Dynamic Simulation and Process Matrix Modeling of Process Intensified Distillation

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Submitted By

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UNDER THE SUPERVISION AND GUIDANCE OF

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ABSTRACT

Reactive Distillation is gaining importance in intensified horizon because of higher conversions and lower cost. Current study represents production of methyl acetate in reactive distillation. Modeling in chemical engineering involves creating mathematical representations of physical and chemical processes to analyze, predict, and optimize the behaviour of chemical systems while simulation in chemical engineering refers to the use of computational tools and techniques to model the behaviour of chemical processes and systems. Here we have defined a novel process matrix modeling method that involves the information in the process row matrix and is a method of conversion of information diagram into numerical form. The contents of that row are the number of the particular unit, the name of the unit computation representing the unit and the input stream number followed by the output streams numbered. This helps in analysis of multiplicity existing in the multiple steady state conditions of reactive distillation. The highest purity achieved is 99%. The time varying rate of reaction and continuous methyl acetate composition with number of stages is studied under dynamic simulation. The results have proven the highest purity of 99% corresponding to reboiler duty of 2kW and reflux ratio of 4.

Keywords: Methyl acetate, Control Strategy, Simulation, Modeling

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ACRONYMS

Abbreviations	Full Forms
RD	Reactive Distillation
ARDTs	Advanced Reactive Distillation Technologies
PID	Process Intensified Distillation
PET	Poly ethylene terephthalate
MOC	Material of Construction
PVC	Poly vinyl chloride
DWSIM	Simulator

NOMENCLATURE

Q_C	Condenser Heat duty
Q_W	Reboiler Heat duty
h_D	Enthalpy of distillate
h_w	Enthalpy of residue
H_W	Enthalpy of vapor leaving the reboiler
ΔHv	Heat due to vaporization
x_D	Mole fraction of distillate
M_D	Holdup of distillate
V_1-	Vapor Molar flow rate on 1^{th} tray
$y_{n,i}$	Vapor mole fraction of component *i* on n^{th} tray
D	Distillate flow rate
RR	Reflux ratio
R	Reflux rate
$x_{n,i}$	Liquid mole fraction of component *i* on n^{th} tray
L_{n+1}	Liquid Molar flow rate of $n+1^{th}$ tray
V_{n-1}	Vapor Molar flow rate on $n\text{-}1^{th}$ tray
$y_{n-1,i}$	Vapor mole fraction of component *i* on $n\text{-}1^{th}$ tray
L_n	Liquid flow rate on n^{th} tray
M_n	Liquid holdup on n^{th} tray
$R_{n,i}$	Net reaction rate of component *i* on n^{th} tray
F_n	Input feed flow rate on n^{th} tray
$z_{n,i}$	Feed mole fraction of component *i* on n^{th} tray
$x_{W,i}$	Liquid composition of bottom product
M_W	Reboiler holdup
W	Residue Flow rate
V_W	Molar Flow rate of vapor leaving the reboiler
$Y_{W,i}$	Mole fraction of vapor leaving the reboiler
h_{n-1}	Enthalpy of liquid at n-1 th plate
H_{n+1}	Enthalpy of vapor at n+1th plate
h_n	Enthalpy of liquid at nth plate
H_n	Enthalpy of vapor at nth plate
h_f	Enthalpy of the Feed
λ	latent heat of the reaction
V_R	Volume of the Reactive Zone

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CHAPTER 1: INTRODUCTION

In our daily life we deal with several products that we are getting from the market and these products are actually being manufactured by different complex processes of chemical or mechanical engineering in a broader way process engineering. Based on the performance criterion these processes have some advantages as well as disadvantages. The performance criterion differs from process to process as they are based on different mechanisms. Generally all such processes are energy extensive process that means it requires a huge amount of energy for smooth functioning of these operations. In current scenario energy is need of the hour as energy is the very crucial phenomenon for any developing nation like ours. The term "Sustainable Energy" has gained a lot of attention in past few decades as a lot of environmental concerns are arising in front of the whole world. [1]

Sustainability is the concept which is based on clean energy resources or renewable energy sources which are present in infinite quantity and will be available for the future generations also even after their huge consumption. Process Intensification deals with the development of such novel techniques or mechanisms which will aim to increase the efficiency of currently existing process along with addressing the environmental concerns. Cost optimization is the one of the building block of Chemical process intensification, as the capital cost is a deciding factor in choosing any process or mechanism. Earlier when limited knowledge and facts were available on any process the only objective was to get the desired product from the raw materials. But now when a lot of information is available on any given topic by the rigorous research it is crucial to modify some orthodox processes which have certain disadvantages which can't be ignored.

The analytical study of any process allows us to implement some process modifications in a structured manner which broadly aims to optimize the waste production, efficient use of energy, use of clean and renewable energy, minimizing the overall plant cost and reduction in equipment size. By reduction of equipment size the overall cost of the plant is largely affected and also the complexity of the plant also decreases because more number of complicated equipment means more number complicated equations which increase the complexity of the plant. From chemical engineering viewpoint these structured strategies largely improves the processing and

manufacturing capabilities of the plant. A sophisticated method of distillation called Process Intensified Distillation (PID) as shown in figure 1 seeks to improve the sustainability, productivity, and efficiency of the conventional distillation process.

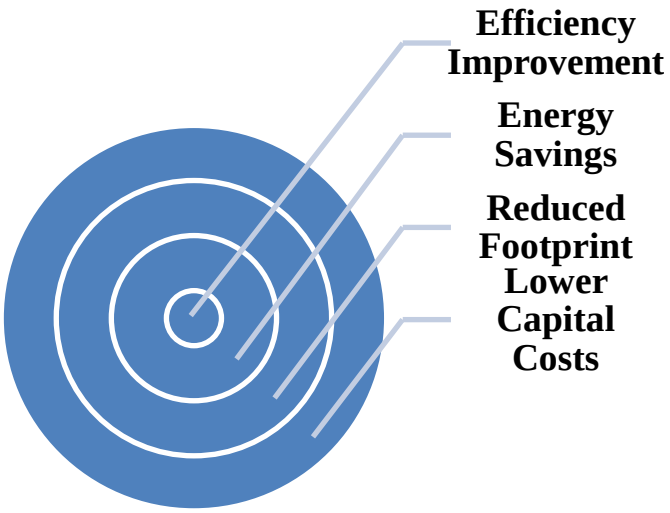

Fig 1 Key advantages of Process Intensification

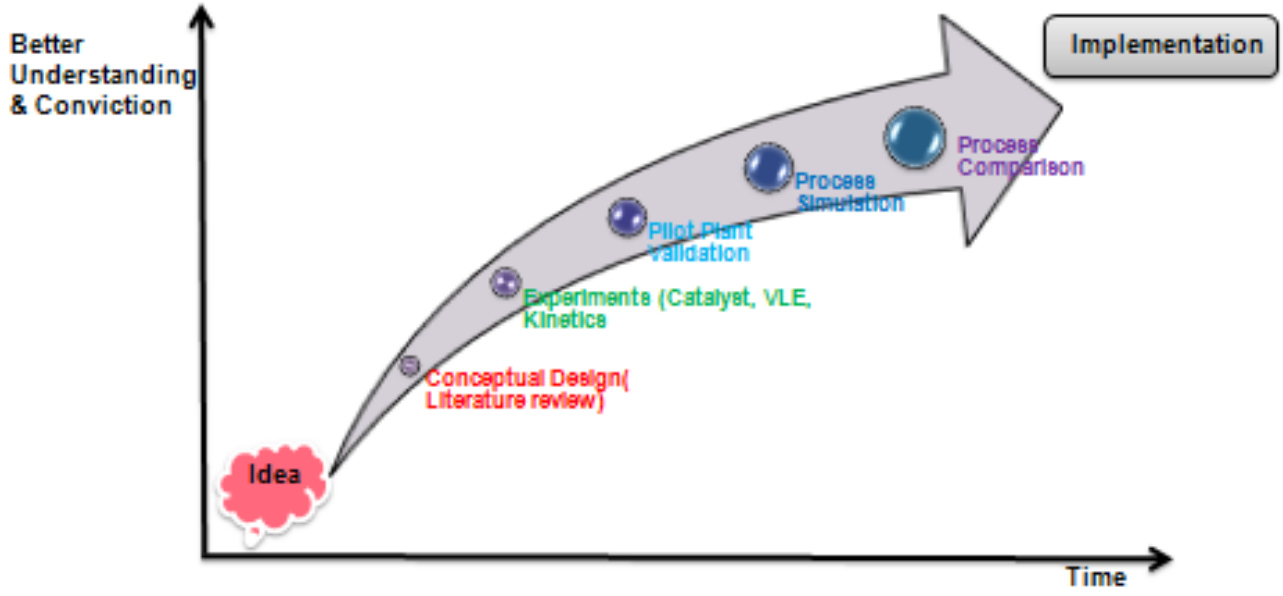

Fig 2 Steps Involved in Process Intensification

The steps involved in process intensification are shown above in figure 2. Chemical engineering mainly deals with conversion of raw materials into useful products in an optimum and a safe way with the help of two major operations i.e. Unit Operations and Unit Process. Unit operations are mainly related to physical changes occurring in the process whereas Unit process involves chemical conversions with the help of some chemical reactions. One of the most popular unit operations is distillation. Distillation is a separation technique which works on the principle of relative volatility or boiling point difference. It is energy extensive process as a huge amount of energy is required to vaporize the mixture. [2]

The Distillation columns alone consumes a lot of energy as compared to other equipments used in the process industries. The major disadvantage with the distillation technique is its energy usage. Normally Reactive Distillation is treated as a special case of distillation such as enhanced distillation like azeotropic or extractive distillation but it is not completely true in a sense because reactive distillation is not only a distillation technique or an enhanced distillation technique because it is not just a separator where only separation of two compounds is taking place but it is an reactor as well where reaction along with separation is taking place.

As its name says reactive distillation is a combination of reactor and a distillation column in a single unit. Process intensification is all about enhancing the currently existing process to the maximum possible extent without compromising the sustainability of the process. Reactive distillation is also called as a Multifunctional Reactor that means our purpose is to perform a desired reaction and the distillation will help reaction so that some enhanced performance is achieved so it is not just an separation methodology, we can refer it to as a reactor in which distillation is employed or it can be a distillation column where reaction is employed depending upon the application we are concerned about. The term Reactive Distillation should be taken in broader sense as far as its applications are concerned because it is not just a theoretical concept just to be studied from books but also a commercially viable and feasible technique.

The design of a multifunctional reactor solely aims to increase the efficiency of the reaction taking place inside the reactor with the integration of two or more operations in order to achieve different objectives which results in reduction of total capital expenditure. This is how chemical process intensification has emerged greatly in recent years because it offers multiple advantages

over the orthodox process. Moreover Process intensifications have some limitations as well which needs to be addressed carefully.

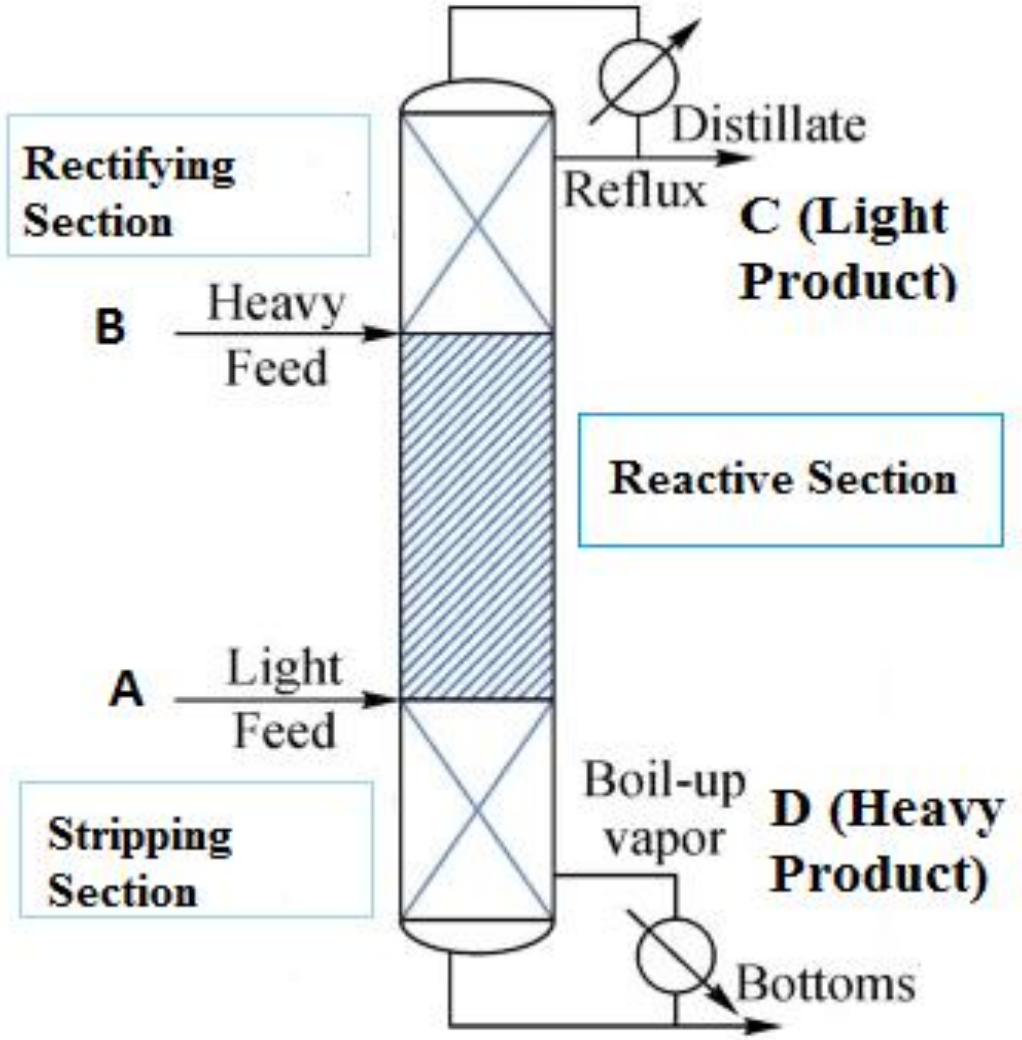

Fig 3 Schematic diagram of Reactive Distillation

Let us consider the following reversible reaction,

$$A+B \leftrightarrow C+D$$

Order of Relative Volatilities,

$$\alpha_C > \alpha_A > \alpha_B > \alpha_D$$

Relative volatilities play a very important role in reactive distillation setup because if there is no difference in vapour pressure then the separation is not possible. The feeding arrangement in the reactive setup is also very crucial because as shown in the figure 2 the reactants are A and B in which the A is the lighter component that means i.e. more volatile than the other reactant B. So the component A is fed from the bottom of the reactive section and B being the heavier is fed from top of the reactive section so that the reactants can have a better contacting in the reactive section. [3]

The reactive section which has catalyst on it will help the reactants to produce products C and D. Now among C and D, C being the lightest component will rise up and it will be collected as top product whereas D being the heaviest product will get collected from the bottom as bottoms. So the first thing you need to check to find whether the reactive distillation can be applied or not is the relative volatilities of all the components. Near about 1970's the United Kingdom based industry named Imperial Chemical Industries (ICI) introduced the concept of process intensification. The objective of the industry was to decrease the size of new chemical plants in order to reduce the total cost of the plant. There has been a significant paradigm shift from 1970's to today's situation regarding the meaning of process intensification because earlier the only objective was to reduce the capital cost by decreasing the equipment size but today the objectives are more diversified towards the increase in overall effectiveness and conversion of the products.

In Chemical engineering the process design is a very crucial step but it is not a single step process, it is carried out in different stages. Broadly process design can be classified in following three stages as shown in figure 4

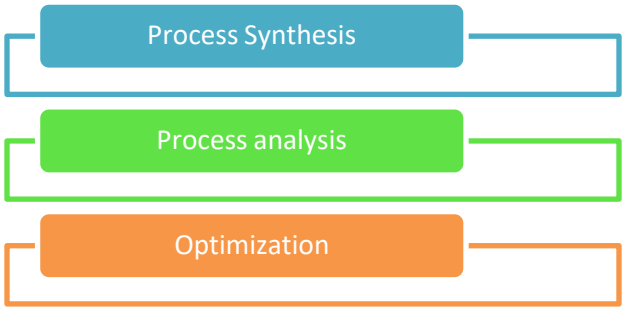

Fig 4 Stages of process design

In the first step the flow sheet of the complete process is prepared keeping all the equipments and their interconnections in mind. This requires good understanding of the complete process which is gained through experience of solving different simple and complex design problems. This step is also referred to as conceptual design step and the main motive of this step is to find the best process flow sheet. After this step the analysis of the process is done by writing several material and energy balances over the complete process. By these set of equations a mathematical model is prepared to observe the changes in output with some sort of input changes.

Mathematical modeling of a process provides some equations which are representative of the whole process and complete study of the process can be done by just observing these equations. These set of equations helps to predict the behaviour of the process more accurately without making significant changes to the existing process.

The last step in the process design is the optimization in this step the complete optimization is done keeping the safe operation of the whole process in mind. Several types of optimization techniques are employed using some algorithms.

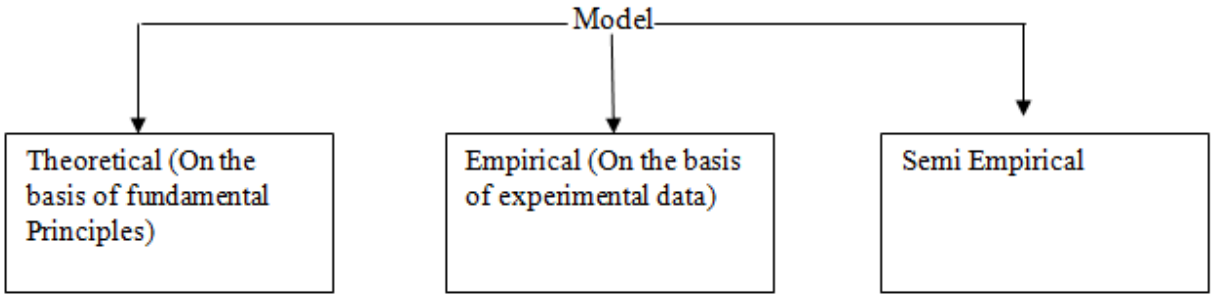

Fig 5 Classification of model

1.1 Systematic Model Building:

A model building starts with identifying the influencing factors like vapour liquid equilibrium, kinetics or we can say the first principle relations. But in case of empirical model, equations itself can be developed using experimental values. Validation of result is must and can be correlated using simulation or historical data. A proper sequence of flow-sheeting for model building is shown in figure 5

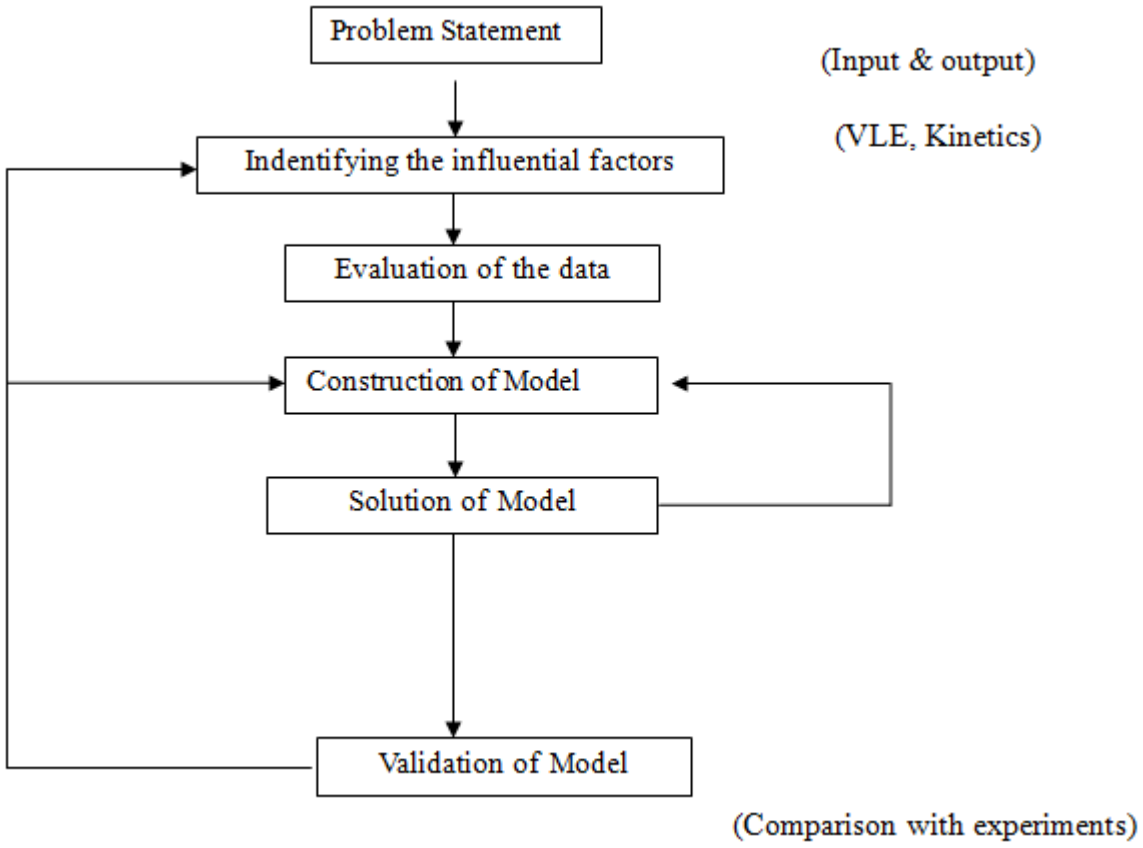

Fig 6 Flow-sheeting for model building

With the availability of various simulation software's it has become easier to perform various process intensification techniques in order to achieve desired output. Earlier when these simulation software were not there one has to make many pilot plants in order to perform experiments, which was a costly as well as time taking process. Today various innovative

methodologies are available to convert the schematic diagrams or complex flow sheets to simple Numerical form. Some of the methods are listed below:

- Process Matrix Technique
- Stream Connection Technique
- Incidence Matrix Technique
- Adjacency Matrix Technique

In the process matrix method, each unit in the information diagram is assigned with a number and each stream is also assigned with a number. The streams entering any unit are assigned with a positive number (INPUT Stream) and streams leaving any unit are assigned a negative number (OUTPUT Stream). A sample flow sheet is shown in figure 6. The matrix has some columns and some rows; each unit is given one row of the process matrix and that row is sufficient to describe all the connections of that unit. The contents of that row is basically the number assigned to the particular unit, the name of the unit (MIXER, DISTLL etc) and their respective associated stream numbers. In order to develop a better picture of this process matrix method let us consider an example

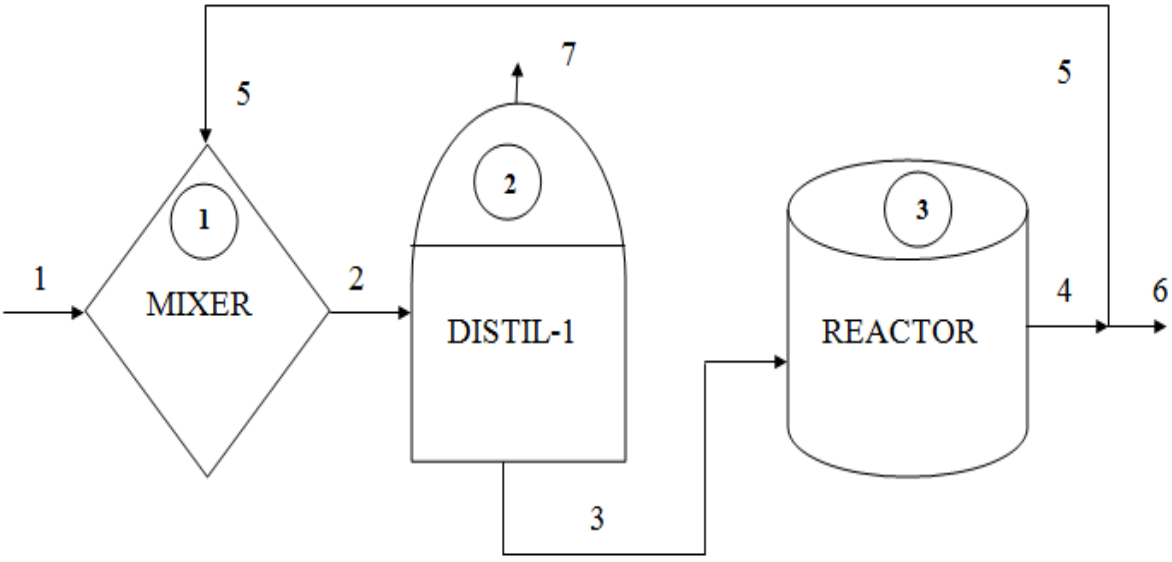

Fig 7 Sample Flow sheet example of process matrix modeling

Table- 1 Process matrix

UNIT	UNIT NAME	ASSOSIATED STREAM NUMBERS		
1	MIXER	1	5	-2
2	DISTIL-1	2	-7	-3
3	REACTOR	3	-4	

Thus the complex flow sheets can be simplified in these types of matrix for easier and better understanding of any process. With the help of process matrix it is easier to understand what stream links what units. The identification of input and output streams can be easily done without in depth analysis of the complete process flow sheet because any stream number with a negative sign clearly indicates that it must be a exit stream with respect to the particular unit. Also the order of the input and output stream plays a significant role in process matrix to understand this let us consider the example of distillation column(2) which has two leaving streams (-7,-3) one is the distillate leaving from the top and the other one is the residue leaving from the bottom. In the process matrix modeling there is a thumb rule that the first output is the overhead or top product whereas the second output is the bottoms. [4]

Such type of thumb rules are necessary to avoid any ambiguity in process modeling because if there is a standard way of writing the process matrix there will be no confusions and generalised process matrix can be written which will be universally accepted and understood. The major benefit with these process matrixes is that the engineer can readily identify all the stream connections and the units employed in the plant in no time. The Stream connection matrix is similar to process matrix method up to some extent. It is an array which contains stream numbers along with the unit numbers (from unit, to unit). The first column contains stream number the second one contains the from unit number and the third one contains the to unit number.

CHAPTER 2: LITERATURE SURVEY

Reactive distillation has gained a lot of lime light recently but it is not a new concept way back in 1860s it was first applied for the recovery of ammonia in the classic Solvay process, although the term reactive distillation was not coined then but it was practised. Reactive distillation is like an Old Wine in a new bottle. Many patents were registered but till then reactive distillation was only a theoretical concept that was only on paper. The industrial application of reactive distillation started in 1980 when Eastman Company started production of high purity methyl acetate from methanol and acetic acid. This was the first time when commercial viability of reactive distillation was in front of the whole world. After that many industries started using reactive distillation in their process and hence reactive distillation gained popularity. Initially the application of reactive distillation was limited only to equilibrium based reactions like methyl acetate production but later on its other applications were also discovered.

Concept of Reactive Distillation

For reversible reactions, where equilibrium is important we can improve equilibrium conversion by removing product in the reactor. (Le Chatelier's Principle)

Let us consider this reaction

$$\mathbf{A+B \leftrightarrow C+D}$$

If a reversible reaction is taking place such that reactants A and B are reacting in order to form products C and D. If we keep on removing the product C the equilibrium conversion to product D increases.

Due to the integration of reaction and distillation for a certain class of reacting systems, the researchers are showing much interest to develop reactive distillation**.** The clubbing of reaction with distillation in a single column was observed by some researchers. Due to his contributions he was awarded for his work for establishment of a continuous process for production of methyl acetate but until 1980s no industry was setup to explore the commercial viability of reactive distillation. In 1984 at Eastman Kodak. One of the pioneers discussed about process for manufacturing of methyl acetate using methanol and acetic acid using a homogenous catalyst. Figure 8 shows the conventional method of methyl acetate production while figure 9 shows the

process intensified reactive distillation for same process. The catalyst proposed was sulphuric acid. Their focus was to reduce the number of units that were being used in the orthodox process. Due to the equilibrium limitations it was found that the nature of the process was very complex, the reason being the formation of two minimum boiling azeotropes. [1]

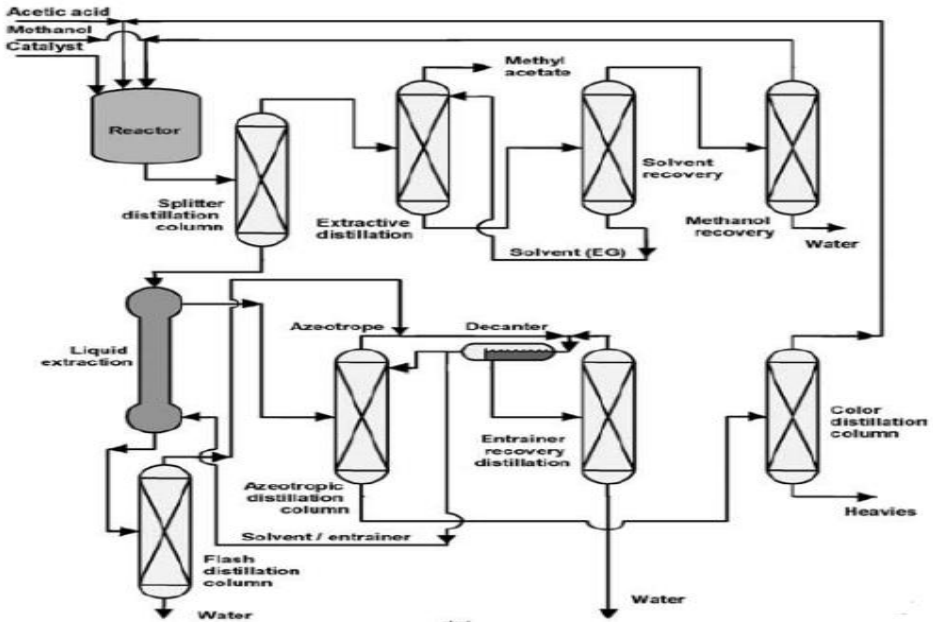

Fig 8 Conventional flow sheet for methyl acetate

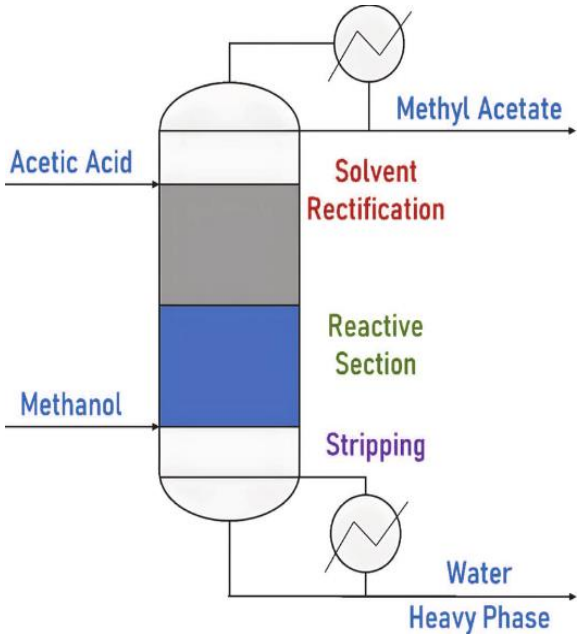

Fig 9 Reactive distillation synthesizing methyl

After the successful production of methyl acetate from reactive distillation people started exploring the phenomenon. People started working on production of fuel oxygenates such as Methyl Tertiary butyl ether popularly known as (MTBE). [4][5]

The thermodynamics solely aims the conversion of low grade energy to high grade energy which means the transformation of heat into work. In order to do so internal combustion engines were developed which requires any fuel. Fuel in a layman's language is any material that has potential to release some amount of energy when burnt. Fossil fuels are the primary source of all types of fuels that are being used in the world such as gasoline, diesel, aviation turbine fuel and many more.

There are two major concerns related to the fossil fuels first is that they are limited and on the second one is that they are not clean sources. The environmental concerns are forcing us to think of some alternative fuels in place of these fossil fuels. Gasoline blending is being practiced keeping the environmental concerns in mind. Blending is basically adding some fixed little quantity of other additives in the fuel in order to enhance their efficiency. Fuel Oxygenates are very crucial for gasoline fuels because as it is very evident from their name that oxygenates is adding oxygen, so oxygenates are added to gasoline in order to increase their octane number. Octane number is a property of gasoline fuels which signifies that how efficient a gasoline is, it is anti knocking quality of a gasoline fuel. So oxygenates are basically octane boosters which on addition of oxygen in the fuel increase the combustion of fuel.

Apart from addition of oxygen the fuel oxygenates also replaces some toxic materials from the gasoline such as lead. This property of oxygenates largely affects the quality of air as it reduces toxic emission in the atmosphere. Tert Amyl Ethyl Ether (TAEE) is one of the best examples of fuel oxygenates which can be used as a octane booster. The region being that the amount of aromatics is very less in the TAEE which makes the fuel to be environment friendly. So these types of fuel oxygenates can be made in reactive distillation setup, which increases the applicability of reactive distillation to great extent.

2.1 Modeling of reactive distillation

Modeling involves in-depth analysis of the whole process considering all the parameters affecting the system. Modeling of reactive distillation is not an easy job because of integration of

reaction and separation in a single unit. Here both reaction kinetics and vapour liquid equilibrium play important role. While modeling the reactive distillation column the assumptions should be in accordance to both VLE and reaction kinetics. The distillation temperature is only governed by the bubble point temperature but in a reactive setup this temperature should match with the favourable temperature for the reaction. [4]

One of the researchers performed a broad literature review regarding the commercial viability of reactive distillation; some of the handpicked published work is tabulated below

Table-2 Commercially Viable Reactions for RD

Reactive System	**Reference**
Acetic Acid + Ethanol → Ethyl acetate + water	Suzuki et al. (1971), Izarraraz et al. (1980), Alejski et al. (1996), Seferlis et al. (2001), Huang et al. (2007)
Acetic Acid + Methanol →Methyl acetate+ water	Barbosa et al. (1988), Yu, Weifang (2004) Sander et al. (2007), Chen et al. (2008)
Isobutylene + ethanol → ETBE	Sneesby et al. (1997), Jhon et al. (2003), Bisowarno et al. (2004),
Methanol + 2-methyl-1-butene → TAME	Baur et al. (2003), Huang et al. (2007) Katariya et al. (2008)
Isobutylene + methanol → MTBE	Doherty et al. (1992), Isla et al. (1996), Hauan et al. (1998), Sneesby et al. (1999), Baur et al. (2000) Qi, et al. (2004) Singh et al. (2005),
Adipic Acid + Hexamethylene diamine → Nylon 6,6	Jacobs et al. (1977), Grosser et al. (1987), Doherty et al. (1992).

Modeling of a reactive distillation system can be broadly divided in five sub categories

1. Equilibrium Stage and Non Equilibrium Stage Modeling
2. Homogenous and Heterogeneous system
3. Dynamic Study of reactive distillation

4. Thermodynamic Modeling
5. Kinetic Modeling

2.1.1 Equilibrium Stage Modeling

In this type of modeling approaches it is assumed that the system follows the Roult's law and at the same stage it is assumed that the leaving vapour and leaving liquid are in equilibrium. In this type of equilibrium stage modeling approach (EQ) broadly two deciding factors are there on the basis of how the reaction is implemented which may be either equilibrium based or rate based. If the methodology is equilibrium based then it is assumed that the liquid phase is in equilibrium and if the methodology is rate based then it is executed by means of a kinetic expression.[5]

2.1.2 Non Equilibrium Stage Modeling

In this type of modeling approach the VLE i.e vapour liquid equilibrium is assumed to be constant in each tray also it is assumed that in each tray there is a thermodynamic equilibrium. The differentiating factor between the both types of modeling approaches is that in non equilibrium stage modeling the effects of mass and heat transfer are to be considered in each tray whereas in equilibrium stage modeling this is not the case. The interfacial transfer rates play very crucial role while deploying this type of modeling approach because proper knowledge of reaction rates at each tray is required.

Several researchers conducted various studies over non equilibrium modeling for the case of esterification of methyl acetate and observed that while writing the balances over a specific tray for developing model equations a term accounting for interfacial mass transfer rate is required. Later they observed that this term can be written as the product of interfacial area and molar flux.

When these both techniques were simulated using some simulation software it was observed that there exists a comparable difference in the concentration profiles of equilibrium modeling and non equilibrium Modeling approaches, thus the extra efforts made by researchers in NEQ modeling were justified.

2.1.3 Homogenous and heterogeneous model

Another bifurcation on modeling of reactive distillation can be made as homogenous and heterogeneous model. In homogenous model in order to reduce the complexity of the system

certain assumptions are made such as pseudo homogenous kinetics where in heterogeneous models this is not the case.

Detailed analysis over the catalyst surface is required in order to understand the intra particle diffusion effects over the catalyst surface. In homogenous type of model it is assumed that the reaction takes is taking place only in liquid phase not in vapour phase. [6]

2.2 Manufacturing of biodiesel by process intensified distillation.

The Environmental concerns such as increased Carbon di oxide emission, pollution and climate change are rising day by day. In such a scenario the whole world is looking for some alternatives of fossil fuels as burning of these fuels produces CO_2. Bio diesel is one of the potential fuels that can replace the fuels based on the fossils. Biodiesel is an environmental friendly option which is made from biological sources typically derived from plant oil animal fats.

Emission of green house gases had forced the engineering enthusiasts to think of some other fuels such as biodiesel. Biodiesel can be blended with the traditional diesel to reduce the carbon footprints. The main ingredients of the biodiesel are Fatty acid mono alkyl esters, the Trans esterification of alcohols with fatty acids. The fatty acids are readily available in animal fats and vegetable oils. The reactive distillation technique employed to the biodiesel production shows impressive results in comparison to the traditional methods.

Two different types of catalyst are used first one is alkali and the other one is heterogeneous catalyst. The technical and economical aspects both play a very crucial role in selecting the catalyst. The reaction between the fatty acids and alcohols is highly reversible in nature which suits the reactive distillation setup. The product so formed in reaction is continuously removed which shift the reaction in forward direction which increases the production and conversion of the reaction.

2.3 Heat and Mass Integration

Distillation is the most energy intensive process as it requires a lot of energy for its smooth functioning so in the current scenario it is very much crucial to efficiently utilize the energy resources due to the environmental concerns. Heat and mass integration primarily focuses on

innovative integrations that will increase the efficiency of the reactive distillation system with reduction in energy usage.

Exothermic reactions are those reactions which liberate some amount of heat when the product is formed with the desired reactants so researchers observed that exothermic reaction can be performed in reactive distillation setup because the heat of reaction can be utilized in the column itself which will reduce the rebioler duty and in turn which will reduce the overall cost of the plant. Mass integration inside the reactive zone can be achieved by enhancing the mass transfer taking place over the catalyst surface.

2.4 Advanced methodologies with reactive distillation

Although it is a relatively novel concept, reactive distillation was initially used in the 1860s to recover ammonia from the traditional Solvay process; the phrase was not yet in use at the time, but the technique was known by that name. Reactive distillation is similar to a freshly opened bottle of old wine. Reactive distillation was merely a theoretical idea that existed only on paper up until a number of patents were registered.

In a research, it was noted that reaction and distillation may be clubbed together in a single column. Despite the fact that no industry had been established to investigate the commercial viability of reactive distillation prior to the 1980s, he was recognized for his achievements for helping to build a continuous process for the manufacturing of methyl acetate. [7]

One researcher discussed the use of a homogeneous catalyst in the methanol and acetic acid manufacturing process of methyl acetate in 1984 at Eastman Kodak. [1] Sulphuric acid was the catalyst that was suggested. Their main goal was to cut down on the quantity of units needed in the conventional procedure. The production of two minimal boiling azeotropes revealed the highly complicated character of the process, which was attributed to the equilibrium limitations. [2][4]

People began investigating the phenomenon once methyl acetate was successfully produced using reactive distillation. The process of producing fuel oxygenates, such as methyl tertiary butyl ether, or MTBE, was initiated. [8] When Modeling, the entire process is thoroughly examined, taking into account every factor that could have an impact on the system. Because

reaction and separation are integrated into a single unit, reactive distillation modeling is a challenging task.

Vapour liquid equilibrium and reaction kinetics are also significant factors in this case. Both VLE and reaction kinetics should be taken into consideration while modeling the reactive distillation column. The temperature at which distillation occurs is solely determined by the bubble point; however, in a reactive system, this temperature must coincide with the reaction's favourable temperature. [9]

Reactive distillation was first exclusively used in equilibrium-based reactions, such as the synthesis of methyl acetate, but other uses were subsequently found for it. By eliminating product from the reactor, we can increase equilibrium conversion for reversible processes where equilibrium is crucial. (The Principle of Le Chatelier)[10]

Let's think about this reaction.

$$\mathbf{A+B \leftrightarrow C+D}$$

If reactants A and B are reacting to create products C and D in a reversible reaction that is occurring, the equilibrium conversion to product D grows if we continue to remove the product C. Researchers are very much interested in developing reactive distillation since it integrates reaction and distillation for a certain class of reacting systems**.** [11]

Till 2010 the concept of reactive distillation was quite familiar to the world and after that people started advanced intensification in reactive distillation mechanism. One study introduces a systematic method for evaluating advanced reactive distillation technologies potential. It uses basic data to guide decision-making through four steps, demonstrated with five case studies for process development. [12]

Researchers have conducted experimental investigations on reactions such as esterification, transesterification, and alkylation in reactive distillation, employing diverse catalytic agents. This review paper summarizes these studies on reactive distillation processes. [13] Over the last thirty years, the design and optimization of reactive distillation have been extensively explored for various reactive mixtures. They categorized methods into graphical, optimization-based, and evolutionary/heuristic approaches, aiming to offer a contemporary review of these techniques.

The article outlines the information sought, advantages, limitations, and modifications of each method, and suggests future research directions for the optimization of reactive distillation processes. [14] Multiplicity analysis is also very crucial in the design of reactive distillation column as the reactive distillation is a highly non linear process so there are multiple steady states. Better understanding of multiple steady states is required in order to optimize the process.

Another literary work presents an overview of the characteristics and industrial outlook of latest reactive distillation technologies. The focus of this investigation encompasses five emerging technologies. [24]. Figure 9 (a-e) shows the emerging technologies coupled with reactive distillation.

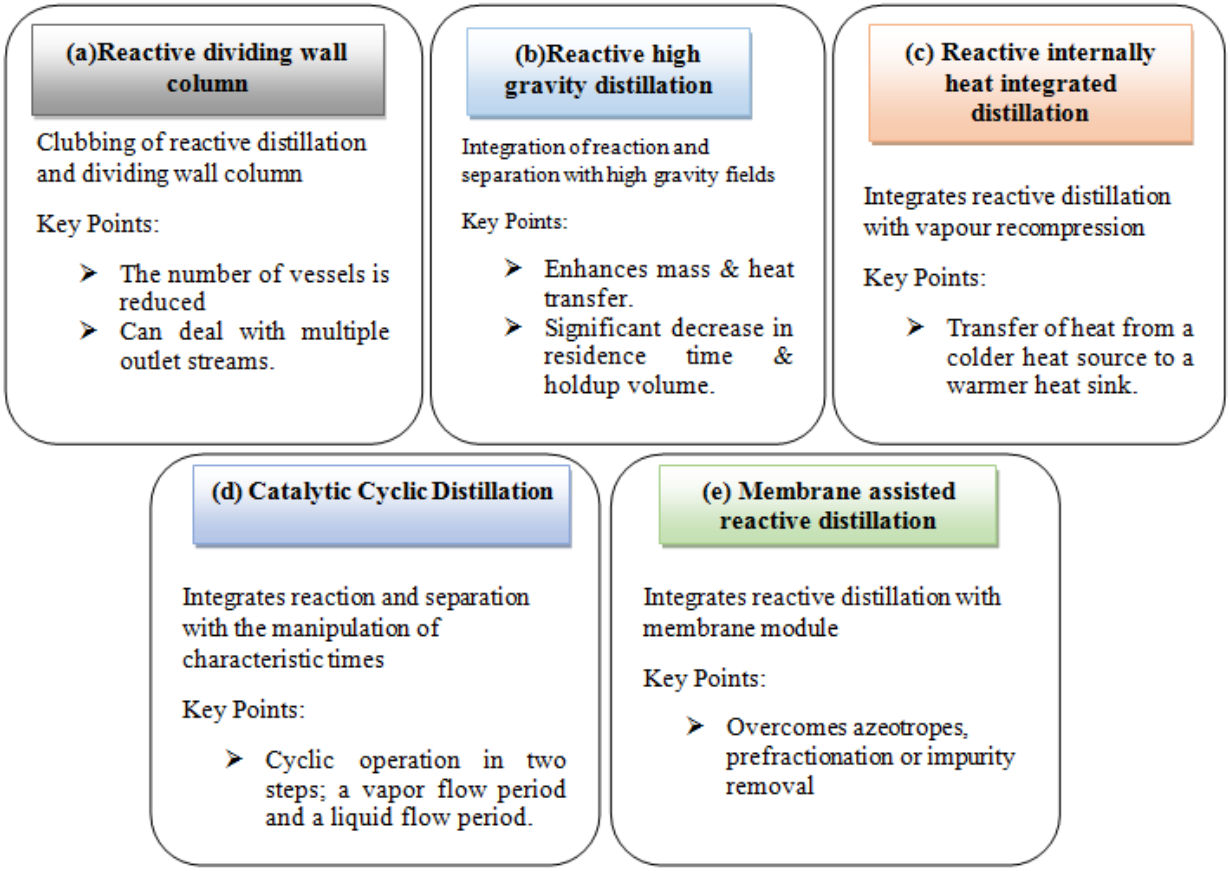

Fig 10 (a-e) Emerging Technologies coupled with Reactive distillation

The term multifunctional reactor can be coined as reaction equipment in which performance of reaction is drastically intensified by means of some or the other additional process function. So the Reactive distillation column also referred to as multifunctional reactor is clubbed with

several process intensification methodologies in order to intensify the process which will result in better conversion and yield. [20] Figure 10 shows the advanced reactive distillation technologies.

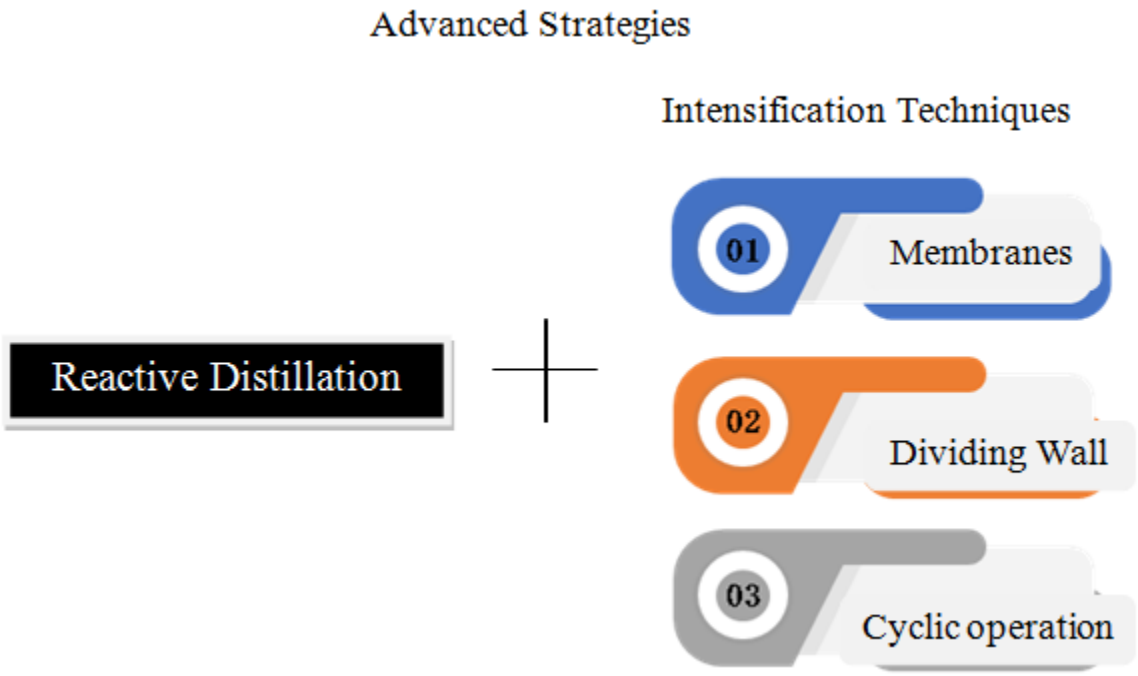

Fig 11 Advanced strategies for reactive distillation

There hasn't been much research published on reactive distillation control. The goals of the reactive distillation column control process should be to maximise reaction performance and achieve the required level of product purity. The choice of control algorithm and control configuration is part of the control system design. It is important to understand why a proper control strategy is required for reactive distillation. The presence of multiple steady states makes the control strategy very crucial as well as complex also because with a small change in input parameters the output conditions can be drastically changed and steady state will be disturbed. Now it is very difficult to find the next steady state because it is not certain that the process will show the next steady state on which input parameters that is why a robust and reliable control strategy is required for the reactive distillation process so that it can deal with existence of multiple steady states.

CHAPTER 3: PROBLEM FORMULATION

The Chemical process industry is responsible for about one third of the total energy used and the associated Carbon di oxide emissions in the industrial sector, distillation alone is responsible for about 40 % of the energy used in the chemical industry. Distillation the undisputed king of industrial separation process is a low thermal efficiency process that currently consumes 4.8 quadrillion BTUs of energy.(Source- Department of Energy U.S)

The Distillation columns alone consumes a lot of energy as compared to other equipments used in the process industries. The major disadvantage with the distillation technique is its energy usage. Normally Reactive Distillation is treated as a special case of distillation such as enhanced distillation like azeotropic or extractive distillation but it is not completely true in a sense because reactive distillation is not only a distillation technique or an enhanced distillation technique because it is not just a separator where only separation of two compounds is taking place but it is an reactor as well where reaction along with separation is taking place.

As its name says reactive distillation is a combination of reactor and a distillation column in a single unit. Process intensification is all about enhancing the currently existing process to the maximum possible extent without compromising the sustainability of the process. Reactive distillation is also called as a Multifunctional Reactor that means our purpose is to perform a desired reaction and the distillation will help reaction so that some enhanced performance is achieved so it is not just an separation methodology, we can refer it to as a reactor in which distillation is employed or it can be a distillation column where reaction is employed depending upon the application we are concerned about. The term Reactive Distillation should be taken in broader sense as far as its applications are concerned because it is not just a theoretical concept just to be studied from books but also a commercially viable and feasible technique. So the problem statement is To develop a process intensified distillation setup & examine the application for synthesis of methyl acetate through modeling, simulation and experiment.

CHAPTER 4: METHODOLOGY

Reactive Distillation offers various advantages but its modeling is quite a tedious job to do because while modeling one has to take in account both the reaction kinetics as well as vapour liquid equilibrium data which makes the whole process more complicated. While doing flow sheeting sometimes it becomes very difficult to understand the inlet and outlet streams so we have proposed a process matrix to ease the flow sheeting of any process.

A typical reactive distillation flow sheet is given below

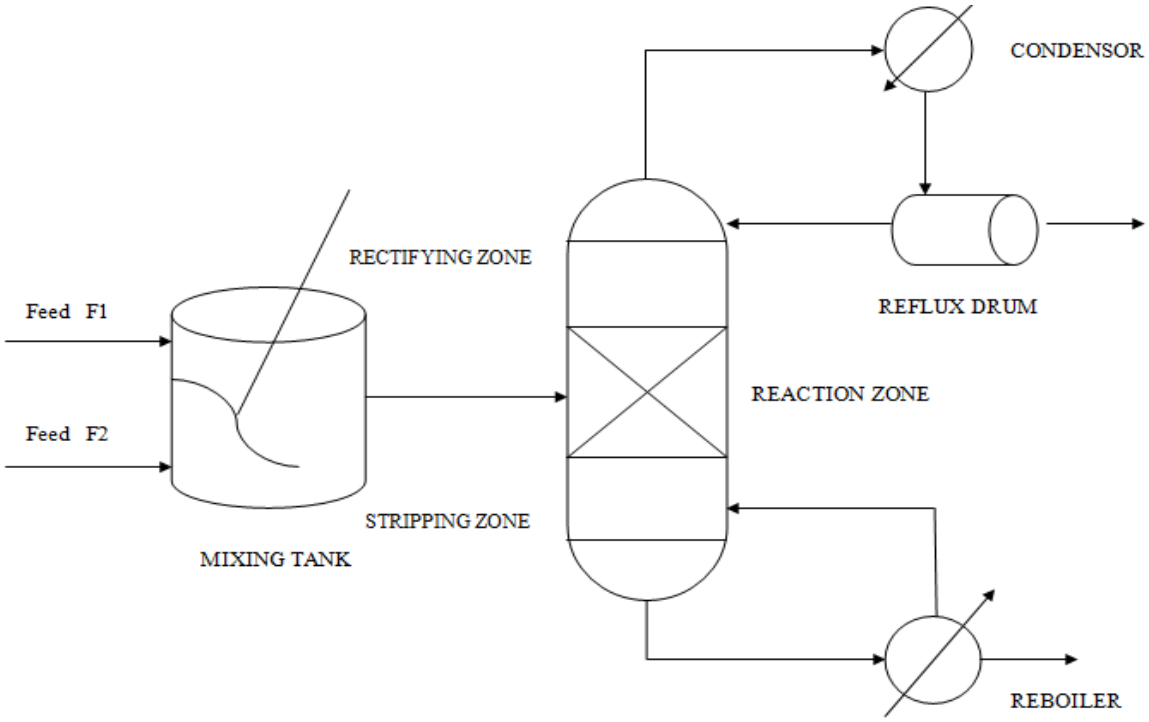

Fig 12 Flow sheet for Reactive Distillation

The reactive distillation arrangement depicted above uses a mixer to thoroughly mix the feed before it enters the column. The column is divided into three sections: the rectification part at the top, the reactive portion in the middle, and the stripping section at the bottom. Below is the information flow diagram for the schematic diagram above.

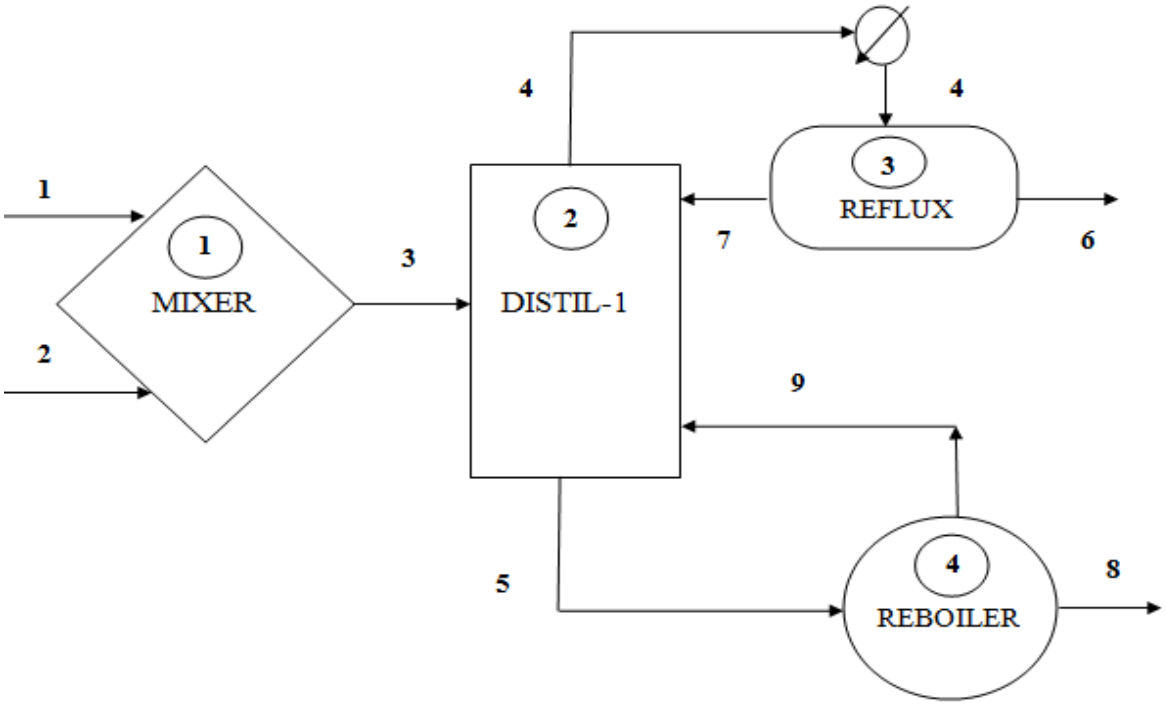

Fig 13 Information flow diagram for Reactive Distillation

Table- 3 Process matrix for reactive distillation

UNIT	**UNIT NAME**	**ASSOSIATED STREAM NUMBERS**		
1	MIXER	1	2	-3
2	DISTIL-1	3	-4	-5
3	REFLUX	4	-6	-7
4	REBOILER	5	-8	-9

Thumb Rules for Process matrix;

- All the incoming streams (inlet) to a particular unit should be numbered with a positive sign.
- All the leaving streams (outlet) to a particular unit should be numbered with a negative sign.

4.1 Modeling of Reactive distillation

The Modeling of reactive distillation was done considering the case of methyl acetate production.

$$CH_3COOH + CH_3OH \rightarrow CH_3COOC_2H_5 + H_2O$$

The following assumptions were made in order to write the balances over the system and to obtain modelled equations:

(1) Assume that every tray is an ideal stage

(2) Take into account non-equal molar overflow

(3) Model the liquid flow from each tray using a hydraulic time constant

(4) Neglect the heat of mixing of water in acetic acid

(5) Assume equilibrium driven reaction kinetics. [17][8]

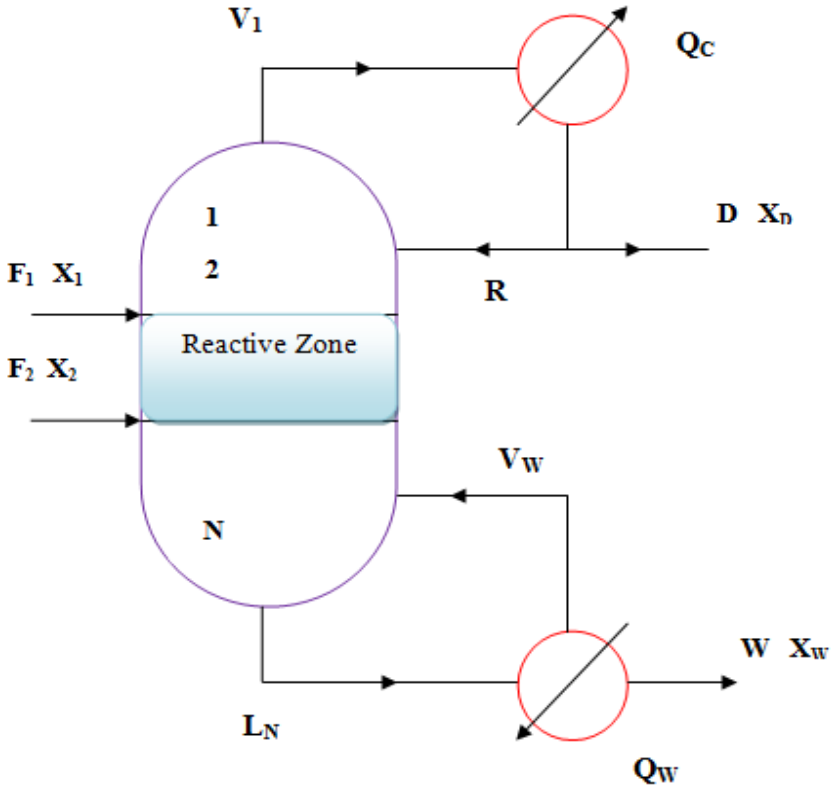

Fig 14 Representative Diagram of Reactive Distillation

For Rectifying and stripping section:

$$\frac{d(x_{n,i})}{dt} = (L_{n+1}x_{n+1,i} + V_{n-1}y_{n-1,i} - L_n x_{n,i} - V_n y_{n,i})/M_n$$

For reactive section:

$$\frac{d(x_{n,i}M_n)}{dt} = (L_{n+1}x_{n+1,i} + V_{n-1}y_{n-1,i} - L_n x_{n,i} - V_n y_{n,i} + R_{n,i})$$

For Feed section:

$$\frac{d(x_{n,i})}{dt} = (L_{n+1}x_{n+1,i} + V_{n-1}y_{n-1,i} - L_n x_{n,i} - V_n y_{n,i} + R_{n,i} + F_n z_{n,i})/M_n$$

Reboiler Heat Duty:

$$Q_W = Wh_{W,i} + V_W H_{W,i} - L_N h_N$$

Condenser Heat Duty:

$$Q_C = V_1 H_1 - (R + D)h_D$$

Energy Balance

$$V_{n+1}H_{n+1} + L_{n-1}h_{n-1} + F_n h_F - V_n H_n - L_n h_n - \lambda V_R R_{n,i} = \frac{d}{dt}(V_R H_R)$$

4.2 Experimental Setup for Reactive Distillation

We tried to make a column on the concept of Packed with Plate reactive distillation setup in order to get a better understanding of the process. The rectifying section and stripping section is designed on the concept of tray or plate column whereas the reactive section is designed on the concept of packed column. The reason for doing so is to get both the advantages of plate as well as packed column. The pressure drop is significantly less in packed column as compared to plate column. In the reactive section Amberlyst-15 solid catalyst is used. In a packed column it is always challenging to decide whether to use structured or random packing's, instead of just dumping the catalyst directly in the reactive section small packets of catalysts are used to avoid excess pressure build up in the reactive section.

Fig 15 Earthen Pot with inbuilt heater for reboiler

Fig 16 Waste teabags as catalyst packaging

Fig 17 Waste PET bottle as Reactive Zone MOC

Fig 18 Waste PVC pipe for full distillation column

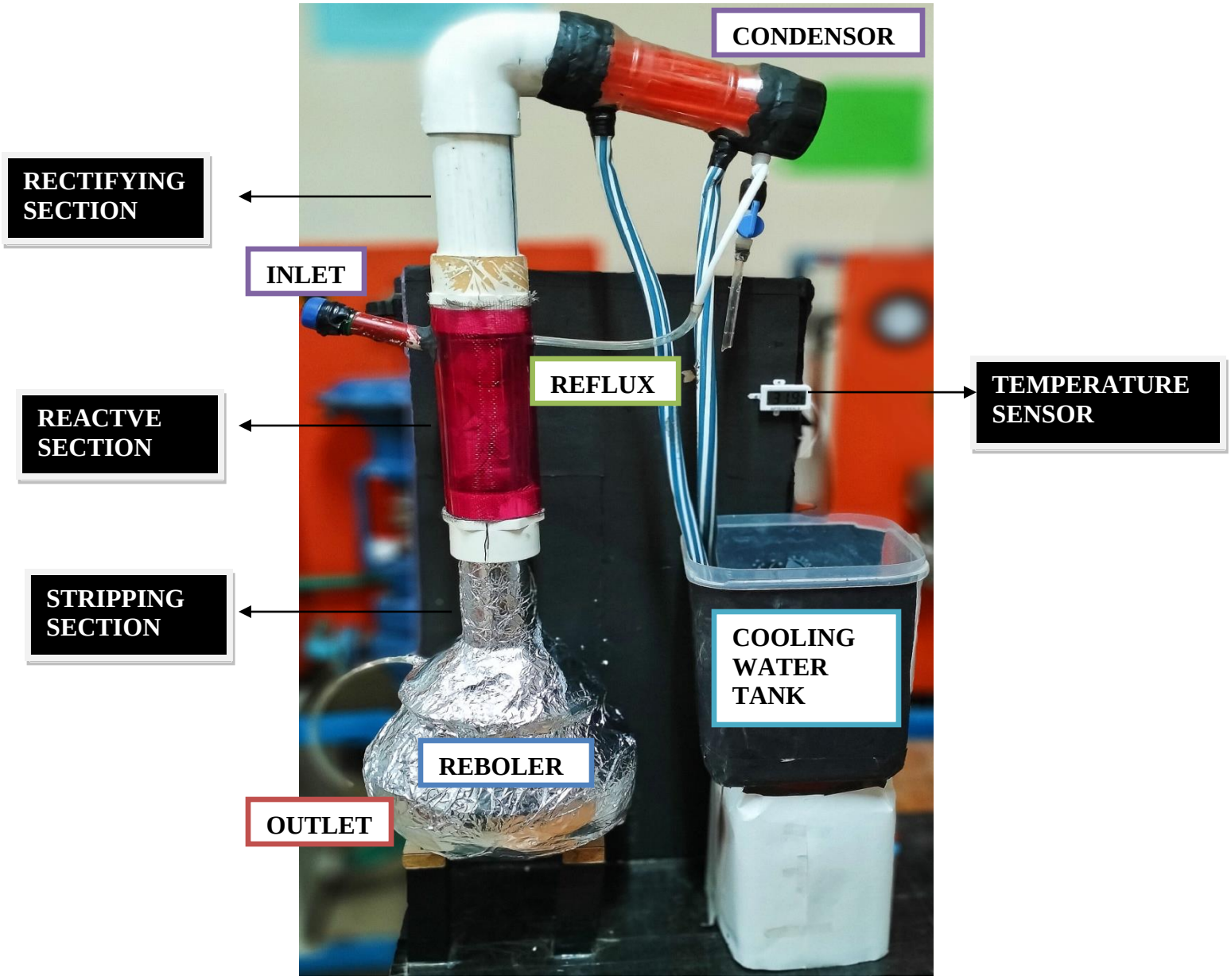

Fig 19 Pilot Plant Setup of Reactive Distillation

The Number of stages used in the experimental setup was 10 (including the reboiler and condenser). Condenser used is a total vertical condenser. The reactive section is between 3-6 stages, the enriching section is between 1-2 stages and stripping section lies between 7-8 stages. Catalyst used is an acidic ion exchange catalyst (Amberlyst-15)

4.3 Simulation

Simulation of methyl acetate esterification process was carried out using DWSIM simulation software. The results obtained from the experimental run and simulation was compared and it was found that the results are verifiable.

Non-ideal vapour-liquid equilibrium has been taken into consideration using the UNIQUAC model of activity coefficient. For vapour pressure, the extended Antoine model has been applied.

The interaction parameter values have been modified based on existing literature. The reaction is a basic reversible pseudo-homogeneous reaction. The flow sheet used is shown in figure 20.

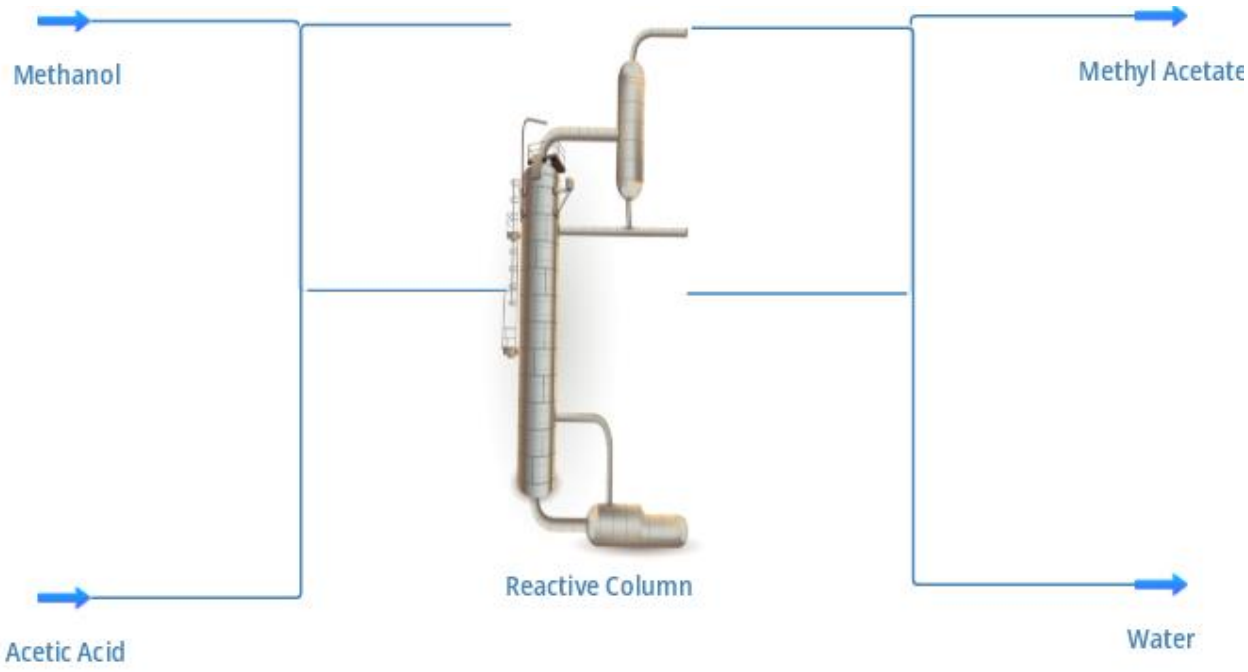

Fig 20 Flow sheet of methyl acetate reactive distillation column

CHAPTER 5: RESULTS & DISCUSSION

5.1 Results of Experimental setup

Both the feed streams were premixed in a mixer and the feed was introduced from the top of reactive section (where catalyst was filled). The Reboiler temperature was fixed to 70^0C, the reason being that the bubble point of methyl acetate is close to this temperature. The reboiler's pressure ranges between 249 and 300 mmHg, whereas the top stage's pressure fluctuates between 108 and 163 mmHg. The Purity of methyl acetate obtained by experimental run was 96%. The change in composition of the product along with rate in reactive zone with respect to time was observed and that is shown below in figure 21 and 22

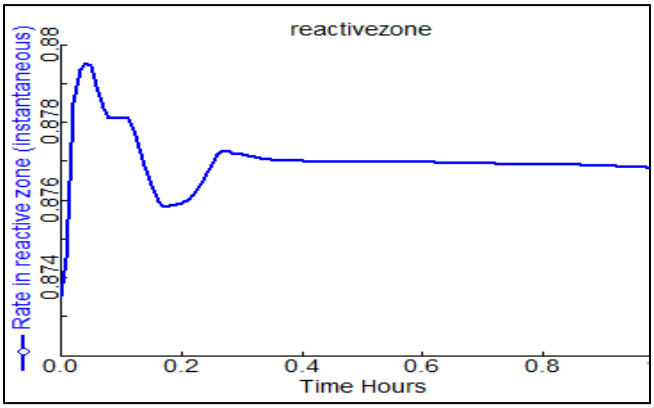

Fig 21 Rate in reactive zone

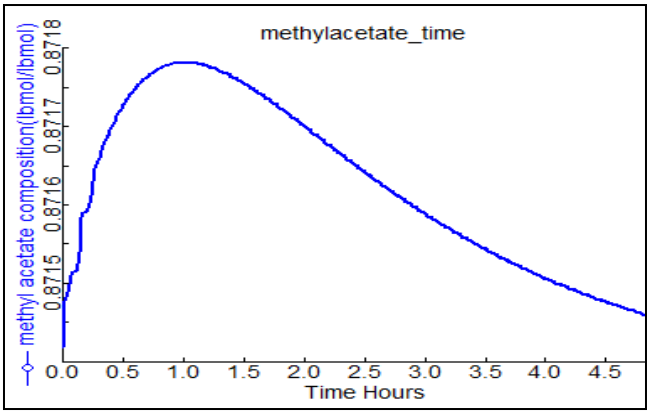

Fig 22 Change in product composition w.r.t time

5.2 Results of Simulation using DWSIM

Two different inlet streams of pure acetic acid and pure methanol were fed with an equal molar flow rate to the reactive distillation column at a pressure of 1 atm and a temperature of 298K. The Distillation column used here is not a simple distillation column but a complex column. It has been imported from ChemSep by using CAPE-OPEN Unit operation. Constant Pressure is maintained throughout the process. The top product obtained is methyl acetate with a purity of 98.7% while water is obtained as a bottom product with a purity of 99.5%.. The Reflux ratio is set to a value of 4.

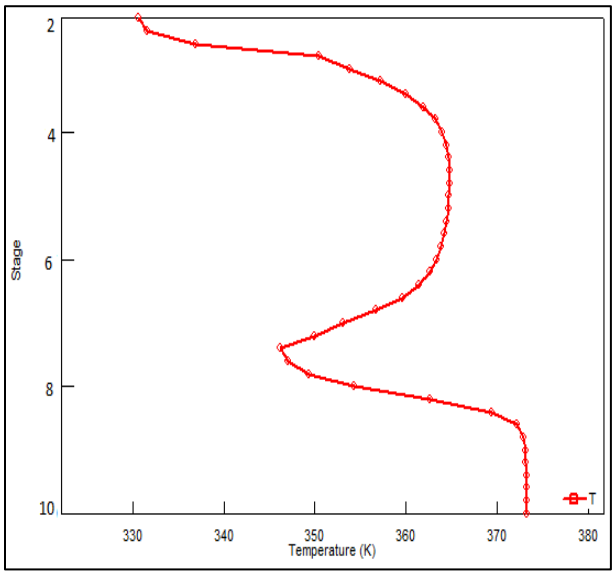

Fig 23 Stage wise Temperature Profile

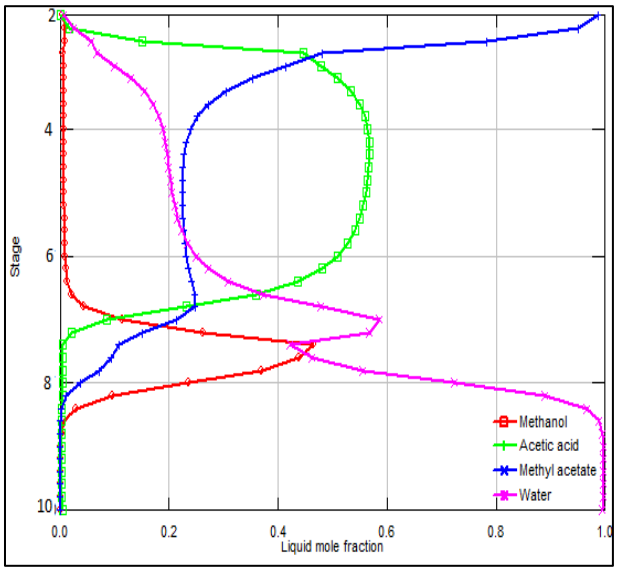

Fig 24 Stage wise Composition Profile

The advanced control strategy was applied in the DWSIM simulation software for the case of methyl acetate formation as shown in the figure. The fundamental reason for the preference for inferential control techniques using measurable temperatures is the unreliability of composition analysers.

Reactive systems often exhibit non-unique relationships between composition and temperature. [13] Input multiplicity can be avoided by proper selection of control strategy. Three control architectures that are used in methyl acetate reactive distillation systems were examined in the current work. Every structure has PI controllers and is SISO.

Tyreus-Luyben tuning technique was used. The reflux flow rate regulates the amount of methyl acetate present in the distillate. The heat input to the reboiler regulates the composition of the water in the bottoms. There is flow control over the acetic acid flow rate. The distillate flow rate and the bottoms flow rate, respectively, regulate the levels in the reflux drum and the column base.

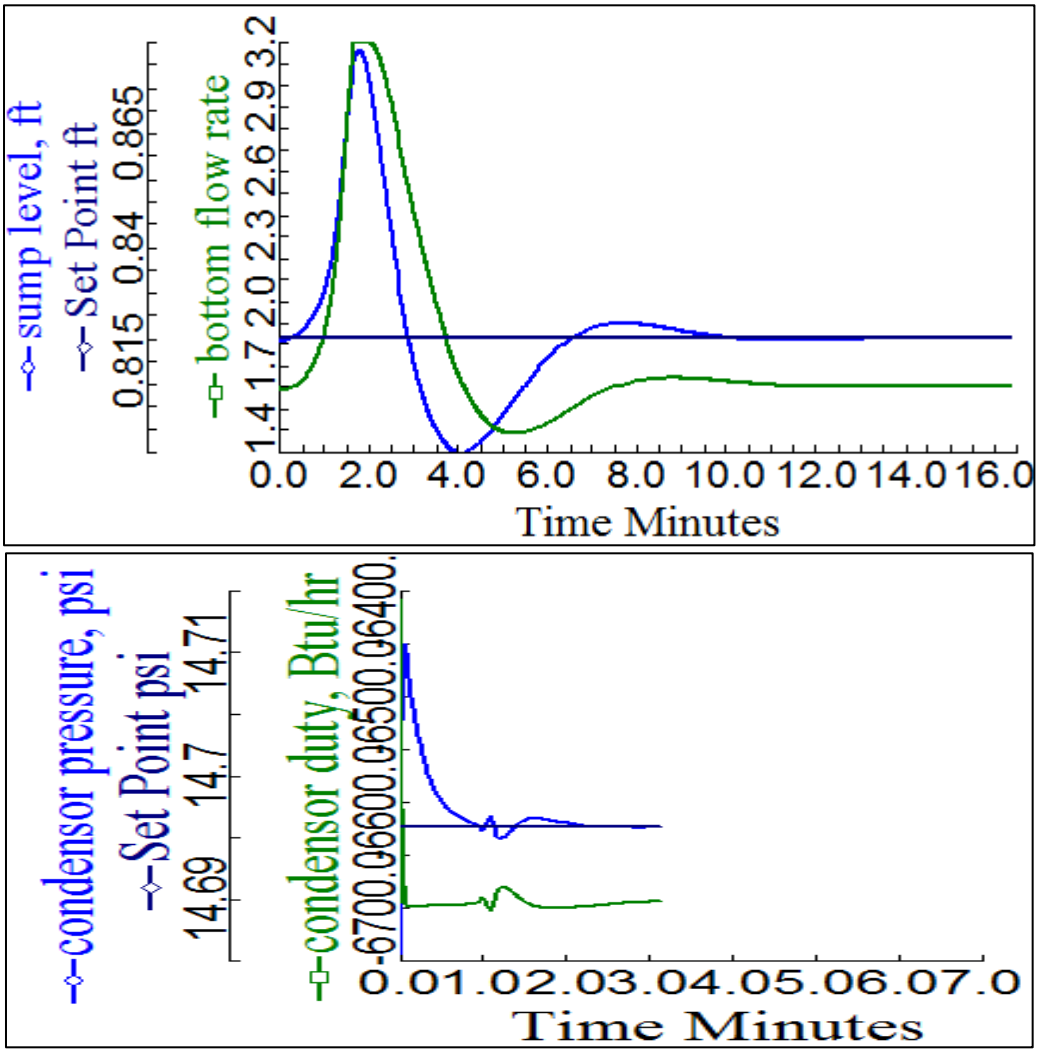

Fig 25 Performance of the Closed Loop Control Strategy for Methyl Acetate RD

This work highlights the advantages of reactive distillation from the process intensification point of view; it was found that reactive distillation is effective for various syntheses and manufacturing. The production of methyl acetate using methanol and acetic acid was studied and

it was found that 95% purity of methyl acetate was obtained. [9] Earlier when the methyl acetate was produced from the traditional method the plant contains 12 to 13 units because of various azeotrops formation. But when the reactive distillation concept was applied the whole process was done in a single unit, which drastically reduced the total expenditure. After that reactive distillation gained more popularity and several patents and papers were registered on reactive distillation. This field has a lot of scope for further research because there are certain limitations which still need to be addressed. The complexity of reactive distillation is due to the integration of vapour liquid equilibrium and reaction kinetics. Some sort of algorithms must be developed to deal with VLE and kinetics in a efficient way.

Some motives behind the applications of Reactive Distillation;

- To Surpass Equilibrium Conversion
- For Selectivity engineering
- For Better energy utilization
- For Higher purity products
- For Difficult separations (azeotrops)
- For better temperature control
- For longer catalyst life

CHAPTER 6: CONCLUSION

In Chemical engineering the process design is a very crucial step but it is not a single step process, it is carried out in different stages. Broadly process design can be classified in following three stages: Process Synthesis, Process analysis and Optimization. In the first step the flow sheet of the complete process is prepared keeping all the equipments and their interconnections in mind. This requires good understanding of the complete process which is gained through experience of solving different simple and complex design problems. This step is also referred to as conceptual design step and the main motive of this step is to find the best process flow sheet. After this step the analysis of the process is done by writing several material and energy balances over the complete process. By these set of equations a mathematical model is prepared to observe the changes in output with some sort of input changes.

Heat Integration: The Chemical process industry is responsible for about one third of the total energy used and the associated Carbon di oxide emissions in the industrial sector, distillation alone is responsible for about 40 % of the energy used in the chemical industry. Distillation the undisputed king of industrial separation process is a low thermal efficiency process that currently consumes 4.8 quadrillion BTUs of energy.(Source- Department of Energy U.S)

Environmental Sustainability: It contributes to green chemistry by enabling more efficient processes, reducing energy consumption, and minimizing waste production. As environmental concerns become more pressing, technologies like reactive distillation offer pathways to cleaner industrial processes.

Moreover identification of reflux and purge streams is easier in these types of process matrix than the orthodox flow sheeting techniques. Process intensification is not only related to the changes made inside the process in order to enhance the performance but also related to the techniques and algorithms employed to study or represent the process.

These types of novel techniques must be adapted by all the industries where flow sheets are used. These connection matrix are very crucial from safety point as well because in case of hazardous material these matrix can clearly depict that where these hazardous material are coming from and

where these streams are going, the workers will be extra cautious when dealing with these tanks and streams. This will reduce the risk of any leakage or spill of any hazardous material

Reactive distillation was studied for the case of methyl acetate formation; simulation was done using DWSIM simulation software. Moreover experimental analysis of methyl acetate was done in a pilot scale plant. Modeling of RD is also shown and in order to reduce the complexity of Reactive distillation for future researchers a systematic work flow for Process Development studies on Reactive Distillation is suggested below,

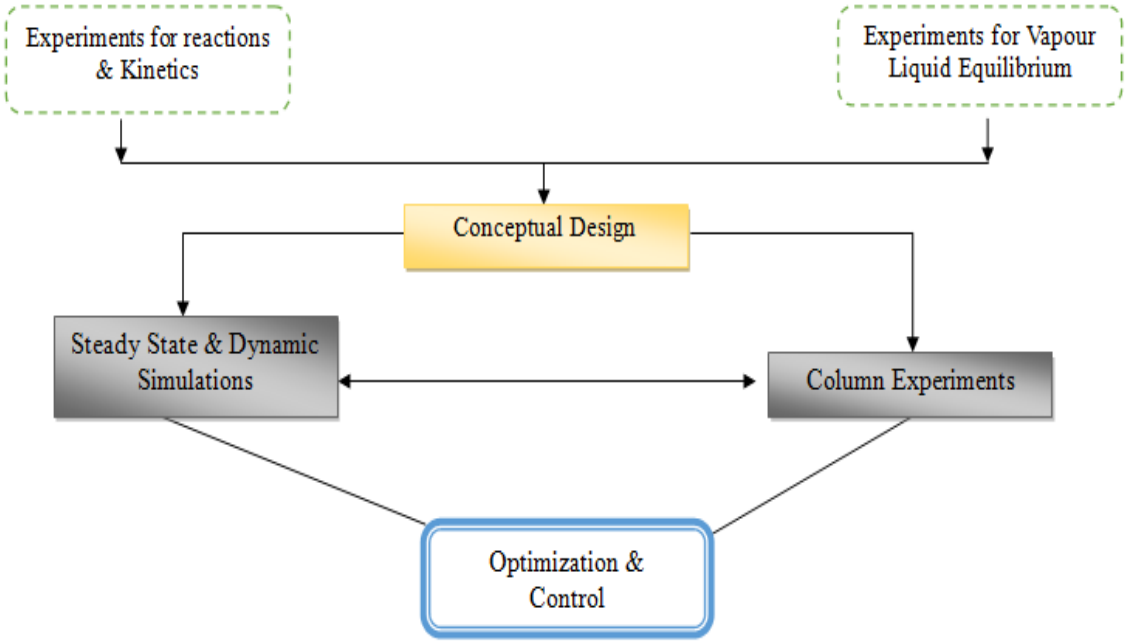

Fig 26 Systematic work flow for Process Development studies on Reactive Distillation

CHAPTER 7: OUTCOMES & SOCIAL RELEVANCE

7.1 Achieved Project Outcomes

- Successfully validated the dynamic simulation model with experimental or industrial data, ensuring its accuracy and reliability
- Highlighted the environmental benefits of the intensified distillation process, such as reduced greenhouse gas emissions and lower energy consumption.
- .Achieved cost savings through process intensification, which reduced the need for extensive equipment and minimized operational expenses.
- Utilized the process matrix modeling approach to systematically analyze and enhance the distillation process performance.
- Gained a comprehensive understanding of the dynamic behavior of the intensified distillation process under various operational scenarios.
- Applied the mass and energy balance over the reactive distillation setup.

7.2 Social relevance of the topic

Heat Integration: The Chemical process industry is responsible for about one third of the total energy used and the associated Carbon di oxide emissions in the industrial sector, distillation alone is responsible for about 40 % of the energy used in the chemical industry. Distillation the undisputed king of industrial separation process is a low thermal efficiency process that currently consumes 4.8 quadrillion BTUs of energy.(Source- Department of Energy U.S)

Environmental Sustainability: It contributes to green chemistry by enabling more efficient processes, reducing energy consumption, and minimizing waste production. As environmental concerns become more pressing, technologies like reactive distillation offer pathways to cleaner industrial processes.

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Daily Diary

* Reactive Distillation

Date 5 /1 /24
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Reactive Distillation is an innovative process that combines chemical rxn and seperation in a single unit, offering several advantages over conventional methods

Objectives:

* Understanding Reactive Distillation
* Analysis and Comparision
* Design and Simulation.

Reactors are the heart of chemical Process engineering. Adeption of an integrated approach to reaction and seperation may provide significant improvments in process design and operations

* Need For Reactive Distillation?

Due to the disadvantages of conventional process such as:

(i) They occupy a-lot of Spac
(ii) Installation costs are more
(iii) Consumes alot of energy
(iv) Consumes alot of time due to large number of distillation columns

In order to overcome these factors and to improve the reaction efficiency we require a technique i.e Reactive Distillation.

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* In a lay man's language RD is a combination of reaction and distillation in a single column.

* The Reactive Distillation consists of reactive section at the middle with non reactive rectifying and stripping section at top and bottom respectively.

RD has been successfully used and investigated in the Past four several rxn such as.

→ Hydrodesulphurization of light oil fractions
→ Transesterification
→ Aldol condensation, Alkylation.

Esterification:
Alcohols react with acetic acid to give corresponding ester and water

$$CH_3COOH + C_4H_9OH \rightleftharpoons C_4H_7COOCH_3 + H_2O$$

As it is reversible, it is difficult to acquire product at required rate and with required quality

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* Catalyst:

Amberlyst

Amberlyst is a brand name for family of solid catalysts used in various chemical processes.

-> High activity, high selectivity and stability in a wide range of chemical rxn

-> It is an amphoteric catalyst

-> Esterification, transesterification, nitration, alkylation, Biodiesel production

Date - 30/1/24

Rate Kinetics

$$CH_3COOH + CH_3OH \rightleftharpoons CH_3COOCH_3 + H_2O$$

Popken et al (2000) investigated the rate kinetics for synthesis of methyl acetate by an acidic ion-exchange resin (Amberlyst - 15).

(1) Pseudo Homogeneous model

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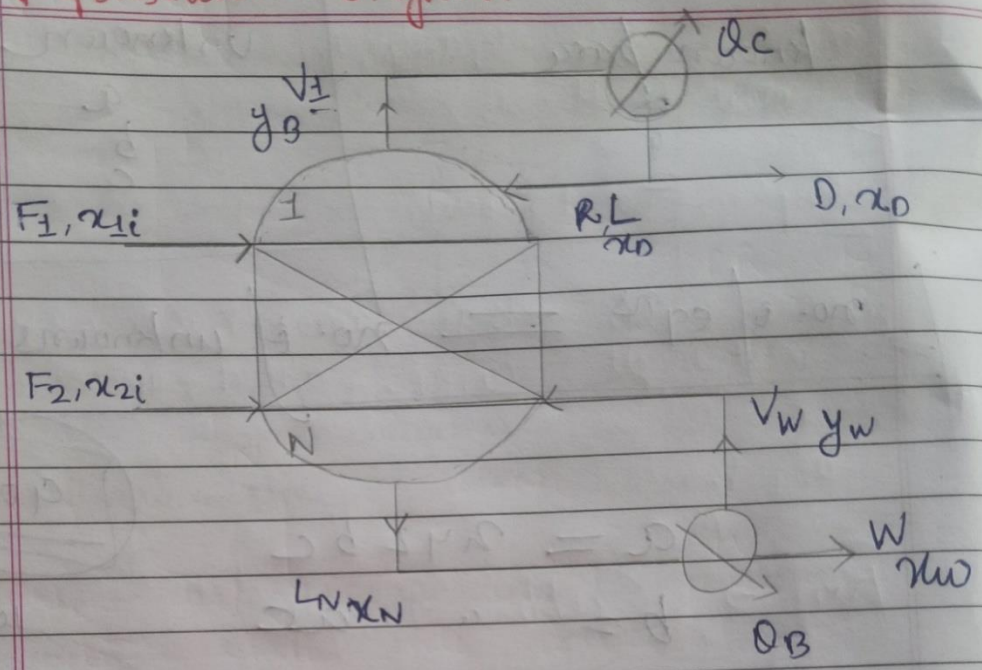
* Representative Diagram:



Nomenclature:

F = Feed Flow rate
D = Distillate Flow rate
W = Bottoms / Residue Flow rate
y_n = Vapour Composition on n^{th} Stage
x_n = Liquid Composition on n^{th} Stage
L_n = Flow rate of liquid on n^{th} Stage
V_n = Flow rate of vapour on n^{th} Stage

Note: (i) Top Down Approach is used for Counting of Plates
(ii) All the Flow rates are Molar Flow rates.
(iii) All the Compositions are mole fraction

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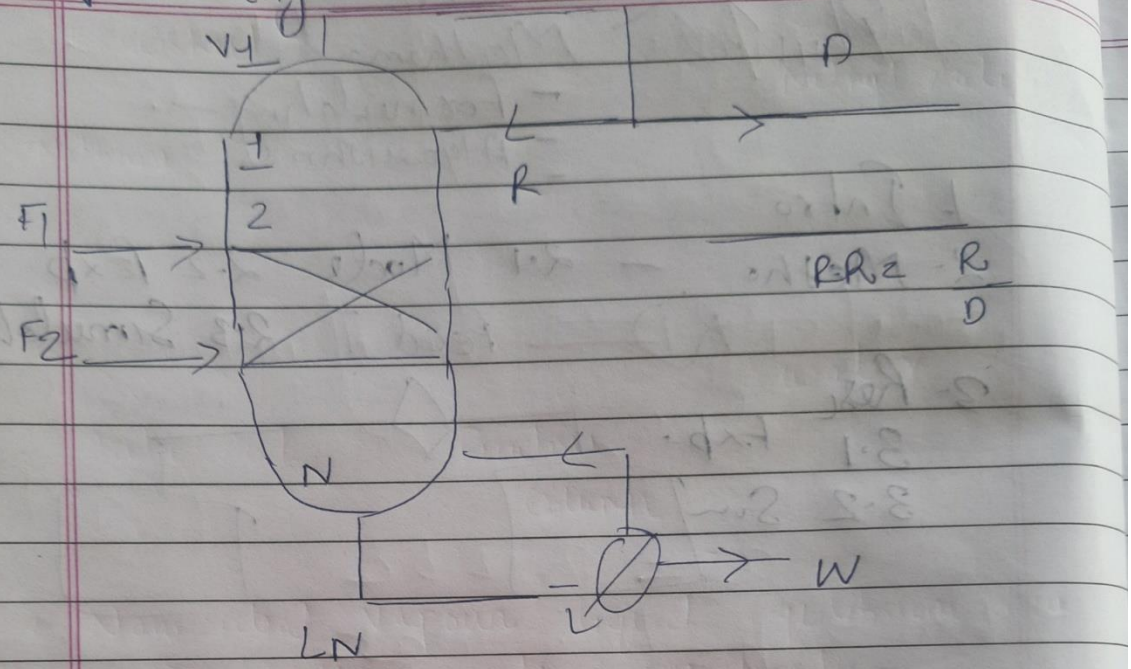
Modelling:



For Rectifying and Stripping Section

Time

Assumptions:

(1) Assume equilibrium & mixed reaction Kinetics
(2) Assume that every tray is an ideal stage
(3) Assume non equal molar overflow
(4) Model the liquid flow from each tray using a hydraulic time constant
(5) Ignore the heat of dilution of acetic acid in water.

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There are number of cutting edge-techniques for Simplifying Complex flowsheets or schmatic designs into numerical form.

* Process Matrix Modelling
* Stream Connection Modelling
* Incidence Matrix Technique
* Adjacency Matrix Technique

* Simulation
Methanol
Acetic acid
Methyl Acetate
Water

Cape-Open Unit operation
Equation-119
Pseudo Homogenous Reactor

* Simulation Using DWSIM

* DWSIM is a Simulation Software which is used to do various types of Simulations.

* The Simulation is done for the case of methyl acetate Formation.

* Methanol + Acetic Acid $\rightleftharpoons$ Water + Methyl Acetate

Results of Simulation:

* The top product obtained is methyl acetate with a purity of 98.7%. while water is obtained as a bottom product with a purity of 99.8%.

X —

Nowadays, the Chemical Industry is responsible for about 1/3 one third of the total energy used and the associated CO_2 emissions in the industrial sector, distillation alone is responsible for about 40% of the energy used in the Chemical industry.

Distillation- the undisputed King of industrial Separation process

Distillation is a low thermal efficiency unit operation that currently consumes 4.8 quadrillion BTUs of energy.

Source → Department of energy U.S.

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This is to certify that **Patanjali Shandilya** of **Madhav Institute of Technology & Science, Gwalior, India** presented the paper in the 2nd International Student Conference on Multidisciplinary and Current Technical Research (ISCMCTR - 2024), held at Madhav Institute of Technology & Science, Gwalior (M.P.), India, during 20 - 21 April, 2024.

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Author(s): Patanjali Shandilya (Madhav Institute of Technology & Science, Gwalior, India)*

Paper ID: 3

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Coordinator, ISCMCTR - 2024

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This is to certify that **Dr./Mr./Ms. Patanjali Shandilya** of **Madhav Institute of Technology, Madhya Pradesh, India** has given Oral Presentation on **Dynamic Simulation and Process Matrix Modeling of Process Intensified Distillation** in the **International Conference on Recent Advances in waste Minimization and Utilization (RAWMU-2024)** held from **23rd April 2024** to **24th April 2024**, organized by Research and Development Cell, Lovely Professional University, Punjab.

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