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Research Paper

MODELING AND SIMULATION OF A DISTILLATION COLUMN USING MATLAB

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This paper presents the modeling and simulation of a distillation column using MATLAB. Simulation studies are often used to examine the operational behavior of distillation columns. A rigorous model for the simulation of the steady-state behavior of the distillation column has been developed. MESH equations, which actually represent the behavior of the distillation column have been solved through MATLAB, in order to study the effect of different parameters. In this paper, the effect of the feed condition and the feed composition on the steady state behavior of a methanol/MTBE/Iso-butylene column have been studied.

Keywords: Distillation, Modeling, Simulation, Steady-state

INTRODUCTION

Distillation is a process that separates two or more components into an overhead distillate and a bottoms product. The bottoms product is almost exclusively liquid, while the distillate may be a liquid or vapor or both. Distillation is the most widely used separation technique in process industry. The separation process requires that (1) a second phase be formed so that both vapor and liquid phases can contact each other on each stage within a separation column, (2) the components have different volatilities so that they will partition between the two phases to different extents, and (3) the two phases can be separated by gravity or other mechanical means. Distillation differs from absorption and stripping in that the second fluid phase is usually created by thermal means rather than by the introduction of a second phase that may contain an additional component or components not present in the feed mixture (Seader and Henley, 2001).

According to Forbes, the art of distillation dates back to at least the first century AD. By the eleventh century, distillation was being used in Italy to produce alcoholic beverages. At that time, distillation was probably a batch process based on the use of just a single stage, the boiler. The word distillation is derived from the Latin word *destillare*, which means dripping or trickling down. By at least the sixteenth century, it was known

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that the extent of separation could be improved by providing multiple vapor-liquid contacts (stages) in a so called Rectifactorium. The term rectification is derived from the Latin words *recte facere*, meaning to improve. Modern distillation derives its ability to produce almost pure products from the use of multi-stage contacting. Throughout the twentieth century, multistage distillation was by far the most widely used industrial method for separating liquid mixtures of chemical components. Distillation becomes energy intensive separation technique when the relatively volatility α, of the components being separated is low (1.50).

VARIOUS ASSUMPTIONS IN DISTILLATION MODEL

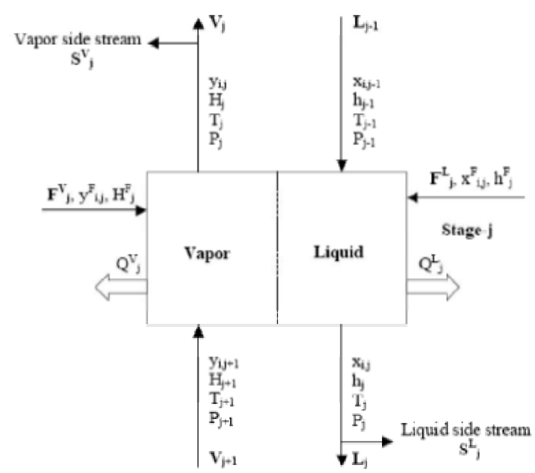
- Each stage is a perfectly mixed stage, i.e., liquid composition at each stage is homogenous and equal to the composition of liquid leaving the stage.
- The vapor and liquid leaving any stage are in physical equilibrium.
- Entrainment of liquid drops in vapor and occlusion of vapor bubbles in liquid are negligible
- Vapor holdup is neglected.
- The energy balance is based on conservation of enthalpy instead of internal energy.
- Perfect mixing in both phases at each stage.

STEADY-STATE MODELING OF A DISTILLATION COLUMN

A rigorous steady-state column model was developed using MESH equations which actually represent the behavior of the column.

Figure 1 shows the schematic of a separation stage. The model consists of mass balance, equilibrium relation, summation equations and energy balance, which are collectively known as MESH equations.

Figure 1: Model of a Separation Stage



Mass Balance

The model equations for a general 'j^th' stage and 'i^th' component are represented as:

$$L_{j-1}x_{j-1i} + V_{j+1}y_{j+1i} + FZ_{j,i} - \left(V_j + S_j^v\right)y_{j,i} - \left(L_j + s_j^l\right)x_{j,i} = 0 \quad ...(1)$$

And in terms of the flow rate of components, above equation can be written as:

$$l_{j-1,i} + v_{j+1,i} f_{j,i} - v_{j,i} - s_{j,i}^l - l_{j,i} - S_{j,i}^v = 0 \quad ...(2)$$

where

$$l_{i,j} = L_j x_{i,j} \quad ...(3)$$

$$v_{i,j} = V_j y_{i,j} \quad ...(4)$$

$$V_j = \sum_{i=1}^{c} v_{i,j} \quad ...(5)$$

$$L_j = \sum_{i=1}^{c} l_{i,j} \quad ...(6)$$

$$s_j = \frac{U_j}{L_j} \quad ...(7)$$

$$S_j = \frac{W_j}{V_j} \quad ...(8)$$

Now substituting the Equations (3) to (8) in Equation (2), we will get:

$$l_{j,i}\left(1+s_j\right)+v_{j,i}\left(1+S_j\right)-l_{j-1,i}-v_{j+1,i}-f_{j,i}=0 \quad ...(9)$$

Equilibrium Relationship

The compositions of the streams leaving a stage are in equilibrium. Therefore, the mole fractions of the component *'i'* in the liquid and vapor streams leaving stage *'j'* are related by the equilibrium relation shown in the equation given below:

$$y_{j,i} = K_{j,i} x_{j,i} \quad ...(10)$$

Substituting Equations (3) to (6) in Equation (10), we get,

$$K_{j,i} l_{j,i}\left(\sum_{k=1}^{c} v_{k,j} / \sum_{k=1}^{c} l_{k,j}\right) - v_{j,i} = 0 \quad ...(11)$$

Summation Equations

Two additional equations arise from the necessity that the mole fractions of all the components, either in vapor or liquid phase must sum to unity.

$$\sum_{i=1}^{c} x_{j,i} = 1 \quad ...(12)$$

$$\sum_{i=1}^{c} y_{i,j} = 1 \quad ...(13)$$

In terms of flow rate of the components, above equations can be written as:

$$\sum_{i=1}^{c} l_{j,i} = L_j \quad ...(14)$$

$$\sum_{i=1}^{c} v_{j,i} = V_j \quad ...(15)$$

Energy Balance

The total energy balance for 'j[th]' stage is given by:

$$L_{j-1}h_{L_{j-1}} + V_{j+1}h_{V_{j+1}} + F_j h_{F_j}$$

$$-\left(L_J + U_j\right)h_{L_j} - \left(V_j + W_j\right)h_{V_j} - Q_j = 0 \quad ...(16)$$

Now using the Equations (3) to (8) in the enthalpy balance Equation (16), we will arrive at a new enthalpy equation in terms of $l_{j,i}$ and $v_{j,i}$ as under:

$$\sum_{i=1}^{c} l_{1,i} - \left(L/D\right)\sum_{i=1}^{c} v_{1,i} = 0 \quad ...(17)$$

$$h_{L_j}\left(1+s_j\right)\sum_{i=1}^{c} l_{j,i} + h_{V_j}\left(1+S_j\right)\sum_{i=1}^{c} v_{j,i} -$$

$$h_{L_{j-1}}\sum_{i=1}^{c} l_{j-1,i} - h_{V_{j+1}}\sum_{i=1}^{c} v_{j+1i}$$

$$-h_{F_j}\sum_{i=1}^{c} f_{j,i} - Q_j = 0 \quad ...(18)$$

$$\sum_{i=1}^{c} l_{N,i} - B = 0 \quad ...(19)$$

Two additional equations, which are known as the replacement equations have been used for the stage 1 (Condenser) and stage N (Reboiler) respectively, which are given here as under:

SIMULATION

The model equations for the distillation process are simple algebraic equations developed by applying mass and energy balance around the column, also known as the MESH equations. These MESH equations have been solved by making use of the solver 'fsolve' in MATLAB, which can solve various non-linear equations simultaneously. The model has been simulated under different simulating conditions, viz., different feed conditions (saturated vapor, half vaporized and (saturated liquid) and different feed compositions. A MATLAB code has been developed in order to simulate the model for different simulating conditions in order to study the impact of the different parameters on the steady-state performance of the methanol/MTBE/iso-butylene column.

RESULTS AND DISCUSSION

Simulation calculations for the distillation column have been made in order to study its behavior when feed of different types are fed, for example, saturated liquid, saturated vapor and half vaporized, with the design and operation of the column remaining unchanged. By running the simulations for the distillation, it has been actually tried to establish the thermal condition of the feed that leads to a greater methanol concentration in the liquid phase inside the column. The simulation calculations indicate that the latter is obtained by means of feeding a saturated liquid feed. It is also economical to feed the saturated liquid feed to the column, which is beneficial from two viewpoints, i.e., from the viewpoint of separation as can be seen from the graphs and also from the heat economy viewpoint.

The following results are obtained for the distillation column simulation for different feed conditions, viz., saturated liquid, saturated vapor and half vaporized, which are discussed here below.

Figure 2: Methanol Liquid Composition Profile in the Column for Rr=1 and $\psi = 0$

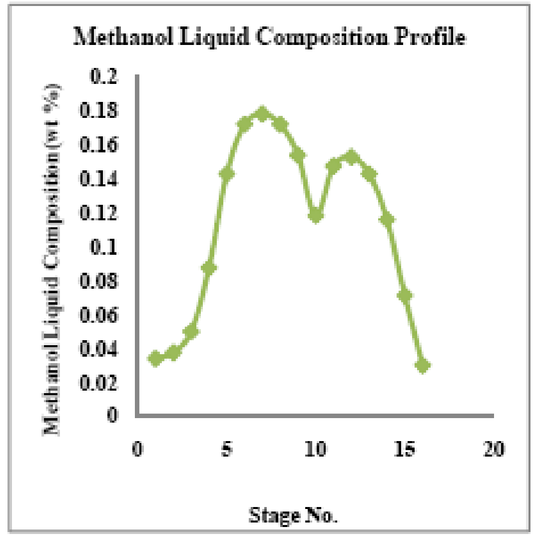
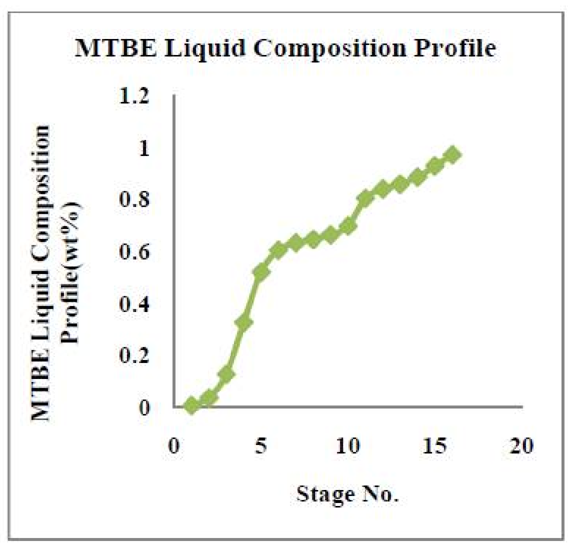


Figure 2 shows the variation of methanol composition inside the column. As can be seen from this graph, two methanol concentration peaks occur inside the column in the liquid phase, one above the feed tray and one below the feed tray. Figure 3 shows the variation of MTBE (Methyl

Figure 3: MTBE Liquid Composition Profile in the Column for Rr=1 and $\psi = 0$



tert-butyl Ether) liquid composition profile inside the column. As can be seen from this graph, MTBE liquid composition increases from top to the bottom of the column. It increases from 1st to 6th stage and then it remains almost constant upto the 10th stage and where from it increases abruptly upto the 16th stage. Infact, it is almost zero concentration at the top of the column and almost 97% composition at the bottom of the column. It is because of the higher boiling point of the MTBE and hence most of it is recovered in the bottom of the column.

Figure 4 shows the variation of isobutylene liquid composition profile inside the column. As can be seen from this graph, iso-butylene composition decreases from top to the bottom of the column. It decreases abruptly from the top of the column upto the 6th stage and then it remains almost constant upto the 10th stage and then it decreases very quickly and then it approaches towards zero at the bottom of the column. Infact, it is almost zero concentration at the bottom of the column and almost 96% composition of iso-butylene at the top of the column, which can be attributed to the low boiling point of the iso-butylene which is around 322°C at the column pressure and hence most of it is recovered at the top of the column as a light key.

Figure 4: Iso-butylene Liquid Composition Profile in the Column for Rr=1 and $\psi = 0$

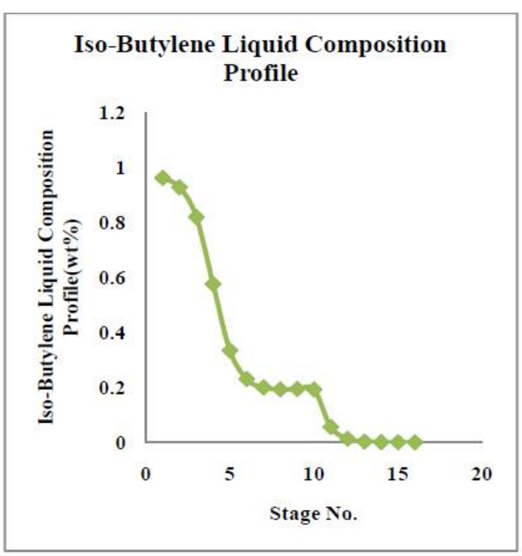
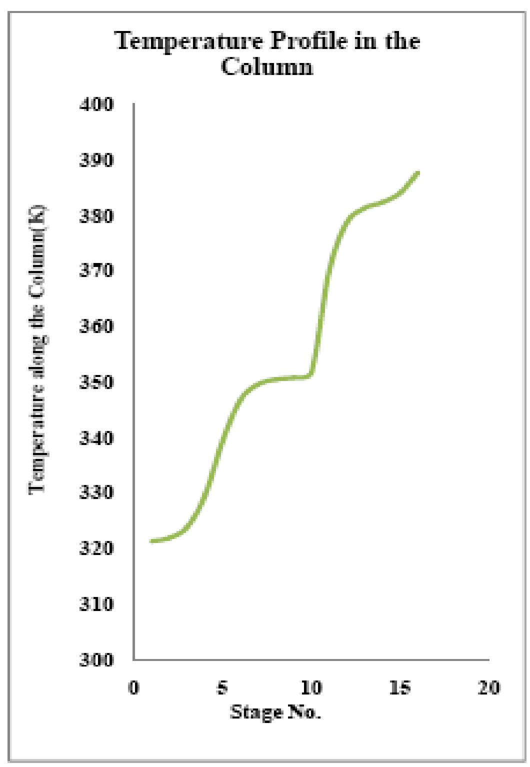


Figure 5 shows the temperature variation along the column. It can be observed from this graph that temperature increases from top to the bottom of the column. There exists a minimum temperature at the top of the column, which is obvious, because of the condenser there at the top through which heat is removed and hence there is minimum temperature and then it increases downwards and shows a sudden increase at the feed stage, which is, because of the feed conditions and the type of the feed that is fed to the column, and then it increases until it reaches its maximum at the bottom of the

Figure 5: Temperature Profile in the Column for Rr=1 and $\psi = 0$



column, which is again obvious, because of there boiler there at the bottom of the column. In nutshell, we can say that temperature.

Figure 6 shows the variation of methanol liquid composition inside the column, when 50% vaporized feed is fed to the column. It can be observed from this graph, again two methanol concentration peaks occur inside the column, one above the feed tray and one below the feed tray, as in the case of saturated liquid feed. It shows the same trend as that of saturated liquid feed except for the values of methanol peak concentrations, which are lower than that obtained in case of saturated liquid feed.

Figure 6: Methanol Liquid Composition Profile in the Column for Rr=1 and $\psi = 0.5$

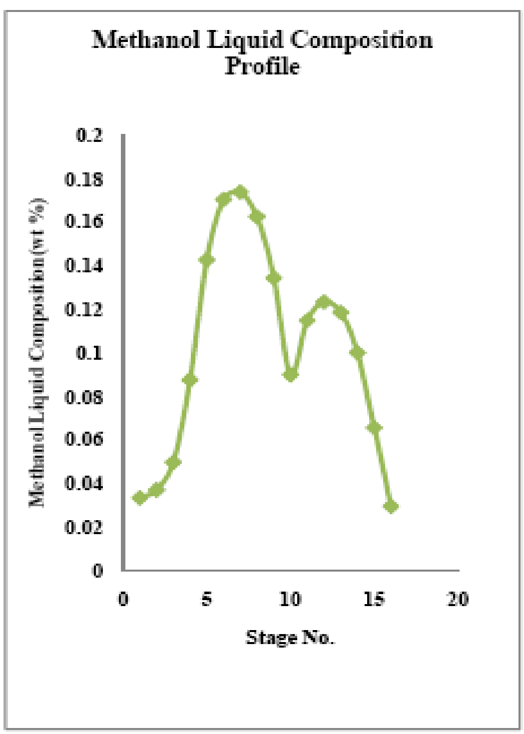
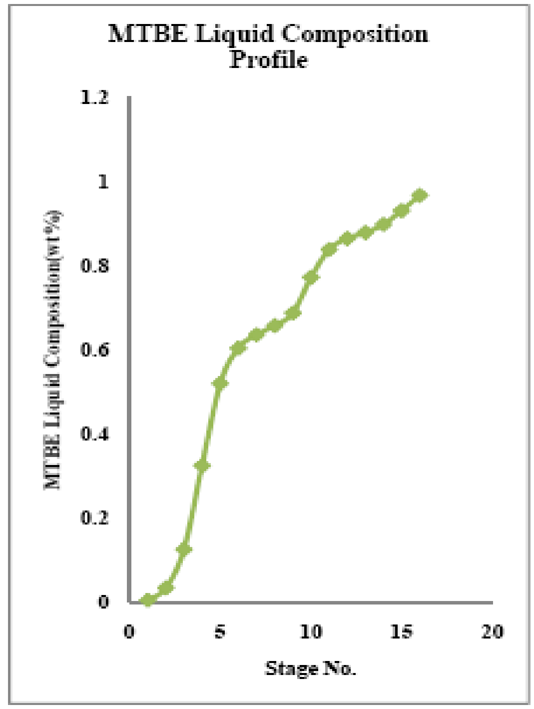


Figure 7 shows the variation of MTBE (Methyl tertiary-Butyl Ether) inside the column, when a 50% vaporized feed is fed to the column. It can be observed from this graph that the MTBE composition increases from the top to the bottom of the column. It is almost in negligible amount in the top and maximum amount of it is present in the bottoms, almost 97%, which can be attributed to its higher boiling point. It is desirable also to get maximum amount of MTBE in the bottom of the column in as much as pure form.

Figure 7: MTBE Liquid Composition Profile in the Column for Rr=1 and $\psi = 0.5$



It can be observed from Figure 8 that the iso-butylene liquid composition decreases from the top to the bottom of the column. It can be observed from this figure that iso-butylene composition is maximum at the top of the column, which is almost 96% composition of iso-butylene in the top and almost negligible amount in the bottom of the column, which is desirable also. It is because of the low boiling point of the isobutylene that, it is mostly obtained in the top.

Figure 8: Iso-Butylene Liquid Composition Profile in the Column for Rr=1 and ψ = 0.5

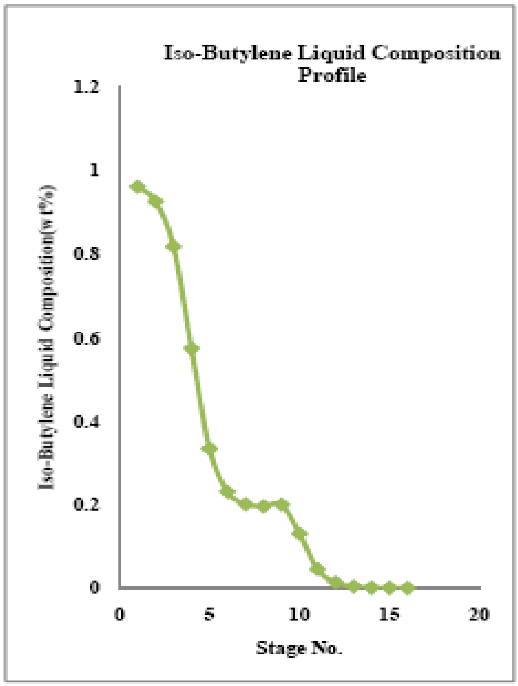


Figure 9: Temperature Profile in the Column for Rr=1 and ψ = 0.5

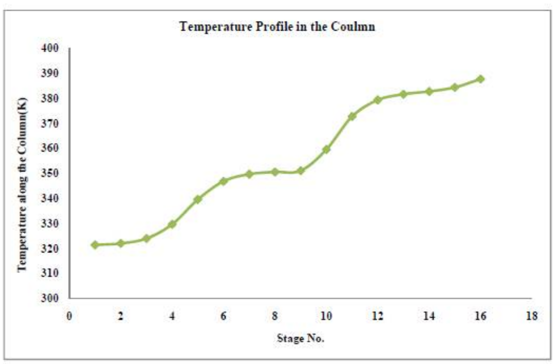


Figure 9 shows the temperature variation along the column, when a 50% vaporized feed is fed to the column. It can be observed from this figure that temperature increases from top to the bottom of the column. It shows the same pattern as for the saturated liquid feed, however, the variation of the temperature near the feed stage is found to be different, because of the different feed condition (50% vaporized feed). In nutshell, we can say that temperature shows an increasing trend from top to the bottom of the column.

Figure 10 shows the comparison of methanol composition profiles inside the column at different feed conditions, i.e., saturated liquid, 50% vaporized and saturated vapor. It can be observed from this figure that the maximum methanol concentration in both the rectifying and the stripping section of the column occurs for the saturated liquid feed. This feed condition is therefore considered as an optimum condition for the rest of the simulation work. A liquid side-draw can be taken from the stage, where this peak in methanol concentration or composition occurs inside the column and this side-draw can be fed to the pervaporation, which can be place parallel to the column so as to remove methanol through the pervaporation membrane which is more selective for the methanol as compared to MTBE. In this way the purity of MTBE can be further increased in the bottom of the column.

Figures 11 and 12 show the effect of the feed condition (saturated liquid, 50% vaporized and saturated vapor) on the composition of the MTBE and Iso-butylene respectively, inside the column.

Figure 10: Methanol Liquid Composition Profile in the Column for Varying Feed Conditions

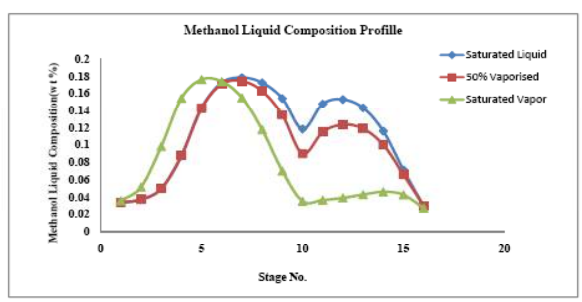


Figure 11: MTBE Liquid Composition Profile in the Column for Varying Feed Conditions

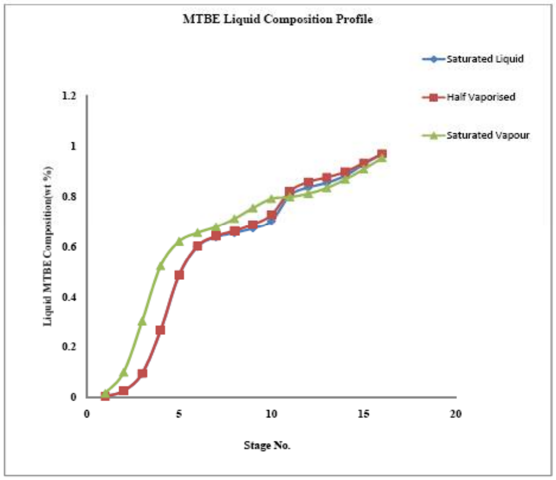
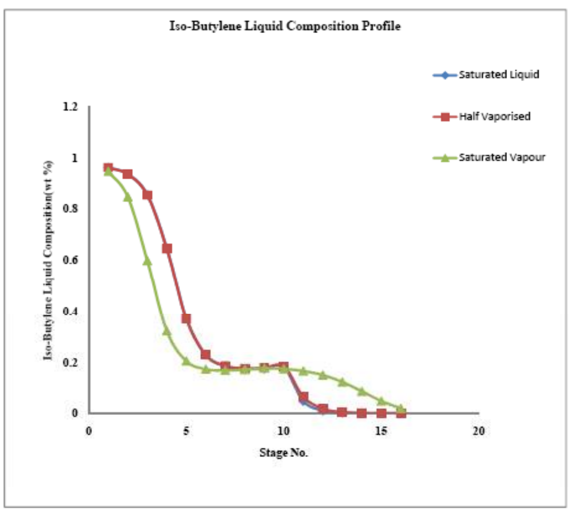


Figure 12: Iso-butylene Liquid Composition Profile in the Column for Varying Feed Conditions



It can be clearly noticed from these graphs that the maximum composition of MTBE in the bottom of the column and maximum composition of Iso-butylene at the top of the column corresponds to the saturated liquid feed. This also confirms that the saturated liquid feed condition is indeed optimum for the distillation operation for the present work. Hence, it can be concluded that it is always better to operate the column for saturated liquid feed for this mixture of methanol/ MTBE/iso-butylene, which is also economical form the heat economy point of view and also from the point of view of MTBE purity in the bottom of the column.

Validation of MATLAB Simulation Results by ChemSep Simulation Software

A comparison of the simulation results for the developed model using MATLAB 7.9.0 Software and those obtained by ChemSep Simulation Software has been made. The results are shown in Figures 13 to 24. These Figures depict a

Figure 13: Comparison Profiles for Methanol Liquid Composition in the Column for $\psi = 0$

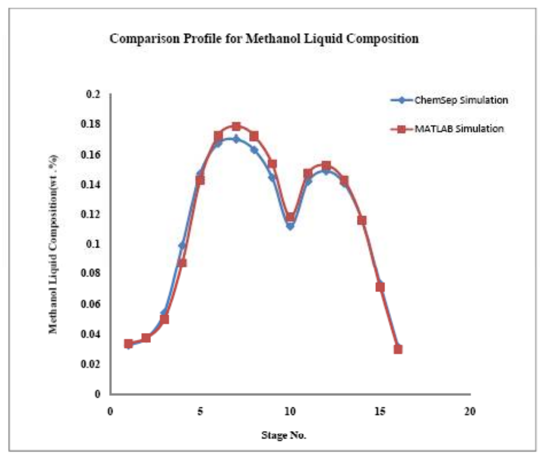


Figure 14: Comparison Profiles for MTBE Liquid Composition in the Column for $\psi = 0$

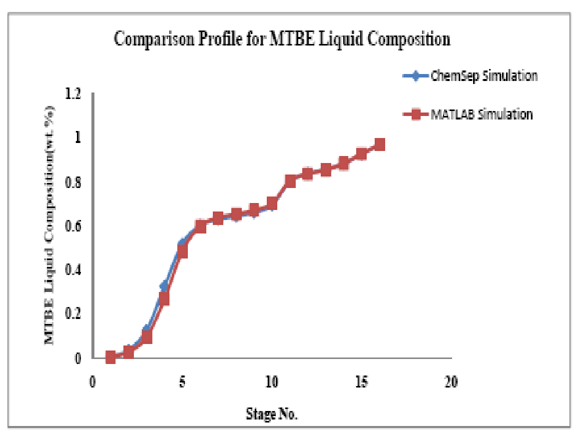


Figure 15: Comparison Profiles for Iso-Butylene Liquid in the Column for $\psi = 0$

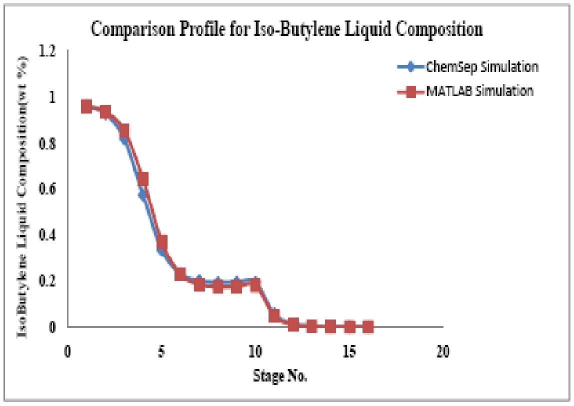


Figure 18: Comparison Profiles for MTBE Liquid Composition in the Column for $\psi = 0.5$

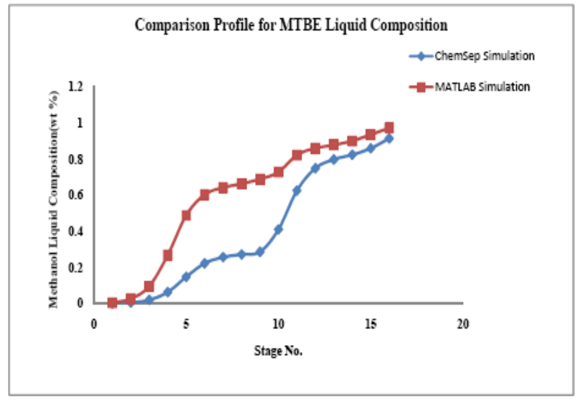


Figure 16: Comparison of Temperature Profiles in the Column for $\psi = 0$

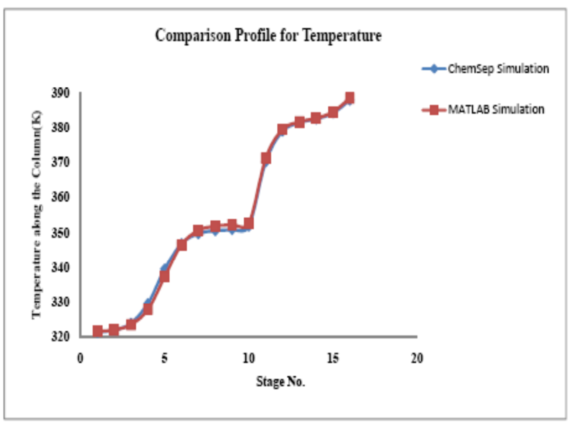


Figure 19: Comparison Profiles for Iso-Butylene Liquid Composition in the Column for $\psi = 0.5$

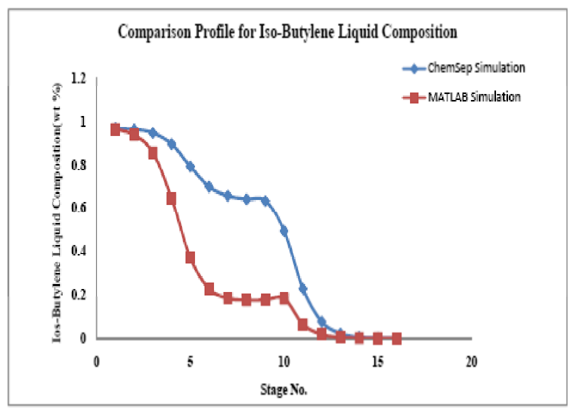


Figure 17: Comparison Profiles for Methanol Liquid Composition in the Column for $\psi = 0.5$

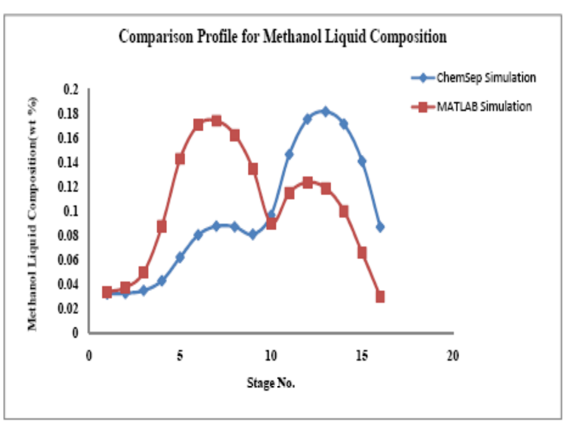


Figure 20: Comparison of Temperature Profiles in the Column for $\psi = 0.5$

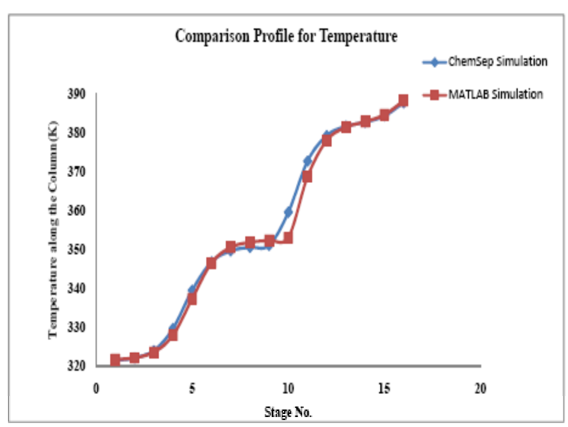


Figure 21: Comparison Profiles for Methanol Liquid Composition in the Column for $\psi = 1$

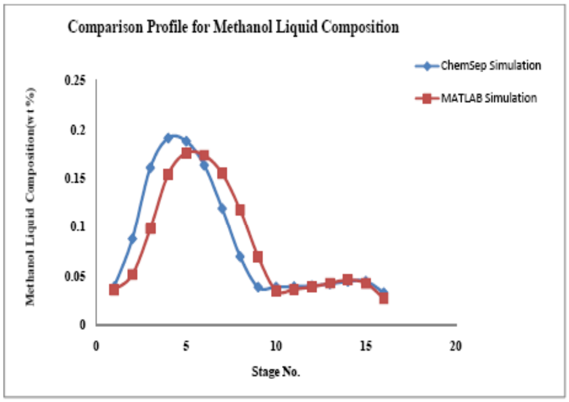


Figure 22: Comparison Profiles for MTBE Liquid Composition in the Column for $\psi = 1$

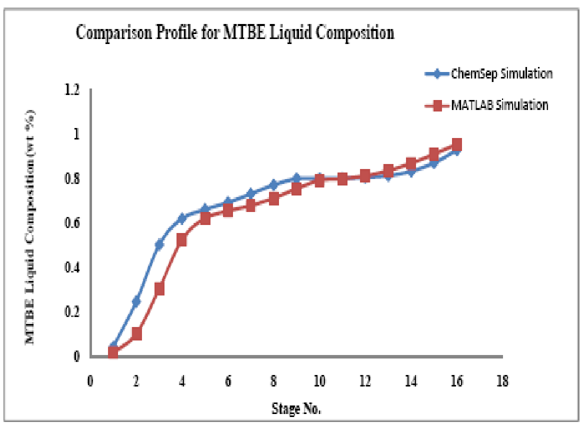


Figure 23: Comparison Profiles for Iso-Butylene Liquid Composition in the Column $\psi = 1$

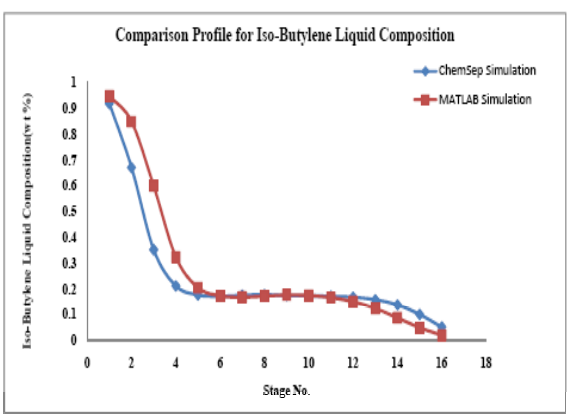
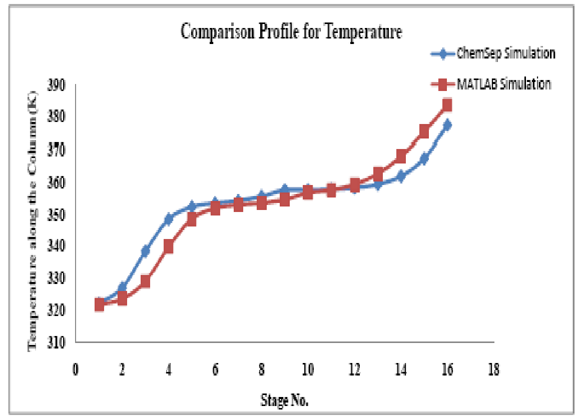


Figure 24: Comparison of Temperature Profiles in the Column for $\psi = 1$

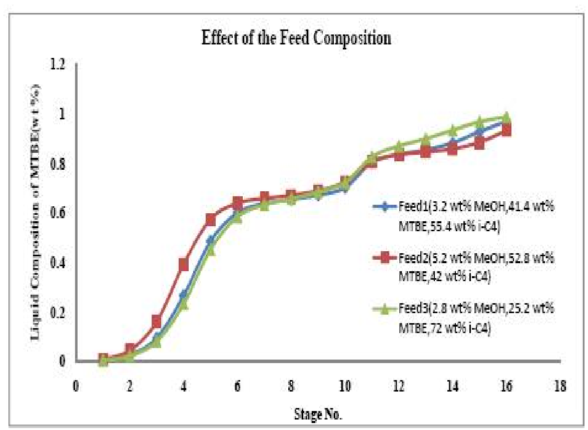


comparison of composition profiles of methanol, MTBE, and iso-butylene and temperature profiles at the different thermal conditions of feed, i.e., saturated liquid, half vaporized and saturated vapor. It can be clearly observed from these Figures that there is a close agreement between the two simulation results for the fixed feed composition, but for the different thermal conditions of feed.

Effect of Feed Composition on MTBE Purity

Figure 25 shows the effect of the feed composition on the purity of MTBE in the bottom of the column.

Figure 25: Effect of the Feed Composition on the MTBE Purity in the Bottom of the Column



It can be observed from this Figure that the purity of MTBE for feed 3 (2.8 wt% MeOH, 25.2 wt% MTBE and 72 wt% i-C4) is maximum in all the three feeds that are fed to the column. It shows that the purity of MTBE increases in the bottom of the column for the low methanol composition and high i-C4 composition in the feed that is fed to the column, which is clearly evident from the above Figure. It can be concluded that in order to obtain high MTBE purity, methanol concentration must be reduced in the feed or inside the column.

CONCLUSION

An equilibrium based steady-state model has been developed for the distillation column and the model equations have been solved by making use of MATLAB 7.9.0 Software. The mathematical model developed has shown satisfactory results in simulating the distillation column for the separation of methanol/MTBE/iso-butylene mixture. The three different types of feed have been fed to the column, viz., saturated liquid, saturated vapor and half vaporized and it was found that the purity of MTBE is maximum in the bottoms, when a saturated liquid feed is fed to the column. The effect of feed composition on the purity of MTBE in the bottom of the column has also been observed and it has been found that the purity of MTBE in the bottom of the column is maximum for the low methanol composition and high i-C4 composition in the feed that is fed to the column. It can further be concluded that in order to obtain high MTBE purity, methanol concentration must be reduced in the feed or inside the column.

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REFERENCES

1. Gonzalez B and Inmaculada Ortiz (2001), "Modeling and Simulation of a hybrid process (pervaporation-distillation) for the separation of azeotropic mixtures of alcohol ether", *Journal of Chemical and Biotechnology*, Vol. 77, pp. 29-42.
2. Homerich U and Robert Rautenbach (1998), "Design and optimization of combined Pervaporation/Distillation processes for the production of MTBE", *Journal of Membrane Science*, Vol. 146, pp. 53-64.
3. Mohamed Z M (2006), "Mathematical Modeling and Simulation for Production of MTBE by Reactive Distillation", M.Tech. Thesis, University of Technology.
4. Seader J D and Ernest J H (2001), "*Separation Process Principles",* 2nd Edition, John Wiley and Sons, Inc. New York, USA.
5. Tahmeed Aijaz (2006), "Modeling and Simulation of Reactive Distillation", M.Tech. Thesis, Chemical Engineering, Aligarh Muslim University, Aligarh.

APPENDIX

NOMENCLATURE

F Molar flow rate of the feed [kmol/hr]

$f_{i,j}$ Feed flow rate of component 'i' tothe column[kmol/hr]

D Total molar flow rate of distillate[kmol/hr]

B Total molar flow rate of bottom[kmol/hr]

Rr Reflux ratio

N Number of stages in the column

N_f Stage at which feed enters the column

P Column pressure [Pascals (Pa)]

P_F Pressure at which feed enters theColumn [Pascals (Pa)]

L_j Total molar flow rate at which liquid phase leaves jth state

V_j Total molar flow rate at which vapor phase leaves jth stage.

W_j Molar flow rate of the vapor side stream leaving jth stage. Please correct it also

U_j Molar flow rate of the liquid side stream leaving jth stage

$W_{i,j}$ Molar flow rate of component 'i' in vapor side stream leaving jth stage

$U_{i,j}$ Molar flow rate of component 'i' in liquid side stream leaving jth stage

$l_{i,j}$ Molar flow rate of component 'i' in liquid phase leaving jth stage

$v_{i,j}$ Molar flow rate of component 'i' in vapor phase leaving jth stage

$Z_{i,j}$ Mole fraction of component 'i' in the feed stream entering jth stage

$x_{i,j}$ Mole fraction of component 'i' in the liquid phase leaving jth stage

$y_{i,j}$ Mole fraction of component 'i' in the vapor phase leaving jth stage

ψ Vapor fraction of the feed

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