

Modeling and Simulation of a Distillation Column using ASPEN PLUS for separating methanol/water mixture

Sohail Rasool Lone & Mushtaq Ahmad Rather

Abstract—Industries are always posed with the problem of separating methanol from water. Distillation is regarded as one of the best processes by which this goal can be achieved. Present study was carried out on these lines to obtain 99.5% composition of methanol in distillate and 99.5 % of water in the bottom product by utilizing ASPEN PLUS simulation software. MESH equations, which actually represent the behaviour of the distillation column, have been solved through ASPEN PLUS in order to study the effect of different parameters. Optimum feed stage location, number of stages and reflux ratio was also established. The optimum conditions found out by our analysis to determine No. of stages (N), feed stage (N_f) and optimum reflux ratio (R_o) were 21, 16 and 1.5 respectively. The paper as such best describes the modeling and simulation of a distillation column using ASPEN PLUS to obtain 99.5% composition of methanol in distillate from 1:1 methanol/water mixture. This analysis will thus prove beneficial for designers in industry who deal with separation of methanol for methanol/water mixture.

Index Terms: Distillation, Modeling, Simulation, Steady-state

1. INTRODUCTION

Distillation is a process that separates two or more components in a mixture 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. The word distillation is derived from the Latin word *destillare*, which means dripping or trickling down. According to Forbes, the art of distillation dates back to at least the first century A.D. 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. By sixteenth century, it was known 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 word *rectefacere*, meaning to improve. Distillation is the most widely used separation process in industry. The separation process requires formation of a second phase by application of heat energy so that both vapor and liquid phases can contact each other on each stage within a separation column. The components have different volatilities so that they partition between the two phases to different extents, and 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 & Henley, 2001). 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

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technique when the relatively volatility, α , of the components being separated is low (1.50).

2. 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.
- The energy balance is based on conservation of enthalpy instead of internal energy.

3. STEADY-STATE MODEL OF A DISTILLATION COLUMN

A rigorous steady-state column model was developed using MESH equations, which actually represent the behaviour of the column. The model consists of mass balance, equilibrium relation, summation equations and energy balance, which are collectively known as MESH equations.

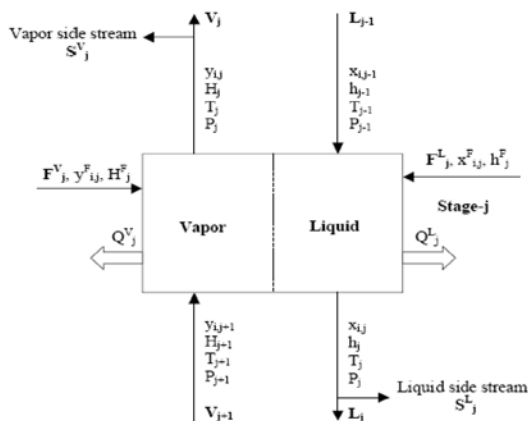


Fig. 1 shows the schematic of a separation stage.

3.1 MASS BALANCE

The model equations for a general 'jth' stage and 'ith' component are represented as:

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

In terms of the flow rates of the 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 get:

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

3.2 EQUILIBRIUM RELATIONSHIP

Since 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:

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

3.3 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:

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

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

3.4 ENERGY BALANCE

The total energy balance for 'jth' stage is given by:

$$L_{j-1} h_{L_{j-1}} + V_{j+1} h_{V_{j+1}} + F_j h_{F_j} - (L_j + U_j) h_{L_j} - (V_j + W_j) h_{V_j} - Q_j = 0 \quad (16)$$

Now using the equations (3) to (9) in the enthalpy balance equation (16), we arrive at a

new enthalpy equation in terms of $l_{j,i}$ and $v_{j,i}$ as under:

$$h_{L_j} (1 + S_j) \sum_{i=1}^C l_{j,i} + h_{V_j} (1 + S_j) \sum_{i=1}^C v_{j,i} - h_{L_{j-1}} \sum_{i=1}^C l_{j-1,i} - h_{V_{j+1}} \sum_{i=1}^C v_{j+1,i} - h_{F_j} \sum_{i=1}^C f_{j,i} - Q_j = 0 \quad (17)$$

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:

$$\sum_{i=1}^C l_{1,i} - (L/D) \sum_{i=1}^C v_{1,i} = 0 \quad (18)$$

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

4. SIMULATION

Aspen Plus was used for the simulation of the distillation column for the separation of water-methanol mixture in this work. In the Aspen Plus, there is an inbuilt model known as RADFRAC, which is meant for the simulation of the distillation columns. Water-methanol mixture with 0.5 mole fraction of each component was considered to get the maximum recovery (99.5%) of Methanol at top. The number of stages and the feed location was changed to suit our purpose. Among a number of thermodynamic property models available in Aspen Plus, which can be used for the estimation of various thermodynamic properties, NRTL property model was used in this work. The results that were obtained upon the simulation of the model are presented in the form of graphs.

5. RESULTS AND DISCUSSION

Simulation calculations for the distillation column have been made in order to study its behaviour when the number of stages and the feed stage location of the distillation column are changed. By running the simulations for the distillation, the optimum feed location and the number of stages so as to maximize the composition of methanol (99.5 % in distillate and 99.5% water in bottom product) was established. In order to separate the water/methanol mixture, the vapor liquid equilibrium of the water/methanol mixture equilibrium data was generated using Aspen Plus simulator, which suggested that distillation is possible for a methanol/water mixture. The

vapor and liquid concentrations vary with temperature as shown in Figure 2. Using this property of water/methanol mixture, it is possible to produce high purity methanol. Figure 3 shows the variation of methanol and water composition profile in the column for ($N=10$, $R_r=1.5$ and $N_f=5$). It can be observed from the figure that the purity of the product is 94.2 % in both the product streams, which is not quite up to requirement of 99.5%, which was basically the main aim of this work and hence in the simulation we kept on changing the number of stages and the feed stage location in order to determine the optimum feed stage location and the number of stages to achieve the desired purity of the products.

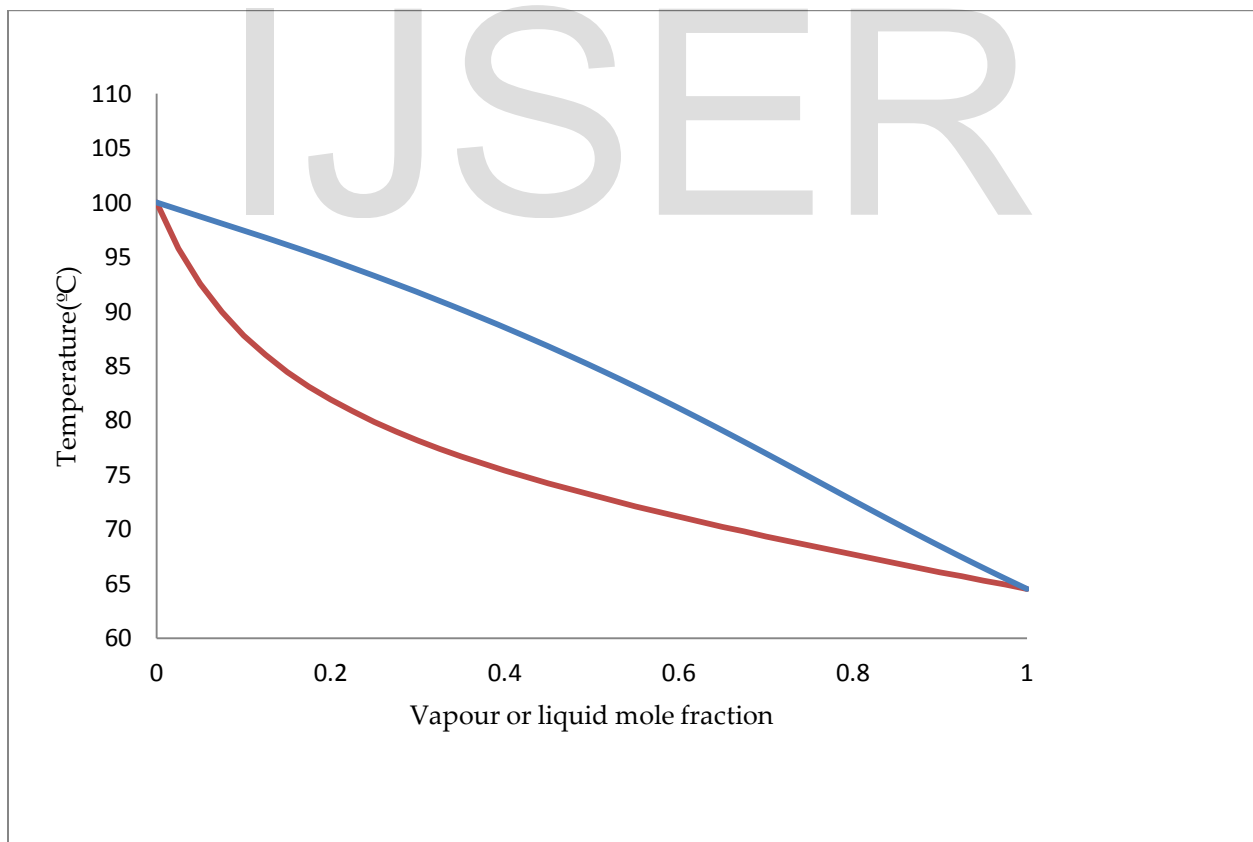


Fig. 2. T-x-y diagram for methanol/water system

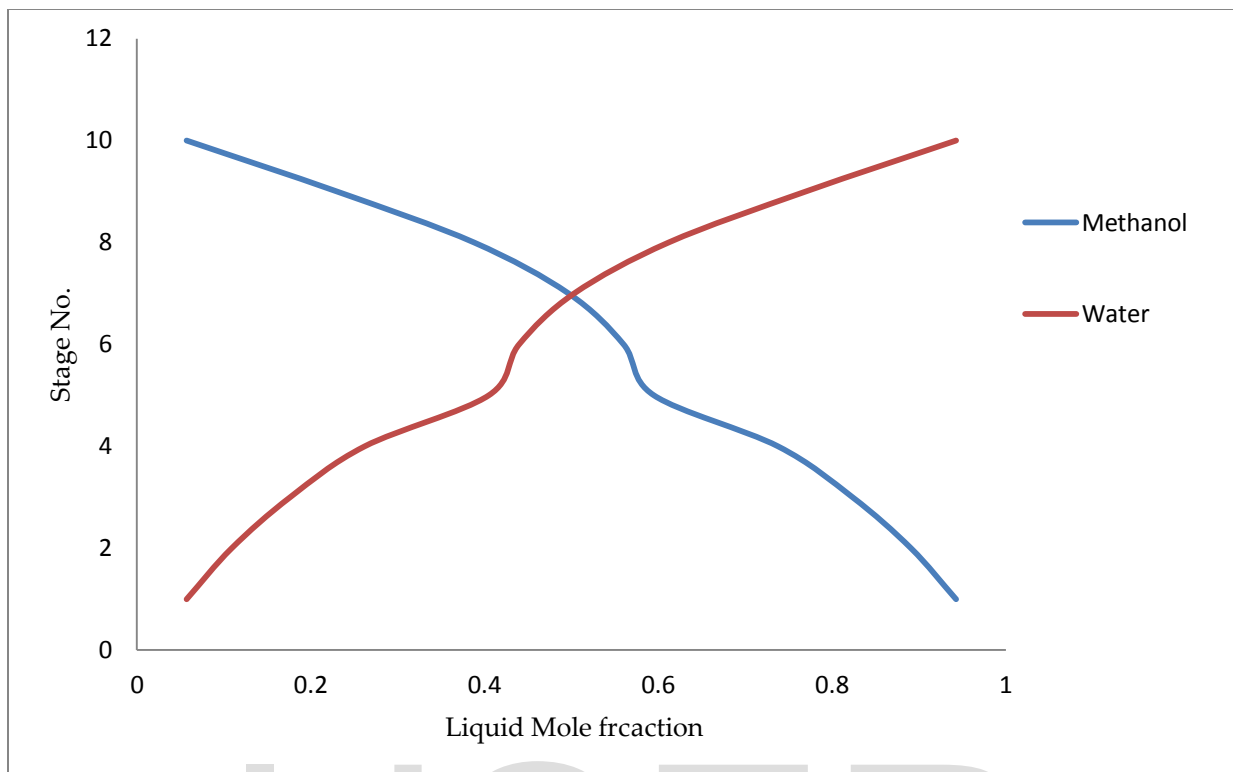


Fig.3. Liquid Composition profile of methanol/water

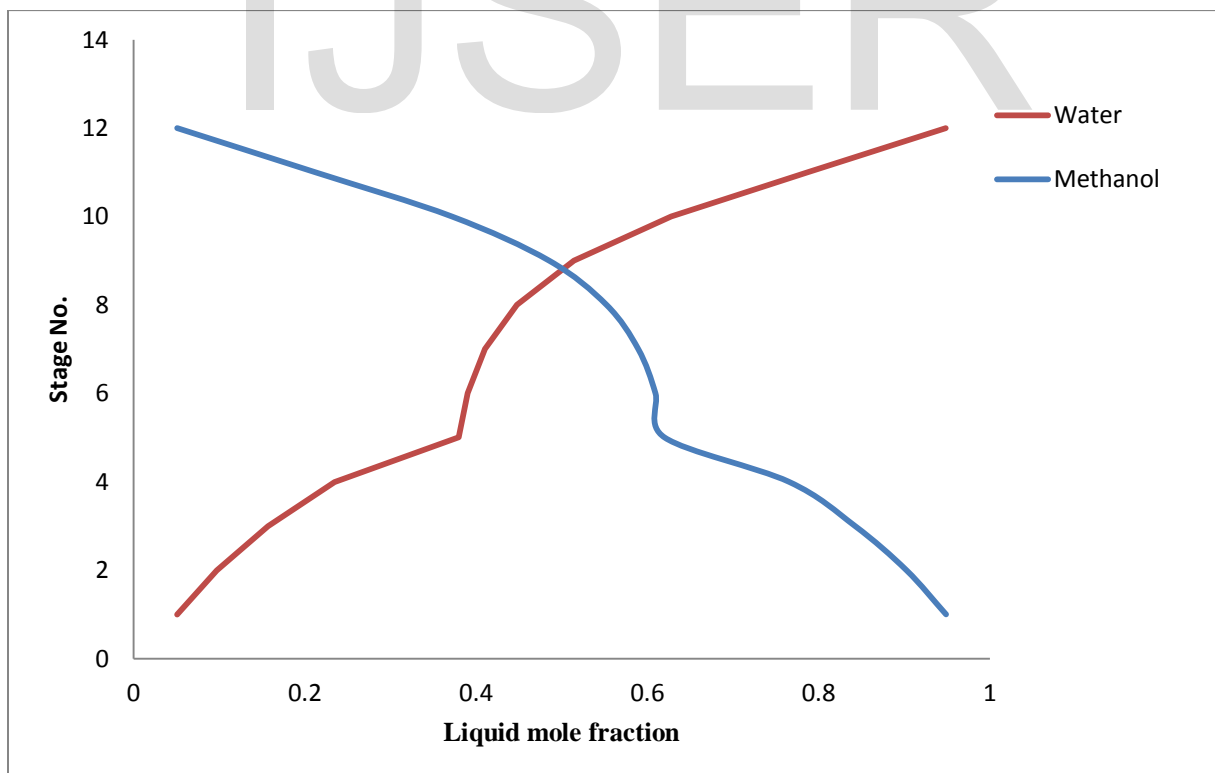


Fig.4. Liquid Composition profile of methanol/water

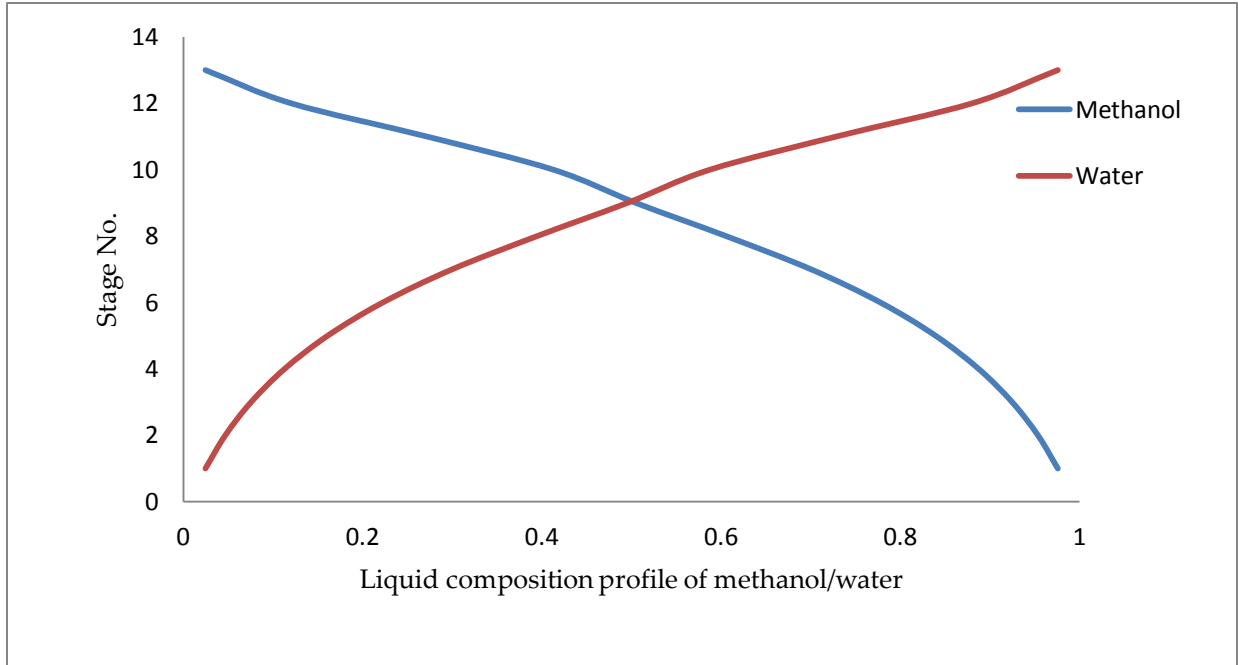


Fig.5. Liquid Composition profile of methanol/water

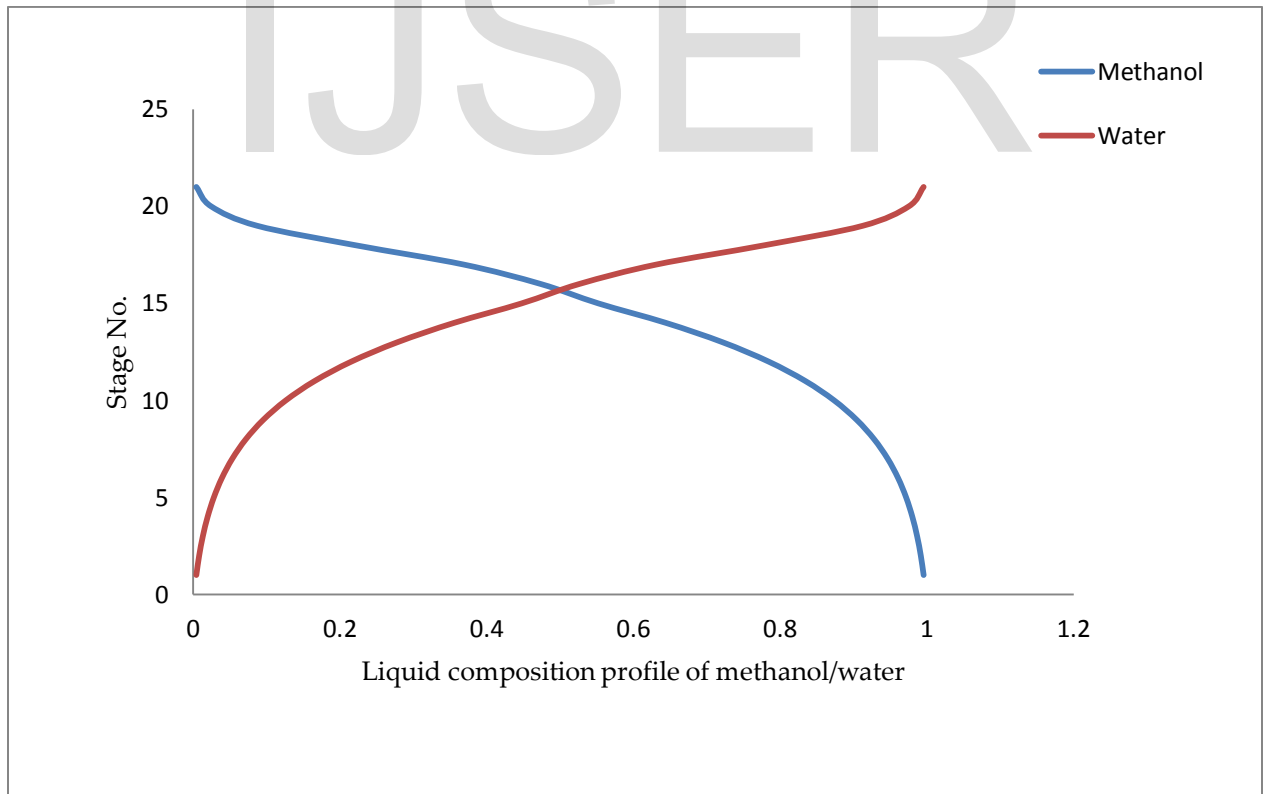


Fig.6. Liquid Composition profile of methanol/water

Figure 4 shows the variation of methanol and water composition profile in the column for ($N=12$, $Rr=1.5$ and $N_f=5$). It can be observed from this figure that the purity of product is 94.9% in both the product streams, which is still not quite up to the required 99.5% and hence we further kept on changing the feed stage location and the number of stages in order to achieve the desired purity of the product. Figure 5 shows the methanol and water composition profile in the column for ($N=13$, $Rr=1.5$ and $N_f=9$). It can be observed from this figure that the purity of product is 97.5%, which has increased by changing the feed stage location

and the number of stages in the column. In order to get the desired purity of the products, the feed stage location and the number of stages in the column need to be further optimized. Figure 6 shows the variation of methanol and water composition profile in the column for ($N=21$, $Rr=1.5$ and $N_f=16$). It can be clearly observed from this figure that the purity of the product obtained is 99.5%, which is the desired purity that was needed. The optimum feed location and the optimum number of stages has also been obtained through the simulation.

5.1 EFFECT OF FEED CONDITION ON THE PURITY OF METHANOL/WATER

Figure's 7, 8 and 9 show the effect of the thermal condition of the feed on the purity of methanol and water in the top and bottom products of the column respectively. It can be clearly observed from figure 7 that the composition of methanol and water is around 99.5% in the top and bottom products respectively, which was the desired purity and hence this was the best feed condition for this simulation work. Also it can be observed from figure's 8 and 9 that the purity of methanol

and water decreases in the top and bottom products as the thermal condition of feed is changed to 0.5 and 1 and the purity of methanol and water decreases in the column and hence they are not the desired thermal feed conditions. Thus, saturated liquid feed condition for which $\psi=0$ is the best thermal feed condition both from the separation view point as well as from the heat economy viewpoint.

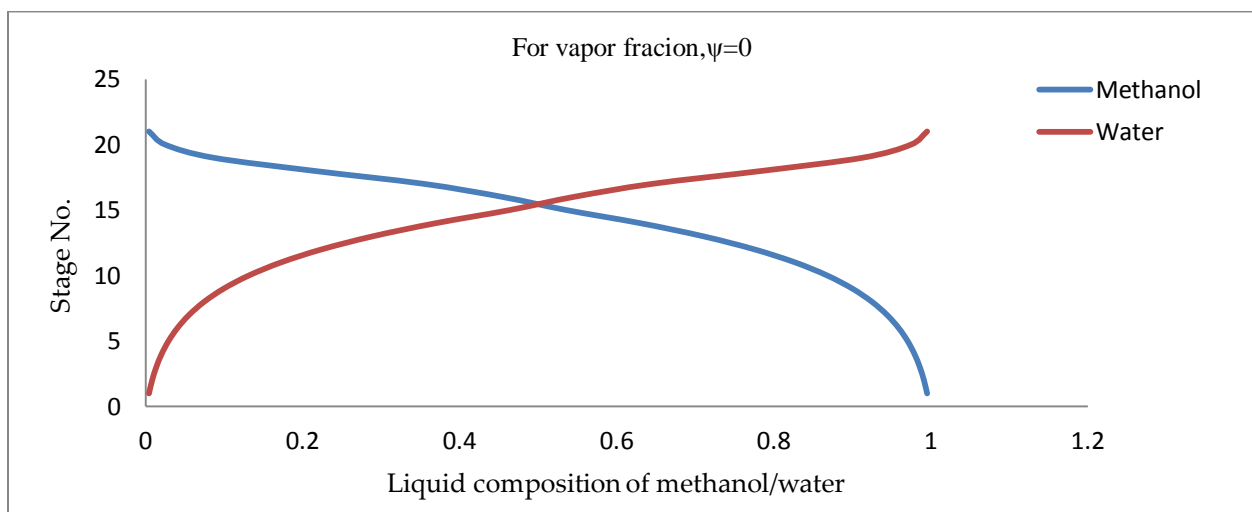


Fig.7. Liquid Composition profile of methanol/water in the column for $\psi=0$

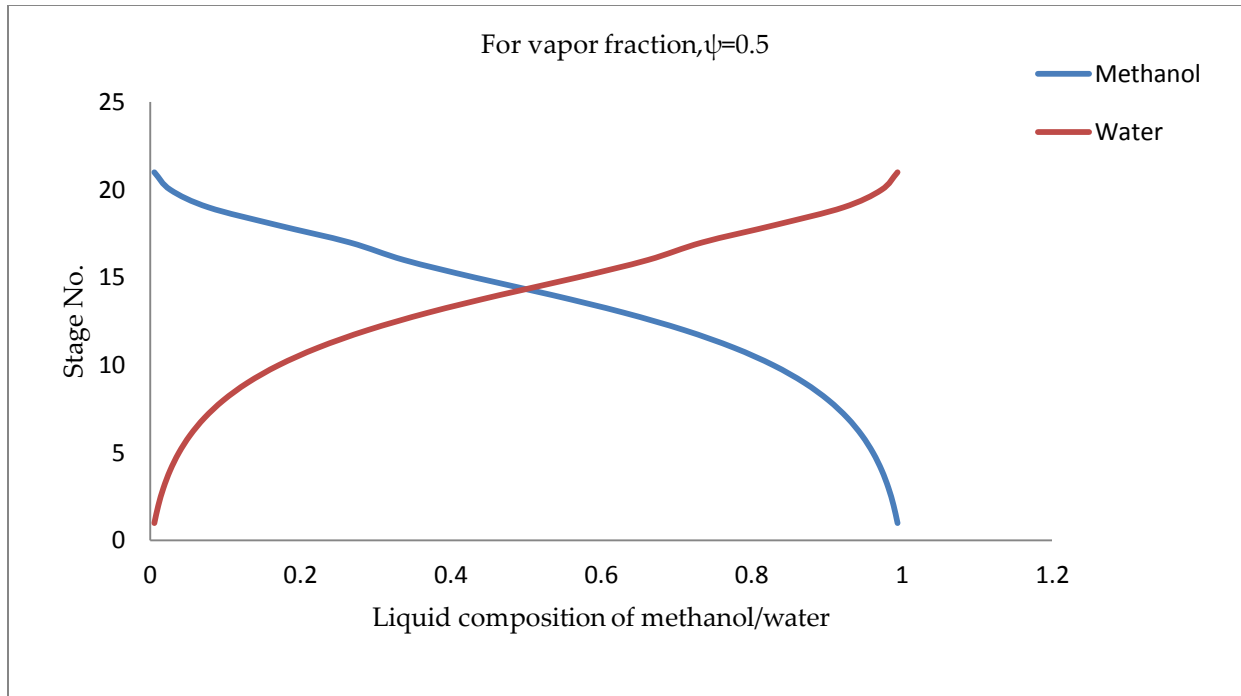


Fig.8. Liquid Composition profile of methanol/water in the column for $\psi=0.5$

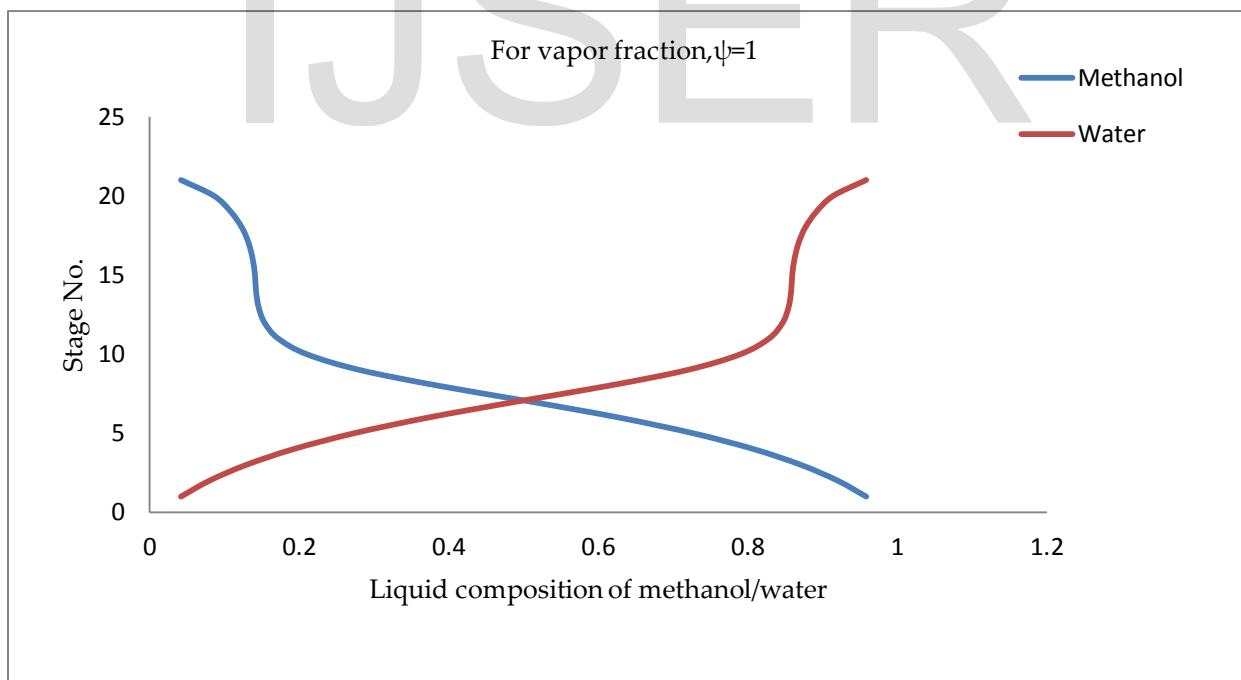


Fig.9. Liquid Composition profile of methanol/water in the column for $\psi=1.0$

6. CONCLUSION

An equilibrium based steady-state model has been developed for the distillation column to separate a mixture of methanol/water in order to get 99.5% methanol in the distillate and same composition of water in the bottoms. The model equations have been solved by making use of Aspen Plus Simulation Software. The VLE data has been generated for this mixture and it was clearly observed from the analysis that the mixture can be separated by distillation to the required 99.5 % of methanol in distillate and 99.5 % water in bottom product. The three different types of simulated feeds have been fed to the column viz. saturated liquid, saturated vapor and half vaporized and it was found that the purity of methanol is maximum in the top, when a saturated liquid feed is fed to the column. Simulations have been carried out further to determine the optimum feed location and optimum number of stages.

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NOMENCLATURE

F	Molar flow rate of the feed [kmol/hr]
$f_{i,j}$	Feed flow rate of component 'i' to the column[kmol/hr]
D	Total molar flow rate of distillate [kmol/hr]
B	Total molar flow rate of bottom [kmol/hr]
R_r	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 the column [Pascals (Pa)]
ψ	Vapor fraction of the feed.
L_j	Total molar flow rate at which liquid phase leaves j^{th} state
V_j	Total molar flow rate at which leaves j^{th} stage
W_j	Molar flow rate of the vapor side stream leaving j^{th}
U_j	Molar flow rate of the liquid side stream leaving j^{th} stage
$W_{i,j}$	Molar flow rate of component 'i' in vapor side stream leaving j^{th} stage
$U_{i,j}$	Molar flow rate of component 'i' in liquid side stream leaving j^{th} stage
$l_{i,j}$	Molar flow rate of component 'i' in liquid phase leaving j^{th} stage

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