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Modeling and Simulation of a Reactive and Pressure Swing Distillation Columns for Methyl Acetate Production using ASPEN PLUS and MATLAB

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ABSTRACT
The models for the production of methyl acetate from the esterification reaction of methanol and acetic acid in a reactive distillation column (RDC) were developed. Six trays were selected as the reactive zone; methyl acetate and water were produced with unreacted acid and methanol in the RDC. Azeotropic mixture of methyl acetate-methanol was formed at the top of the reactive distillation column. The constant boiling mixture of Methyl acetate-methanol was eliminated using pressure swing distillation (PSD) principle simulated in aspen plus. In aspen plus, the reactive distillation was configured as high pressure column (HDC) operated at 14bar and 70^{o}C and a second column as low pressure column (LPC) operated at 0.56 bar 44 ^{o}C. The results obtained from two simulation software (ASPEN PLUS and MATLAB) were compared as 0.3967 mole methanol and 0.5983 mole methyl acetate using Aspen Plus and 0.4408 mole methanol and 0.5592 mole methyl acetate using Mat lab before PSD and 0.2710 mole methanol and 0.7290 mole methyl acetate after PSD. The results obtained were validated using literature data, 0.2154 mole methanol and 0.7846 mole methyl acetate were compared with 0.2710 and 0.7290 obtained from aspen plus with percentage deviation of 20.50 for methanol and -7.63 for methyl acetate.

KEYWORDS: Azeotrope, Methyl acetate-methanol, Reactive distillation column, Pressure swing Distillation.

I. INTRODUCTION

Liquid methyl acetate is flammable and colorless. It is a significant organic material that is used as a food flavor enhancer, solvent, plasticizer, lubricant, and other additives. Throughout the projected period of 2022–2027, the global demand for methyl acetate is anticipated to increase at a compound annual growth rate (CAGR) of about 10.1%. [1] Pressure-swing distillation is one of the improved distillation technologies that can overcome azeotropes by using columns that run at various pressures. However, for this procedure to be feasible, the required separation mixture's azeotropic composition needs to be pressure-sensitive, which is an uncommon occurrence. In pressure-swing distillation, methyl acetate and methanol combine to generate an azeotrope that satisfies the pressure-sensitivity requirement. Usually, two or more phases are created to separate mixtures. The physical characteristics of these phases, such as temperature, pressure, composition, and/or phase state, vary depending on the kind of species that needs to be separated.

[2] created a steady state software simulator employing the reactive extension of the McCabe-Thiele approximation. The behavior of methanol-methyl acetate leaving the top of the RDC in a close boiling state was not explicable by the model simulator developed by [2] Models of a packed reactive distillation column using equilibrium-based and rate-based approaches were compared by [7]. They didn't look into the system's control framework, and they didn't say anything about how azeotropic was eliminated. In order to improve selectivity and yield of the desired product, [5] integrated the separation and reaction processes into a single processing component. They did this by creating equilibrium phases with the beneficial energy produced by the exothermic reaction routes. His study focuses on how the heat produced by a chemical reaction affects the

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product's separation in RDC. The most adequate and effective setup for methyl acetate synthesis utilizing a reactive distillation column was created by [10]. They used a single column for both the separation and reaction operations in their reactive distillation column arrangement. The azeotropic interaction between methyl acetate and methanol could not be eliminated. The elimination of azeotrope production was neither explained nor demonstrated by earlier studies on the methanol and methyl acetate system, nor was a prospective strategy proposed. The aims of this work to model and simulate a reactive and pressure swing distillation columns for methyl acetate production using ASPEN PLUS and MATLAB.

II. MATERIALS AND METHODS

Development of mathematical model

Figure 1 shows a hypothetical representation of reactive distillation trays

Where,

F_j=Feed flow rate; L_{j+1} =Liquid flow rate on (j+1)th tray; L_j=Liquid flow rate on jth tray; V_j=Vapour flow rate on jth tray; V_{j-1} =Vapour flow rate from (j-1)th tray; h_{Fj}=Specific enthalpy of feed to jth tray; h_j=Specific enthalpy of vapour/liquid on jth tray; h_{j+1}=Specific enthalpy of liquid from (j+1)th tray, h_{j-1}=Specific enthalpy of vapour from (j-1)th tray

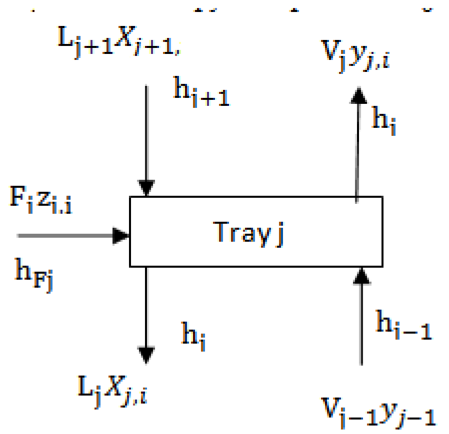

Figure 1: Representative Tray j

2.2. Model Assumptions

i. The system is well lagged
ii. Constant relative volatility of the components
iii. Constant liquid hold up
iv. Reaction occurs on 3 stages
v. Negligible vapour hold up
vi. Thorough mixing of vapour and liquid
vii. The composition of the reacting mixture is uniform.
viii. No conversion of reactant prior to flow into the reactive zone.
ix. The column is divided into six envelope for easy analysis
x. Mass and energy balance is taken on a representative stage for rectifying section, stripping section, reactive stage, feed stage

2.3. Overall material balance

Applying the principle of conservation of mass, we have

$$\frac{dM_j}{dt} = F_j + L_{j+1} + V_{j-1} - L_j - V_j + R_{j,i} \quad (1)$$

Taking component balance for any species i, from equation (1), we have

$$\frac{dM_jX_{j,i}}{dt} = F_jZ_{j,i} + L_{j+1}x_{j+1,i} + V_{j-1}y_{j-1,i} - L_jx_{j,i} - V_jy_{j,i} + R_{j,i} \quad (2)$$

(2)

Phase Equilibrium Relationships

$$y_{j,i} = K_{j,i}x_{j,i} \quad (1 \le j \le Nt,\ 1 \le i \le n) \quad (3)$$

Summations of Mole Fractions

$$\sum_{i=1}^{n} x_{j,i} = 1, \qquad \sum_{i=1}^{n} y_{j,i} = 1$$
$$(1 \le j \le Nt,\ 1 \le i \le n) \quad (4)$$

Combining equation (2) and equation (3), we have

$$\frac{dM_jX_{j,i}}{dt} = F_jZ_{j,i} + L_{j+1}x_{j+1,i} + V_{j-1}K_{j-1,i}x_{j-1,i} - L_jx_{j,i} - V_jK_{j,i}x_{j,i} + R_{j,i} \quad (5)$$

(5)

$$K_n = K_{n+1} = K_{n-1} \quad (6)$$

$$y_n = Kx_n \quad (7)$$

$$\frac{dM_jX_{j,i}}{dt} = F_jZ_{j,i} + L_{j+1}x_{j+1,i} + V_{j-1}Kx_{j-1,i} - L_jx_{j,i} - V_jKx_{j,i} + R_{j,i} \quad (8)$$

(8)

Rectification Section

At the rectifying section of column, there is no feed flow rate, and no chemical reaction

$$\frac{dM_jX_{j,i}}{dt} = V_{j-1}Kx_{j-1,i} - L_jx_{j,i} - Dx_D \quad (9)$$

(9)

Stripping Section

At the stripping section of column, there is no feed flow rate, and no chemical reaction

$$\frac{dM_jX_{j,i}}{dt} = L_{j+1}x_{j+1,i} - V_jKx_{j,i} - B \quad (10)$$

(10)

Feed Tray

$$\frac{dM_jX_{j,i}}{dt} = F_jZ_{j,i} + L_{j+1}x_{j+1,i} + V_{j-1}Kx_{j-1,i} - L_jx_{j,i} - V_jKx_{j,i} + R_{j,i} \quad (11)$$

(11)

Reactive Trays

$$\frac{dM_jX_{j,i}}{dt} = L_{j+1}x_{j+1,i} + V_{j-1}Kx_{j-1,i} - L_jx_{j,i} - V_jKx_{j,i} + R_{j,i} \quad (12)$$

Reflux Drum

$$\frac{M_Dd(x_D,i)}{dt} = V_{Nt}Kx_{Nt,i} - D(1+R)x_{D,i} \quad (13)$$

Column Base

$$\frac{M_Bd(x_{B,i})}{dt} = L_1x_{1,i} - Bx_{B,i} - V_SKx_{B,i} \quad (14)$$

2.3.2 Energy Balance over Tray j

Applying principle of conservation of energy, we have

$$\frac{dM_jh_j}{dt} = F_jh_{Fj} + L_{j+1}h_{j+1} + V_{j-1}h_{j-1} - L_jh_j - V_jh_j + (-\Delta H_R)R_{ji} \quad (15)$$

Rectification Section

At the rectifying section of column, there is no feed flow rate, and no chemical reaction

$$\frac{M_jC_{P_j}dT_j}{dt} = V_{j-1}C_{P_{j-1}}T_{j-1} - L_jC_{P_j}T_jDC_{P_D}T_D \quad (16)$$

(16)

Stripping Section

At the stripping section of column, there is no feed flow rate, and no chemical reaction

$$\frac{M_jC_{P_j}dT_j}{dt} = L_{j+1}C_{P_{j+1}}T_{j+1} - V_jC_{P_j}T_j - BC_{P_B}T_B$$

(17)

(17) **Feed Tray**

Reactive Trays

$$\frac{M_jC_{P_j}dT_j}{dt} = L_{j+1}C_{P_{j+1}}T_{j+1} + V_{j-1}C_{P_{j-1}}T_{j-1} - L_jC_{P_j}T_j - V_jC_{P_j}T_j + (-\Delta H_R)R_{ji} \quad (19)$$

Reflux Drum

$$\frac{M_DC_{P_D}dT_D}{dt} = V_{Nt}T_{Nt} - D(1+R)C_{P_D}T_D - Q_{COND} \quad (20)$$

Column Base

$$\frac{M_BC_{P_B}dT_B}{dt} = L_1C_{P_1}T_1 - BC_{P_B}T_B - V_SC_{P_B}T_B + Q_{REB} \quad (21)$$

2.3.3 Kinetics model

Consider the reversible reaction taking in the distillation column

$CH_4O + C_2H_4O_2 \leftrightarrow C_2H_6O_2 + H_2O$(22)

Let A is CH_4O ; B is $C_2H_4O_2$; C is $C_2H_6O_2$; D is H_2O

The rate of the reaction is given as:

$$R_{ji} = \frac{(v_iM_j)^2}{V_{Rj}}(k_{1,j}x_{j,A}x_{j,B} - k_{2,j}x_{j,C}x_{j,D}) \quad (23)$$

2.4 Solution Technique

The model equations were solved using mat lab and also simulated using aspen Plus

Table1: Simulation Input Data (Vandana, 2019)

Input Parameters	Methanol	Acetic Acid
Inlet stage	6	3
Temperature (^oC)	50	70
Pressure(Bar)	14	14
Flowrate (Kmol/hr)	400	400
Mole fraction	1.0	1.0

Table 2: Columns Process Condition

Parameters	**HP Column**	**LP Column**
No of stage	10	10
Reflux ratio	3	2.5
Pressure (Bar)	14	0.51
Reboiler Temperature(^oC)	70	44

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2.5 Simulation Method in ASPEN PLUS

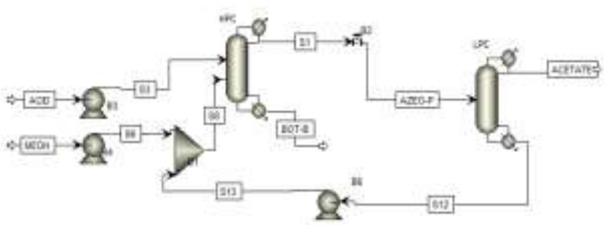

Figure 2: Reactive and Pressure Swing Distillation Columns

III. RESULTS AND DISCUSSION

Table 3 shows the product streams composition from aspen plus and that of Mat lab

Table 3: Comparison of Aspen Plus and Mat lab Stream Composition from High Pressure Column (RDC)

Component	Aspen Plus	Mat Lab
Acetic Acid	0	0
Methanol	0.3967	0.4408
Methyl Acetate	0.5983	0.5592
Water	0.0050	0

Table 4 shows the pressure swing results of figure 2, simulation using ASPEN PLUS

Table 4: Azeotrope Model Results

COMPONENTS	BEFORE PSD	AFTER PSD
METHANOL	0.3967	0.2710
METHY ACETATE	0.5983	0.7290

Table 6: Simulation Validation

COMPONENTS	AFTER PSD	Literature Data	% Deviation
METHANOL	0.2710	0.2154	20.50
METHY ACETATE	0.7290	0.7846	-7.63

3.1 Composition Profile with Reaction Time

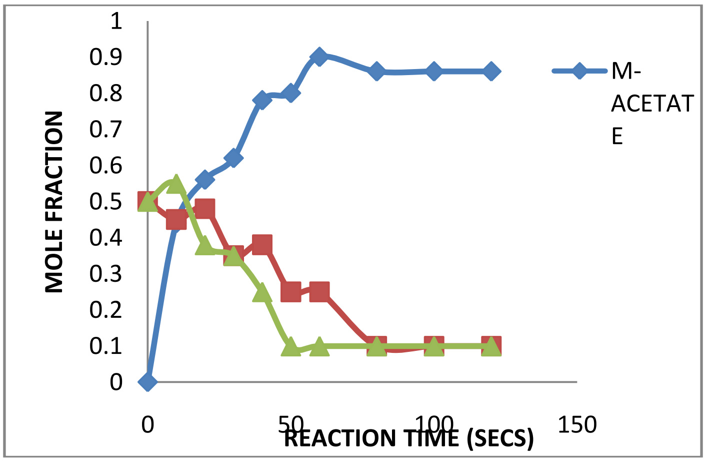

Figure 3: A Graph of Component Mole Fraction against Reaction Time

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The variation of components composition with time as shown in figure 3, from the figure, it was obvious that the product composition continuously increases with respect to time, and reactant concentration decreased with time. This was an indication that good reaction conversion and separation in the high pressure column.

3.2Variation of Components Concentration along the Tray in LPC

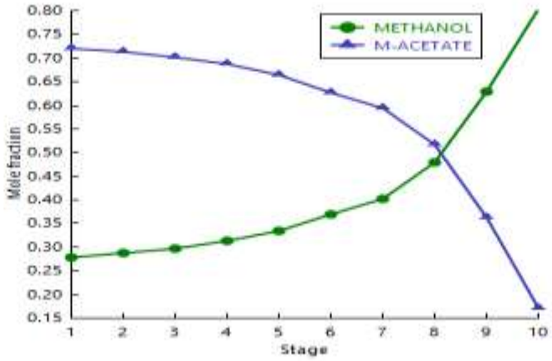

Figure 4: Graph Methyl Acetate and Methanol Mole Fraction against Tray Position

The distillate from (HPC) was fed into a low pressure column (LPC) to separate methanol-methyl acetate using the principle of pressure swing distillation on azeotropic mixture.

This principle was applied due to the pressure sensitive nature of this azeotrope. Separation was enhanced by swinging from higher pressure to a lower pressure as shown in figure 4. From figure 4, it is seen that the concentration of methanol increases down the column whereas that of Acetate decreases down the column and vice versa.

3.3 Temperature Variation along the Stages in HPC (RDC)

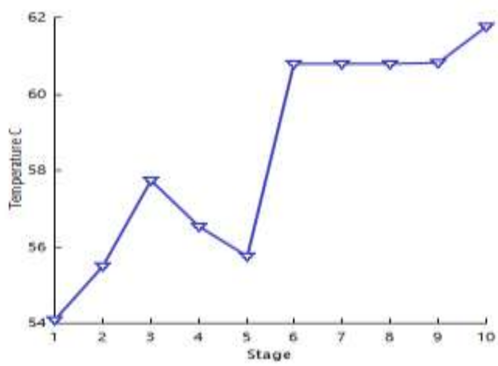

Figure 5: Temperature Progression along the Stages in RD

The temperature profile in reactive distillation column as shown in figure 5; the temperature increased from the top to the bottom of the column as a result the high heat duty generated in reboiler strippe off methyl acetate. The three stages that were selected as the reactive zone where acetic acid and methanol reacted to produced methyl acetate and water. In the reactive zone, the component had sufficient residence time for effective esterification reaction. The temperature increases due the huge amount of heat liberated in the reactive zone as a result of the exothermic nature the reaction. it was observed from the figure 5, the condenser temperature which is 54.5°C is lower than reboiler temperature which is 63.7°C. The temperature of the reactive zone is varied between 58.9 and 63.7°C, making it compatible to the exothermic nature of the esterification reaction.

3.4 Variation of Temperature along the Lower Pressure Colum (LPC)

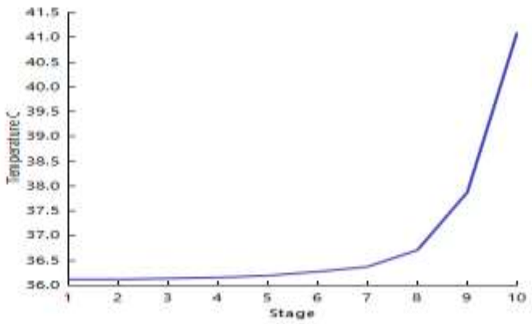

Figure 6: Variation of Temperature along the Lower Pressure Colum (LPC)

Temperature in the LPC varied from 36.4 ^{o}C to 41 ^{o}C along the column from the top to the column base. As seen from figure 6, temperature increases exponentially from the top stage to the column base. This variation in temperature in the Lower pressure column harmonized with the temperature trend in most organic mixture separation column.

3.5 Variation of Mole Fraction with Pressure

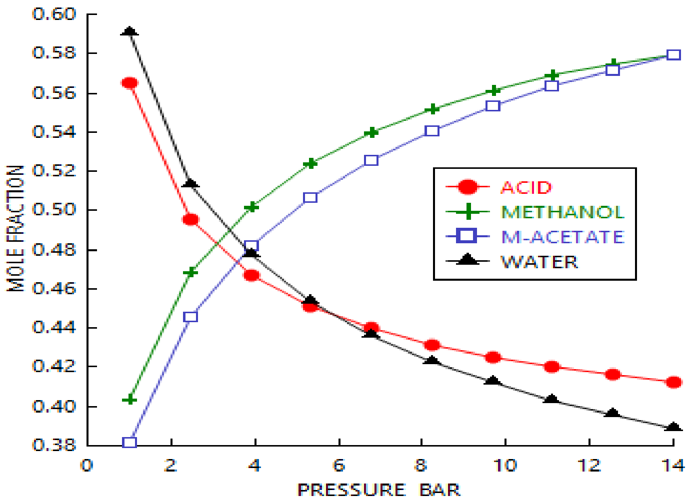

Figure 7: A Plot of Mole Fraction against Pressure

The concentration of various components varied with the increased in column pressure as seen from the plot of mole fraction versus column pressure in figure 7. In the high pressure column, higher pressure of 14bar favoured product formation as good residence time was available for reactant depletion and new species are formation. However, for an azeotropic components that are formed: methanol and methyl acetate, the increased in pressure inhibit the separation of azeotrope.

3.6 Effect of methanol feed Stage on distillate composition

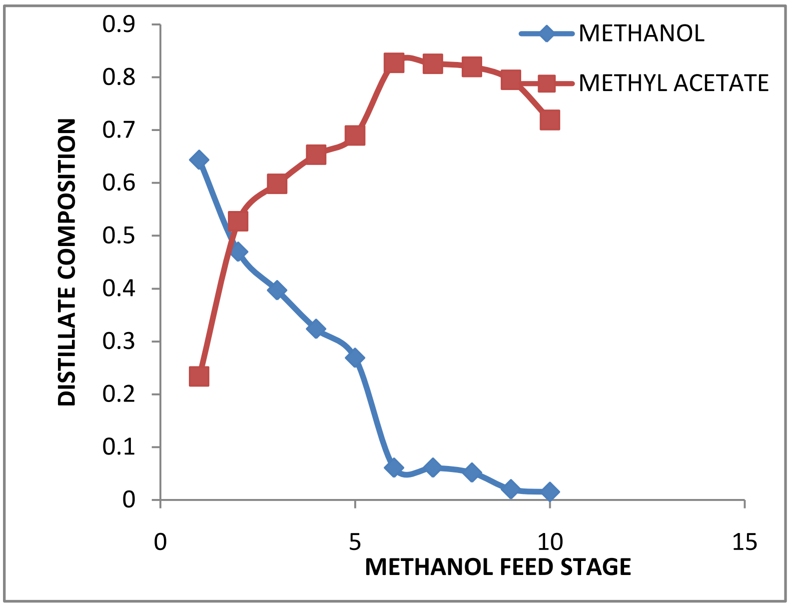

Figure 8: **Effect of methanol feed Stage on distillate composition**

From figure 8, the distillate composition of methyl acetate increased rapidly with methanol feeding stage of 3. From stage 3 to stage 6, the composition methyl acetate is at maximum value of 0.8256. Whereas the distillate composition of methanol decreased progressively with methanol feed stage.

3.7 Effect of Acetic Acid Feed Stage on Distillate Composition

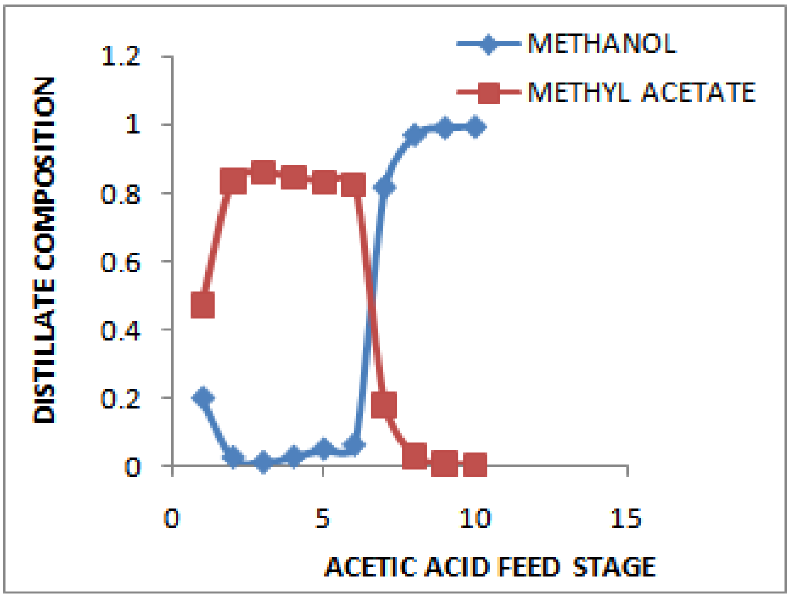

Figure 9: Effect of Acetic Acid Feed Stage on Distillate Composition

The significant of feed stage location was observed in the plot of distillate composition against acetic acid feed stage in figure 9. From the plot in figure 9 , the desire product methyl acetate distillate composition changed from 0.471 to 0.8373 in stage 1 to stage 2 and then decreased slowly from stage 3 to stage 6 with composition of 0.8608 to 0.8270. There was rapid decreased of methyl acetate distillate composition from stage 6 to stage 7 as acetic acid feed stage. In figure 9, methanol distillate composition varied from 0.1989 at stage 1 to 0.0243 at stage 2. From stage 3 to stage 5 the variation in methanol composition in the distillate increased gradually with the change in acetic acid feed stage, from 0.0099 to 0.049. From stage 6 to stage 10 the variation in methanol composition in the distillate increased rapidly with the change in acetic acid feeding stage, from 0.061 to 0.997.

3.8 Comparison of Mat lab and Aspen plus Methyl Acetate Composition Profile along the Trays

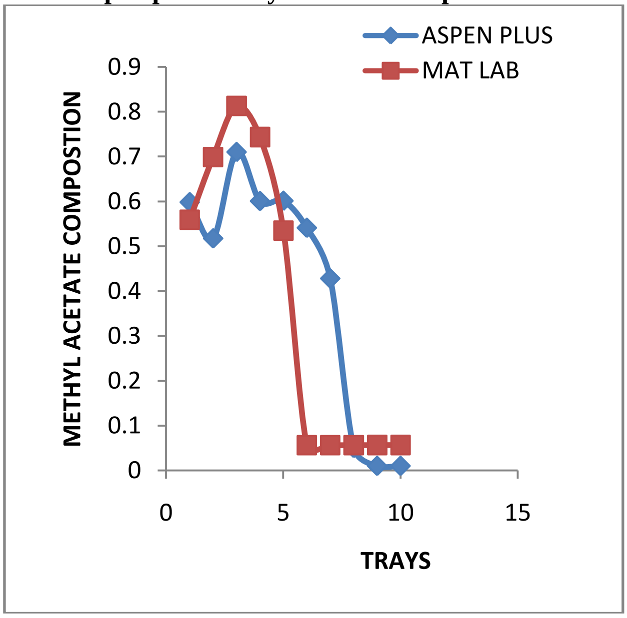

Figure 10: Comparison of Mat lab and Aspen plus Methyl Acetate Composition Profile along the Trays

In figure 10, the composition profile of methyl acetate along the reactive distillation column was studied using simulation software (Aspen plus and Mat lab) and comparison was made with the results obtained from the two simulation software. From the comparison, methyl acetate composition profile results obtained aspen plus and Mat lab were in agreement

3.9 Comparison of Mat lab and Aspen plus Methanol Composition Profile along the Trays

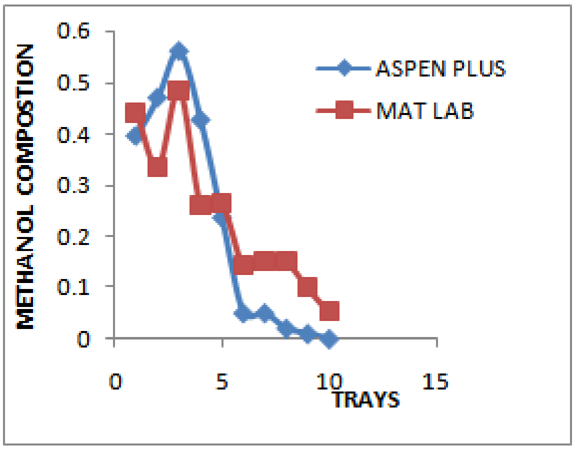

Figure 11: Comparison of Mat lab and Aspen plus Methanol Composition Profile along the Trays

In figure 11, the composition profile of methanol along the reactive distillation column was studied using simulation software (Aspen plus and Mat lab) and comparison was made with the results obtained from the two simulation software. From the comparison, methanol composition profile results obtained aspen plus and Mat lab were in agreement.

IV. CONCLUSIONS

Mathematical models were developed for the six envelopes: (reflux drum, rectification section. reactive section, feed section, stripping section and column base). Reactive and pressure swing distillation columns were simulated using aspen plus as chemical engineering tool for simulation and process modeling. The effect of pressure on methanol-methyl acetate system was simulated using aspen plus and azeotrope was removed at 0.56bar.

Nomenclature

Symbols	Meaning	Units
$\mathbf{B}$	Bottom flow rate	Kmol/hr
$\mathbf{C_p}$	Specific heat capacity at constant pressure	Kj/Kmol-K
$\mathbf{D}$	Distillate flow rate	Kmol/hr
$\mathbf{F}$	Feed flow rate	Kmol/hr
$\mathbf{h_{Fj}}$	Specific enthalpy of feed to jth tray	KJ/Kmol
$\mathbf{h_j}$	Specific enthalpy of vapour/liquid on jth tray	KJ/Kmol
$\mathbf{h_{j+1}}$	Specific enthalpy of liquid from (j+1)th tray	KJ/Kmol
$\mathbf{h_{j-1}}$	Specific enthalpy of vapour from (j-1)th tray	KJ/Kmol
$\mathbf{-\Delta H_R}$	Heat of reaction	KJ/Kmol
$\mathbf{i}$	Species/Component	
$\mathbf{j}$	Representative tray	
$\mathbf{K}$	Distribution coefficient	
$\mathbf{k_1}$	Rate constant of forward reaction	
$\mathbf{k_2}$	Rate constant of backward reaction	
$\mathbf{L_{j+1}}$	Liquid flow rate on (j+1)th tray	Kmol/hr
$\mathbf{L_j}$	Liquid flow rate on jth tray	Kmol/hr
$\mathbf{M_j}$	Molar hold up on jth tray	mol
$\mathbf{M_B}$	Molar hold up in the column base	Mol
$\mathbf{M_D}$	Molar hold up in the reflux drum	Mol
$\mathbf{n}$	Total number of components/species	
$\mathbf{Nt}$	Total number of trays	
$\mathbf{Q_{Cond}}$	Condenser heat duty	KJ/hr
$\mathbf{Q_{Reb}}$	Reboiler heat duty	kJ/hr
$\mathbf{(-r_{j,i})}$	Rate of reaction of species i on jth tray per unit volume	Kmol/m^6-hr
$\mathbf{R_{j,i}}$	Rate of reaction of species i on jth tray	Kmol/m^3-hr
$\mathbf{T_{ref}}$	Reference temperature	K
$\mathbf{T_j}$	Tray temperature	K
$\mathbf{V_j}$	Vapour flow rate on jth tray	Kmol/hr
$\mathbf{V_{j-1}}$	Vapour flow rate from (j-1)th tray	Kmol/hr
$\mathbf{V_{Nt}}$	Vapour flow rate from condenser tray	Kmol/hr
$\mathbf{V_s}$	Vapour flow rate from reboiler	Kmol/hr
$\mathbf{x_{B,i}}$	Bottoms composition of species i	
$\mathbf{x_{D,i}}$	Distillate composition of species i	
$\mathbf{x_{j,i}}$	Liquid composition of species i on jth tray	
$\mathbf{x_{j+1,i}}$	Liquid composition of species I on (j+1)th tray	
$\mathbf{x_{Nt,i}}$	Liquid composition of species i on Nt tray	
$\mathbf{y_{j,i}}$	Vapour composition of species i on jth tray	
$\mathbf{y_{j-1,i}}$	Vapour composition of species i on (j-1)th tray	
$\mathbf{z_{j,i}}$	Feed composition of species i	

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