

## **Simulation Study on the Application of Reactive Distillation (RD) Column for Producing Ethyl Acetate via Esterification of Acetic Acid with Ethanol**

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### **Abstract**

Reactive distillation (RD) is an attractive way of improving process economics by combining distillation and reaction, especially for equilibrium limited reactions such as esterification. In this work, a simulation model for esterification of acetic acid by ethanol in a RD column was developed and verified against published data. Upon confirming the applicability of the simulation model, the effects of changing various operating and design parameters on the column performance were studied. It was found that independent changes in several parameters should enhance the overall conversion and purity. However it was discovered that the performance of the column could not be enhanced significantly with conventional RD column. Finally, a new configuration that involves the introduction of extractive zones in the RD column with extraneous component as an extractive agent was proposed. It was found that higher conversion and significant product purity enhancement could be attained with new configuration as compared to the conventional RD column.

*Keywords: Reactive Distillation, Mathematical Modeling, Ethyl Acetate, Parametric Analysis, Reactive Extractive Distillation*

### **1.0 Introduction**

Reactive distillation is a combination of reaction and separation in a single unit operation. It has captured the imagination of many researchers due to the demonstrated potential over the conventional method of processing. There are two major benefits of the reactive distillation operation. Firstly, the in-situ removal of product from the reaction zone causes equilibrium-limited reactions to shift further to product side, thus allowing higher conversion. Secondly, improved selectivity of the reaction was obtained due to product removal from the reaction zone. For a properly designed reactive distillation column, virtually 100 % conversion can be achieved [1]. There have been a number of successful commercial applications such as the synthesis of methyl acetate, methyl ethyl tertiary ether, ethyl tertiary butyl ether and ethylene glycol. Nevertheless, there are constraints that have to be met prior to considering its application [1,2].

The selected system for the study is the synthesis of ethyl acetate. Ethyl acetate is an industrially important bulk chemical used primarily as a solvent in the paints, coating and inks industry. Though ethyl acetate system is suitable for application of reactive distillation, it is not commercially attractive due to the inability to operate at or near the ideal condition to meet the best reaction and separation requirements. Most of the modeling works on ethyl acetate reactive distillation column available in past literature emphasise on model development followed by simulation using various solution strategies for model validation [3

- 5]. There was also a study conducted on the control aspects of the ethyl acetate reactive distillation column [6]. Huseyin and Mahmut conducted a more fundamental study looking at the effects of liquid phase activity model on the simulation of ethyl acetate reactive distillation column [7]. It is worth noted that none of the studies has reported the success of attaining high conversion and product purity i.e., in the order of 95% and above, from the application of the column.

Thus, an attempt is made in this study to explore further on improving the performance of ethyl acetate reactive distillation column. A mathematical model representing the RD column was developed and validated against published data available from past literature. Parametric study was then conducted on the model to analyse the impact on changing few critical design and operating parameters on the column performance. From the understanding developed in the parametric analysis, a new configuration known as ethyl acetate reactive extractive distillation column was proposed. It was found that significantly higher ethyl acetate purity and conversion was attained compared to the conventional reactive distillation column.

## 2.0 Materials and Methods

### 2.1 Mathematical Modeling

For the purpose of the study, a mathematical model was developed for the synthesis of ethyl acetate using reactive distillation column based on homogeneous catalyst. Several assumptions were made to ensure the simulation model is practically solvable. However care is taken to ensure that it will not have significant affect on the model effectiveness in representing the system. The set of assumptions made are as follows:

- Process is treated as in physical equilibrium i.e., vapor and liquid leaving any stages are in equilibrium, with kinetically controlled reaction.
- Constant enthalpy per stage thus allows enthalpy derivatives to be excluded from the model
- Constant tray liquid holdup thus allows molar flow derivatives to be excluded from the model.
- Ideal vapor phase due to moderate column operational pressure i.e., 1-4 atm.
- Reaction occurs in liquid phase, with each stage acting as a perfectly mixed CSTR reactor.
- Vapor molar holdup and vapor phase chemical reactions were neglected.
- Adiabatic operation and no heat losses to surrounding.
- Heat of mixing at each stage is considered negligible.

The equations used to model the equilibrium stages are known as the **MESH** equations (**M**aterial balance, **E**quilibrium relationship, **S**ummation (constraint equation) and **H**eat (energy) balance). To account for the reaction, the changes in the number of moles of component as a result of chemical reaction were introduced into the MESH equations. The enthalpy balances are expressed in terms of enthalpies of formation, which excludes the need for reaction enthalpies in the energy balance equation. In light of these assumptions, the model equations in terms of the molar and liquid flow rates are as follows:

### Condenser (stage 1)

$$0 = V_2 - L_1 - L_D + \sum R_{i1} \quad (1)$$

$$(hp_1)d(x_i)/dt = V_2 y_{i,2} - L_D (RR + 1)x_{i,1} + R_{i1} \quad (2)$$

$$0 = V_2 H_2^v - (L_1 + L_D) H_1^L + Q_c \quad (3)$$

### Trays

$$0 = F_j + L_{j-1} + V_{j+1} - L_j - V_j + \sum R_{ij} \quad (j=2,3,\dots,N-1) \quad (4)$$

$$(hp_j)dx_{i,j}/dt = F_j + x_{i-1,j-1} L_{j-1} + y_{i,j+1} V_{j+1} - x_{i,j} L_j - y_{i,j} V_j + R_{ij} \quad (j=2,3,\dots,N-1) \quad (5)$$

$$0 = L_{j-1} H_{j-1}^L + V_{j+1} H_{j+1}^v + F_j H_{z,j} - L_j H_j^L - V_j H_j^v \quad (j=2,3,\dots,N-1) \quad (6)$$

### Re-boiler (Stage N)

$$0 = L_{N-1} - L_N - V_N + \sum R_{iN} \quad (7)$$

$$hp_N d(x_i)/dt = L_{N-1} x_{i,N-1} - L_N x_{i,N} - V_N y_{i,N} + R_{iN} \quad (8)$$

$$0 = L_{j-1} H_{j-1}^L - L_N H_N^L - V_N H_N^v + Q_R \quad (9)$$

$$y_i P = x_i \gamma_i P_i^o \quad (10)$$

$$\sum_{i=1}^c x_{ij} = 1.0 \quad (11)$$

$$\sum_{i=1}^c y_{ij} = 1.0 \quad (12)$$

Equations 1, 4 and 7 are overall balances; equations 2, 5 and 8 are component balances; equations 3, 6 and 9 are enthalpy balances; equation 10 is vapor liquid equilibrium relationship; and finally equations 11 and 12 are summation equations.

The rate equation for the un-catalyzed reaction is [7]:

$$r = k_1 C_A C_B - k_2 C_C C_D \quad (\text{mol/sec m}^3) \quad (13)$$

where

$$k_1 = 0.485 \exp(-7186/T) \quad (\text{m}^3/\text{mol sec}) \quad (14)$$

$$k_2 = 0.123 \exp(-7186/T) \quad (\text{m}^3/\text{mol sec}) \quad (15)$$

and the rate of equation for the catalyzed reaction is [7]:

$$r = k_1 C_A C_B - k_1/K_c C_C C_D \quad (\text{mol/sec m}^3) \quad (16)$$

where

$$k_1 = (4.195 C_k + 0.08815) \exp(-6500.1/T) \quad (\text{m}^3/\text{mol sec}) \quad (17)$$

and

$$K_c = 7.558 - 0.012T \quad (18)$$

Special attention was given in the selection of liquid phase activity coefficient model. Among the various correlations available in literature, the empirical model as proposed by Suzuki et al. was used in the simulation study [8]. The developed simulation model was implemented on MATLAB<sup>TM</sup> for the purpose of conducting the steady state simulation. Relaxation algorithm was used to solve the modeling equations.

### 3.0 Results and Discussion

#### 3.1 Simulation Model Verification

For the purpose of verifying the simulation model, a similar configuration for the RD system as published in literature was applied to the model [6]. Basically, the proposed configuration involves feeding the two reactants in countercurrent direction and using homogeneous catalyst to aid the reaction that finally allows the attainment of higher conversion and purity. Table 1.1 summarises the simulation basis for the double feed catalytic ethyl acetate reactive distillation column.

Table 1.1 Column Configuration and Operating Conditions

Quantity	Units	Specifications
Feed 1 Flowrate	mol min <sup>-1</sup>	414
Feed 1 Phase		Saturated Liquid
Feed 2 Flowrate	mol min <sup>-1</sup>	411.9
Feed 2 Phase		Saturated Vapor
Feed 1 Temperature	K	391.8
Feed 1 Pressure	atm	1.00
Feed 1 Stage		4
Feed 2 Temperature	K	351.4
Feed 2 Pressure	atm	1.00
Feed 2 Stage		11
Number of Stages, N		13
Column Pressure, P	atm	1.00
<u>Liquid Holdup</u>		
Condenser, Tray	mol	4.4108 x 10 <sup>4</sup>
Re-boiler	mol	1.4703 x 10 <sup>5</sup>
Reflux Ratio, r		2.023
Re-boiler Heat Duty, r <sub>b</sub>		6.868 x 10 <sup>6</sup> cal/min
Bottom Flow, B	mol min <sup>-1</sup>	425.1

Table 1.2 provides the comparison between the simulation results of the study against the published results. The results were found to be consistent with those obtained from literature. The achieved conversion was 75.6%, which is higher compared to the equilibrium conversion for conventional arrangement i.e., a reactor followed by a separator. The product purity

achieved was 68.2% and it is higher than the azeotrope composition. Figure 1.1 and Figure 1.2 depict the liquid concentration profile in the column and the reaction rate profile for the double feed catalytic reactive distillation column respectively.

Table 1.2 Simulation Results For Catalytic Double Feed Ethyl Acetate Reactive Distillation Column.

Quantity	Units	Proposed Model		Nishith & Daoutidis (2001)	
		Top	Bottom	Top	Bottom
<b>Composition</b>					
Acetic acid (Ac)		0.019	0.2231	0.003	0.2100
Ethanol (Et)		0.1318	0.1123	0.080	0.1400
Ethyl Acetate (Ea)		0.6820	0.0896	0.650	0.1300
Water (W)		0.1672	0.5749	0.240	0.5200
Temperature	K	343.73	364.92	-	-
Product flow	mol /min	400.8	425.1	400.8	425.1
<b>Conversion and Purity</b>					
Et conversion	mole %		75.6		76.8
Ea purity	mole %		68.2		65.0
Reflux flow	mol/min		810.7		810.6

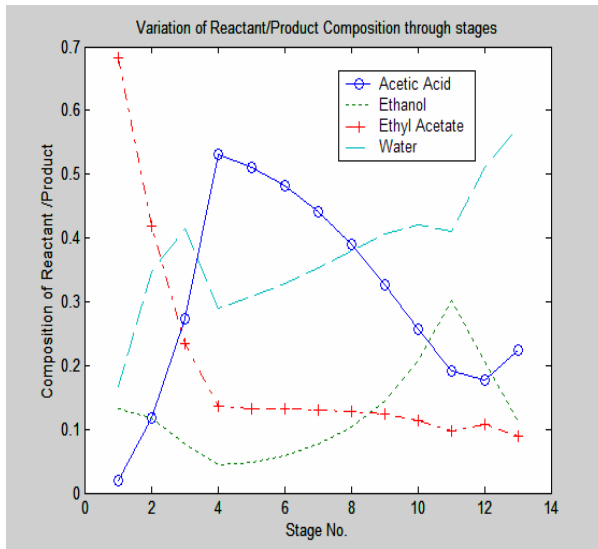


Figure 1.1 Steady State Temperature Profile Along The Column

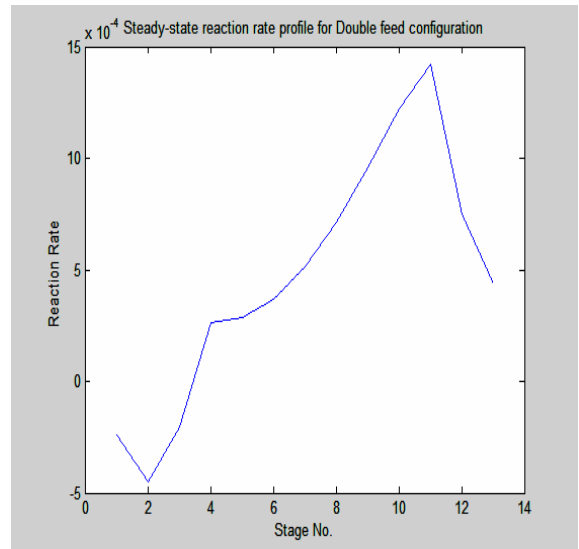


Figure 1.2 Steady State Reaction Rate Profile

As shown in the Figure 1.1, the acetic acid concentration reduces whilst the ethanol concentration increases in the upward direction in the column. This is as expected, as much of the reactants were consumed as the reaction proceeds. Ethanol feed travels up the column mainly in the vapor phase and is absorbed by the down-coming liquid, rich in acetic acid thus allowing reaction to take place. As the products were formed, the ethyl acetate is stripped from the liquid phase and travels with the vapour phase to the top of the column. Water formed from the reaction, moves along with acetic acid in the liquid phase down the column. As shown in the same graph, the concentration of acetic acid is much higher when compared to ethanol in the middle section of the column. This tends to limit the reaction achieved in the

zone. Steady state reaction rate profile indicates, in the first 3 stages from the top of the column, the reaction rates are negative as reverse reaction is prevalent in this zone. Low concentration of the reactants, ethanol and acetic acid, couple with high concentration of products in these stages has led to the situation. This significantly affects the performance of the column in terms of conversion and product purity.

### 3.2 Parametric Study

Reactive distillation column behaves significantly different from the conventional distillation columns due to the simultaneous interaction between the chemical reactions and the vapor liquid equilibrium. A parametric study looking at the effects of key design and operating variables were conducted using the above configuration. The selected parameters used for the column's performance measurement were conversion and the overhead ethyl acetate product purity. Conversion was selected in view of the indication needed for the extent of reaction whilst the top product purity was selected as the indication for separation performance for the column. In this parametric study, only variables involved in the study are varied while all other variables are fixed at its base case values.

#### 3.2.1 Variation in Number of Stages in Rectifying Zone.

Ideally, the rectifying zone of the ethyl acetate reactive distillation column is expected to remove the heavy components from the rising vapor stream to give pure ethyl acetate distillate, to recycle the heavier un-reacted reactants back to the main reaction zone and to remove ethyl acetate from the reaction zone to maintain favorable reaction conditions.

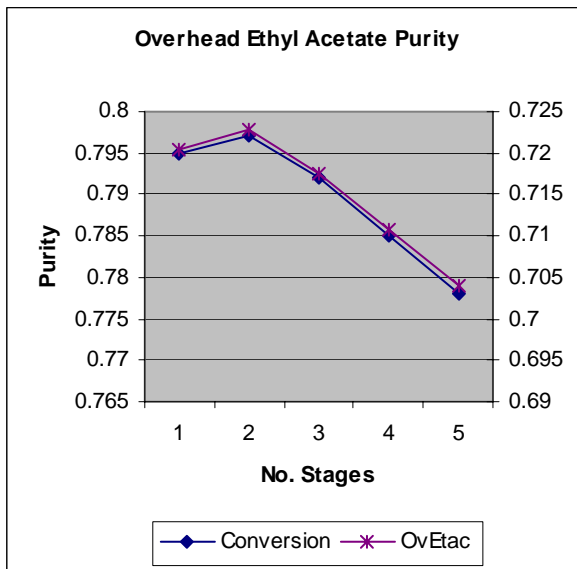


Figure 1.3 Effect Changes in Number of Rectifying Stages

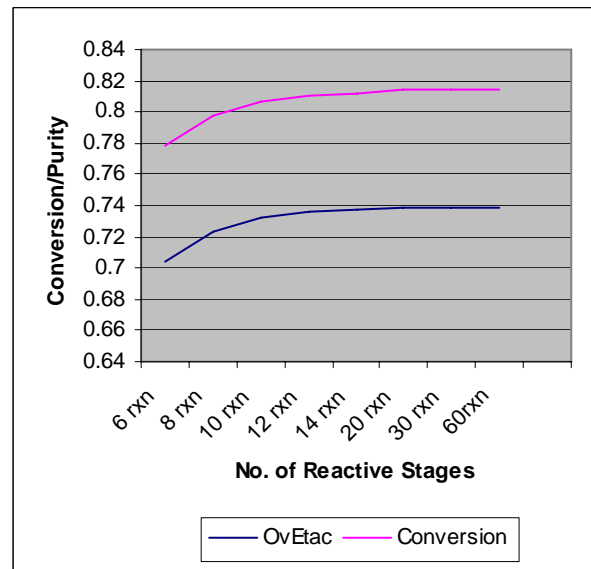


Figure 1.4 Effect of Changes in Number of Reactive Stage

However, in practice, this is almost impossible to achieve mainly because the esterification reaction still takes place in the rectifying zone. Since acetic acid has a low relative volatility compared to the other components in the system, it will have the tendency to flow down the column from its feed point. Thus only small amount is expected to be in the rectifying zone. Given the high concentration of ethyl acetate present in the rectifying zone, it then encourages the reverse reaction, which in turn reproduces the acetic acid reactant. This

negative production rate of ethyl acetate increases as the number of stages is increased in the zone, thus lowering the column conversion and affecting the product purity. Another undesirable effect of increasing the number of rectifying stages is the lost of ethanol reactant in the distillate, which also affects the conversion achieved to a certain extent and the ethyl acetate purity.

### 3.2.2 Variation in Number of Stages in Reactive Zone.

Figure 1.4 shows the simulation results obtained for the changes in the number of stages in the reaction zone. Higher conversion and ethyl acetate distillate purity were observed with increasing number of stages in the reaction zone. Additional stages in the reaction zone provide more sites for the esterification reaction to take place and in turn improve the conversion. Also, the additional stages led to better separation thus increasing the purity of ethyl acetate distillate. Nevertheless, there is a limit of doing so beyond which diminishing improvement was observed i.e., twenty stages for the system studied.

### 3.2.3 Variation in Number of Stages in Stripping Zone.

As shown in the Figure 1.5, the conversion and the ethyl acetate overhead purity were found to increase as a result of increasing number of stages in the stripping zone. Theoretically, the stripping zone in the ethyl acetate reactive distillation column has the following functions: 1) Removal of the heavy reaction product from the reaction zone to maintain favorable reaction conditions, 2) Prevent losses of ethanol to the bottom product by vaporizing and recycling it back to the reaction zone, 3) Prevent losses of ethyl acetate to the bottom product, 4) Provides a medium for forward reaction to proceed. As a result, increasing the number of stages in the stripping zone leads to favorable effect on the column performance. Again, there is a limit in increasing the number of stages in the stripping zone beyond which the performance starts to deteriorate i.e., 44 stages for the system studied. This is to be expected because increase in stripping stages results in more acetic acid, which is heaviest component in the system being discarded from the column via bottom stream. As a consequence, the column suffers loss of reactant acetic acid that in turn reduces the conversion of the column.

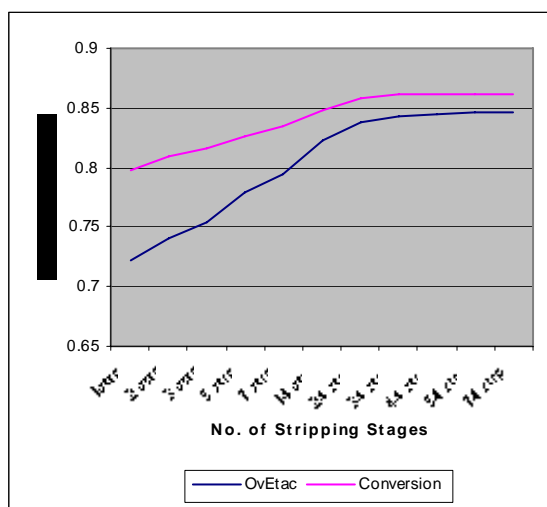


Figure 1.6 Effect of Changes in Column Operating Pressure

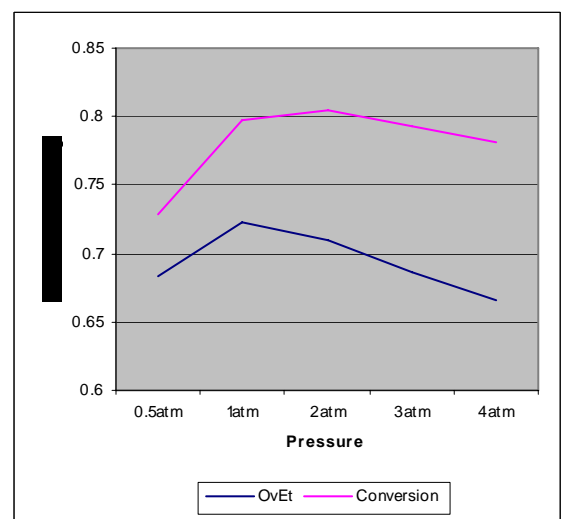


Figure 1.5 Effect of Changes in Number of Stripping Stages

### *3.2.4 Effect of Changes in Number of Stripping Stages*

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### *3.2.5 Effect of Changes in Column Operating Pressure*

In reactive distillation, the choice of operating pressure is made complicated by the indirect effects of pressure on the reaction equilibrium constant and the rate constant for kinetically controlled reaction via changing phase equilibrium temperatures. Increasing the pressure raises the boiling point temperatures along the column and these results in increase in forward reaction constant and decrease in reaction equilibrium constant (for exothermic reaction) and vice versa for decrease in pressure. In both cases, one produces a favorable effect on the conversion while the other produces a contrary effect. As a result of this interaction between the two parameters (forward reaction constant and reaction equilibrium constant), it is expected that there will be an optimal pressure for the system. This is clearly depicted in Figure 1.6, which indicates the presence of an optimum pressure with respect to ethyl acetate purity and reaction conversion achieved in the parametric analysis conducted on the column pressure. The optimal pressure was found to be at 1 atmosphere.

### *3.3 Process Enhancement*

The parametric analysis conducted earlier indicates that increasing the number of stages in rectifying, reactive or stripping stages could only marginally improve the column performance. The same was observed for changing the column operating pressure. Thus, it can be concluded that it is not possible to achieve the ideal performance desired just by manipulating the process parameters further. A modified configuration is thus introduced with the intention to further improve the conversion of both reactants i.e., acetic acid and ethanol while at the same time, achieving significantly higher product purity. From the analysis on the parametric study, it was found that the main constraints leading to the failure of the normal reactive distillation configuration system consists of the followings;

- Close relative volatility of ethanol and water in the stripping zone results in reactant ethanol being washed away into the bottom stream. Therefore, not all of the ethanol could react with the acetic acid to produce ethyl acetate product.



- Close relative volatilities of ethyl acetate, ethanol and water and the formation of azeotropes in the rectifying zone causing difficult separation in order to obtain high purity ethyl acetate at distillate.

These facts suggest that lifting up more ethanol to main reaction zone couple with breaking of azeotropes in the rectifying zone would result in higher conversion and purity. Breaking of azeotropes in these sections could be potentially realised using a suitable extractive agent. An additional component namely ethylene glycol was introduced as the extractive agent in view of it being a suitable extractive agent to break the different azeotropes formed in the system and the ability to simply recover it through distillation.

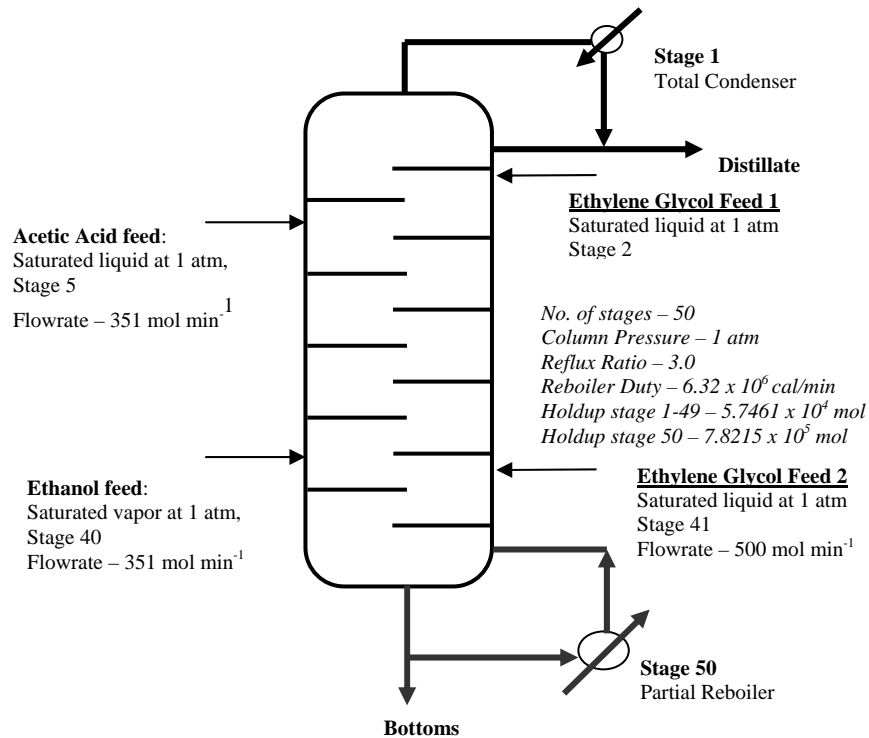


Figure 1.7: The Double Feed Reactive Distillation Column Configuration And Specifications For Ethyl Acetate Synthesis.

Figure 1.7 above shows the proposed configuration of the modified double feed ethyl acetate reactive extractive distillation column. Through the modification, it is expected that purer ethyl acetate could be produced as the overhead product while water and ethylene glycol will be produced as the bottom product. Also higher conversion could be realised. A simulation study was then conducted to prove the expected outcome.

### 3.3.1 Simulation Study of the Ethyl Acetate Reactive Extractive Distillation Column.

Table 1.3 summarises the steady state simulation results of the proposed modified double feed ethyl acetate reactive extractive distillation column.

Table 1.3 Simulation Results For Catalytic Double Feed Ethyl Acetate Reactive Extractive Distillation Column.

Quantity	Units	Distillate	Bottom
<b>Composition</b>			
Acetic acid (Ac)		0.0006	0.0052
Ethanol (Et)		0.0083	0.0030
Ethyl Acetate (Ea)		0.9815	0.0002
Water (W)		0.0096	0.2724
Ethylene Glycol (Eg)		0.0000	0.7192
Temperature	K	350.71	405.33
Product flow	mol /min	350.52	1251.5
Et conversion	mole %	98.07	98.07
Ea purity	mole %	98.15	0.02
Reflux flow	mol/min	1051.6	

Figure 1.7 and 1.8 display the liquid phase concentration profile and the temperature profile in the column respectively.

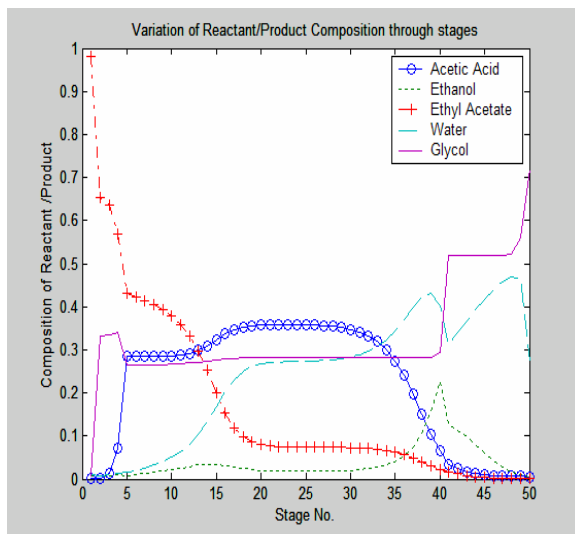


Figure 1.8 Steady State Liquid Phase Concentration Profile

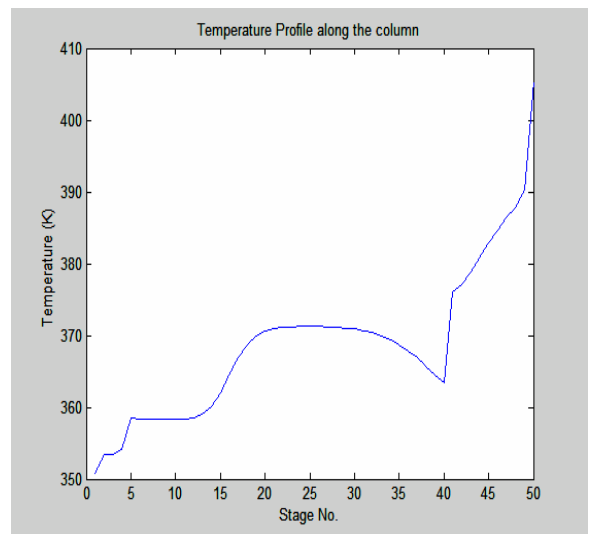


Figure 1.9 Steady State Temperature Profile Along The Column

The results obtained from the simulation have demonstrated favorable results in terms of achieving the outcomes as expected earlier. Using the modified configuration, the achieved ethyl acetate product purity has increased significantly to 98% whilst the conversion based on equal reactants fed to the system has also increased to 98%. As shown earlier, such achievements would not be possible using a conventional ethyl acetate reactive distillation system. The ethylene glycol fed at two locations in the column has provided the required effect needed to produce such performance. The presence of ethylene glycol prevents the formation of azeotrope between ethanol and water in the bottom half of the column as encountered in the conventional reactive distillation column, which significantly limits the performance of the column. Thus more ethanol could be lifted up to participate in the reaction within the reaction zone and hence increasing the overall conversion of the system. Also, it

has caused the separation to be easier as reflected by the reduced reboiler duty required for the column operation in comparison to the conventional reactive distillation configuration simulated earlier.

The temperature profile in Figure 1.9 shows two upper locations in the column where significant temperature changes were observed. Understandably, this is due to the introduction of high boiling components, acetic acid and ethylene glycol into the system. Higher concentration of acetic acid, ethylene glycol and water in the reaction active zone has also led to higher temperature profile in this part of the column. In the lower section of the column, a sudden drop in temperature was noted at ethanol feed due to the introduction ethanol, a low boiling component into the system. Also, another drastic temperature change was observed due to the introduction of ethylene glycol in the system.

#### **4.0 Conclusion**

The study conducted has shown that it is not possible to produce high purity ethyl acetate product with high conversion via conventional reactive distillation process. Conventional reactive distillation configuration has failed to separate the reactants and products of reaction efficiently in the column especially in the zone identified as susceptible for azeotrope formation (i.e. above acetic acid feed point and below ethanol feed point). Due to inefficient separation most of the reactants are washed away in distillate and bottoms of the column, thus the achieved conversion of the system is low even with more number of stages and higher residence time for reaction. On the other hand, reactive extractive distillation configuration (figure 1.7) proposed in this study was able to perform better in terms of achieved conversion and purity in a single column due to introduction of two extractive sections in the column. Presence of ethylene glycol in these zones prevents formation of azeotropes through extractive action, which ensures more of the valuable reactant being pushed to reactive active zone and avoid lost of reactants with product of reaction through distillate and bottoms stream. In addition, extractive action above acetic acid feed point ensures high ethyl acetate product purity obtained from the distillate by breaking the azeotropes formed in this section of the column. Overall, a modified configuration involving introduction of ethylene glycol aimed at breaking the azeotrope formed in the conventional configuration has led to significant increase in column performance.

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## NOTATION

C	concentration of reactant/product	(mol/m <sup>3</sup> )
r	rate of reaction	(mol/sec m <sup>3</sup> )
C <sub>k</sub>	Catalyst Concentration	(vol%)
T	Temperature	(K)
K <sub>c</sub>	constant of reaction equilibrium	
k <sub>1</sub>	forward reaction rate constant	(m <sup>3</sup> /(mol sec))
k <sub>2</sub>	reverse reaction rate constant	(m <sup>3</sup> /(mol sec))
F <sub>j</sub>	Feed flowrate into stage j	(mol/min)
V <sub>j+1</sub>	Vapor flowrate from stage j+1	(mol/min)
V <sub>j-1</sub>	Vapor flowrate from stage j-1	(mol/min)
V <sub>j</sub>	Vapor flowrate from stage j	(mol/min)
V <sub>1</sub>	Distillate flowrate	(mol/min)
V <sub>N</sub>	Re-boiler vapor flowrate	(mol/min)
V <sub>2</sub>	Vapor flowrate from column top	(mol/min)
L <sub>j</sub>	Liquid flowrate from stage j	(mol/min)
L <sub>j-1</sub>	Liquid flowrate from stage j-1	(mol/min)
L <sub>j+1</sub>	Liquid flowrate from stage j+1	(mol/min)
L <sub>1</sub>	Reflux flowrate	(mol/min)
L <sub>N</sub>	Bottom flowrate	(mol/min)
h <sub>pj</sub>	Liquid hold up on stage j	(mol)
R <sub>j,i</sub>	number of moles generated or disappear through reaction for component i on stage j	(mol/min)
x <sub>i,j</sub>	mole fraction of component i in liquid flow L <sub>j</sub> ,	
y <sub>i,j</sub>	mole fraction of component i in vapor flow V <sub>j</sub>	
z <sub>i,j</sub>	mole fraction of component i in feed flow F <sub>j</sub>	
∑R <sub>iN</sub>	net rate of change in the number of moles in the mixture due to participation in chemical reaction	(mol/min)
H <sup>L</sup> <sub>j</sub>	molar enthalpy of liquid phase on stage j	(cal/mol)
H <sup>V</sup> <sub>j</sub>	molar enthalpy of vapor phase on stage j	(cal/mol)
H <sub>z,j</sub>	molar enthalpy of feed introduced into stage j	(cal/mol)
Q <sub>c</sub>	Condenser heat duty	(cal)
Q <sub>R</sub>	Reboiler heat duty	(cal)
γ <sub>i</sub>	Liquid phase activity coefficient of component i	
P	Total pressure of the system	(psia)
P <sub>i</sub> <sup>o</sup>	Saturated vapor pressure of component i	(psia)