;Y[3]=0.1611;Y[4]=0.0069;
G[1]=1.001394164; G[2]=4.355161873; G[3]=2.566596348; G[4]=1.747485518;
a[1]=18.5875;b[1]=3626.55;c[1]=-34.29;;
a[2]=16.8080;b[2]=3405.57;c[2]=-56.34;
a[3]=16.1295;b[3]=2601.92;c[3]=-56.15;
a[4]=18.3036;b[4]=3816.44;c[4]=-46.13;

while(1)
{ SUMX=0; DIFFX=0;
for(i=1;i<=NC;i++)
{ K[i]=exp(a[i]-(b[i]/(c[i]+T)))/P;
X[i]=Y[i]/(K[i]*G[i]);
SUMX+=X[i];
DIFFX-=X[i]*((b[i]/pow((c[i]+T),2)));
} if(fabs(SUMX-1)<=0.000001) break;
T=T-((SUMX-1)/(DIFFX));
}
```

```
sanju<<"DEW Temp= "<<T<<endl;
sanju<<"Liquid compositions "<<endl;
for(i=1;i<=NC;i++)
{ sanju<<X[i]<<endl; }
sanju.close();
}
```

Output file:

DEW Temp= 379.882

Liquid compositions

0.395268

0.4988

0.0924685

0.0134631

7. REFERENCE

1. Separation Process by Seader
2. Reactive Distillation by Kai Sundmacher, Achin Kienle
3. Reactive Distillation Design and Control by William L. Luyben, Cheng – Ching Yu.
4. Design and minimum reflux calculations for single feed multi component reactive distillation column by Domingos Barbosa, Micael F. Doherty (August 11, 1987)
5. A graphical method for designing Reactive Distillation Columns I. The Ponchon – Savarit Method by J. W. Lee, S. Haunan, K. M. Lien, A. W. Westerberg (Aug 8, 2000).
6. A graphical method for designing reactive distillation columns II. The McCabe – Thiele method by J. W. Lee, S. Haunan, K. M. Lien and A. W. Westerberg (January 20, 2000).
7. Extreme Conditions in Binary Reactive Distillation by Jae W. Lee, Steinar Haunan and Arthur W. Westerberg.
8. Graphical methods for Reactive Distribution in a Reactive Distillation Column by Jae W. Lee, Steinar Haunan, Arthur W. Westerberg (June 2000).
9. Process alternatives for methyl acetate conversion using reactive distillation, 1. Hydrolysis by Yu – Der Lin, Jun – Hong Chen, Jian – Kai Cheng, Hsiao – Ping Huang, Cheng – Ching Yu (November 5, 2007).
10. Aspen HYSYS Tutorial.
11. Reactive Distillation for methyl acetate production by Robert S. Huss, Fengrong Chen, Michael F. Malone, Michael F. Doherty (June 12, 2003).
12. Conceptual design of reactive distillation for selectivity improvement in multiple reactant systems by Suman Thotla, Sanjay M. Mahajani.
13. New tools for the design of kinetically controlled reactive distillation columns by Michael F. Doherty and George Buzad.
14. A generalized reactive separation unit model by Rafiquil Gani, Thomas S. Jepsen and Eduardo S. Perez – Cisneros.
15. Reactive distillation: The front – runner of industrial process intensification. A full review of commercial applications, research, scale – up, design and operation by G. Jan Harmsen.
16. Reactive and catalytic distillation from an industrial perspective by Hartmut G. Schoenmakers, Bernd Bessling.

17. Phase equilibria and excess properties for binary systems in reactive distillation process part I. methyl acetate synthesis by Sven Horstmann, Tim Popken, Jurgen Gmehling.
18. Comparison of computer simulation of reactive distillation using ASPEN PLUS and HYSYS software by Q. Smejkal, M. Soos.
19. Reactive distillation – industrial applications, process design and scale – up by A. Tuchlenski, A. Beckmann, D. Reusch, R. Dussel. U. Weidlich, R. Janowsky.
20. Increase MeOAc conversion in PVA production by replacing the fixed bed reactor with a catalytic distillation column by Jian Xiao, Jiaqi Liu, Juntai Li, Xinghua Jiang, Zhibing Zhang.