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Mathematical Modelling of Binary Distillation Column for Petrochemical Industries

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***Abstract:** Distillation is a method of separating mixtures based on differences in volatility of components in a boiling liquid mixture. It is defined as a process in which a liquid or vapour mixture of two or more substance is separated in to component fractions of desired purity by the application and removal of heat. In this work importance is given to Binary distillation columns. In the Binary Distillation, the feed to the process consist of mixture of two components (A & B) and after the distillation two products will be generated. It is very important to model a distillation column and perform its analysis before the distillation column is practically implemented. Distillation columns are generally considered as chemical systems, for modelling chemical systems one can use mass balance equations.*
***Keywords:** Binary Distillation, Top product, Bottoms, Modelling, Trays*

I. INTRODUCTION

In a binary distillation column, binary mixture is fed into the column as a saturated liquid(at its bubble point)with molar flow rate(mol/min) F_f and molar fraction of component 'A'(lighter component) is C_f. The overhead vapour stream is cooled and completely condensed and then flows into the reflux drum. The cooling of the overhead vapour is accomplished with the cooling water. The liquid from the reflux drum is partly pumped back into the column (top tray N) with a molar flow rate F_R (reflux stream) and is partly removed as the distillate product with a molar flow rate F_D. M_{RD} is the liquid holdup in the reflux drum, x_D is the molar fraction of component 'A' in the liquid of reflux drum which is the composition for both reflux and distillate streams. At the base of the column a liquid product stream (the bottoms) is removed with a flow rate F_B and a composition x_B(molar fraction of 'A'). A liquid stream with a molar flow rate *V* is also drawn from the bottom of the column and after it has been heated with steam, it returns to the base of the column. The composition of re-circulation back to column stream is x_B and M_B is the liquid holdup at the base of the column.

II. MATHEMATICAL MODELING

A mathematical model is a mathematical representation of a physical system which is to be implemented. After developing the mathematical model one can test the performance of the proposed system using different test signals under simulation platform.
The principle of conservation in general, say a quantity 'S',

$$\frac{\begin{bmatrix}\text{Accumulation of } S \\ \text{within a system}\end{bmatrix}}{\text{Time period}} = \frac{\begin{bmatrix}\text{Flow of } S \\ \text{in the system}\end{bmatrix}}{\text{Time period}} - \frac{\begin{bmatrix}\text{Flow of } S \text{ out} \\ \text{of the system}\end{bmatrix}}{\text{Time period}} + \frac{\begin{bmatrix}\text{Amount of } S \\ \text{generated within} \\ \text{the system}\end{bmatrix}}{\text{Time Period}} - \frac{\begin{bmatrix}\text{Amount of } S \\ \text{consumed within} \\ \text{the system}\end{bmatrix}}{\text{Time period}}$$

A. *Assumptions*

1) Vapour holdup on each tray will be neglected
2) The molar heats of vaporization of both components A&B are approximately equal.
3) The heat losses from the column to the surroundings are assumed to be negligible.
4) The above three assumptions imply that, $V = V_1 = V_2 = \dots = V_N$ (V = molar flow rate) and there is no need for energy balance on each tray.
5) The relative volatility 'α' of two components remains constant throughout the column.
6) Each tray is assumed to be 100% efficient (That is vapour leaving each tray is in equilibrium with the liquid on the tray)
7) Neglect the dynamics of the condenser and the reboiler.
8) Neglect the momentum balance for each tray.

B. Modelling of trays

1) Feed Tray (i = f)

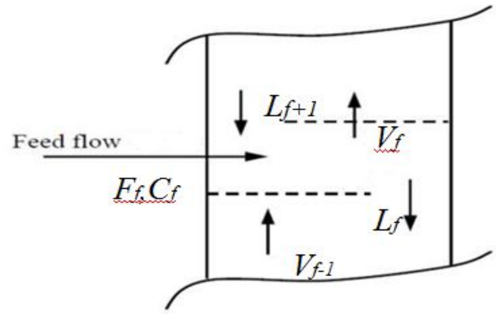

Fig.1 feed tray

Feed or input to the column is given to the feed tray, feed flow is represented by F_f and its composition is C_f.Then the feed is split into liquid and vapour components *L* and *V* respectively.

Total mass and component balance equations are:

$$\frac{d(M_f)}{dt} = F_f + L_{f+1} + V_{f-1} - L_f - V_f \quad (1)$$

$$\frac{d(M_f x_f)}{dt} = F_f C_f + L_{f+1}X_{f+1} + V_{f-1}Y_{f-1} - L_f X_f - V_f Y_f \quad (2)$$

2) Top tray (i = N)

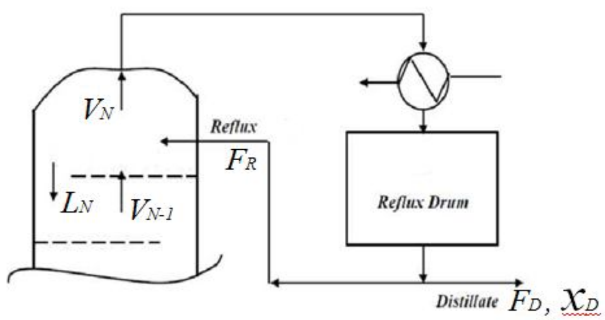

Fig. 2 Schematic of top tray

Vapour which is releasing out of the Nth tray is V_N. Reflux flow to the top tray is F_R, then the total mass and component balance equations are:

$$\frac{d(M_N)}{dt} = F_R + V_{N-1} - L_N - V_N \quad (3)$$

$$\frac{d(M_N x_N)}{dt} = F_R x_D + V_{N-1}y_{N-1} - L_N x_N - V_N y_N \quad (4)$$

3) Bottom Tray (i = 1)

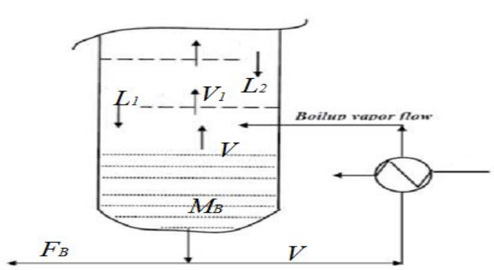

Fig. 3 Schematic of bottom tray

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Column is numbered from bottom to top therefore the bottom tray has the influence of rebioler and is also considered in the balancing equations. Mass and component balance equations are:

$$\frac{d(M_I)}{dt} = L_2 - L_1 + V - V_1 \quad (5)$$

$$\frac{d(M_I x_I)}{dt} = L_2 x_2 + V y_B - L_1 x_1 - V_1 Y_1 \quad (6)$$

4) i^{th} Tray ($i = 2\ldots N\text{-}1$ and $i \neq f$):

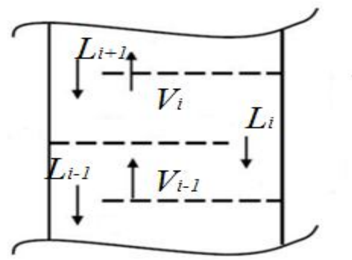

Fig. 4 Schematic of i^{th} tray

For i^{th} tray that is trays other than feed, top and bottom tray, the expressions for developing the balancing equations are same. Generally, mass and component balance equations are:

$$\frac{d(M_i)}{dt} = L_{i+1} - L_i + V_{i-1} - V_i \quad (7)$$

$$\frac{d(M_i x_i)}{dt} = L_{i+1} x_{i+1} + V_{i-1} y_{i-1} - L_i x_i - V_i y_i \quad (8)$$

5) Reflux Drum

Reflux drum is a reservoir that collects the condensed vapour in the form of liquid. Mass and component balance equations are:

$$\frac{d(M_{RD})}{dt} = V_N - F_R - F_D \quad (9)$$

$$\frac{d(M_{RD} x_D)}{dt} = V_N y_N - F_R x_D - F_D x_D \quad (10)$$

6) Column Base

Column base represents the base of the column basic component of the column base is the re-boiler. Mass and component balance equations are:

$$\frac{d(M_B)}{dt} = L_1 - V - F_B \quad (11)$$

$$\frac{d(M_B x_B)}{dt} = L_1 x_1 - V y_B - F_B x_B \quad (12)$$

Vapour-liquid equilibrium relationship can be used to relate the molar fraction of lighter component (A) in the vapour leaving the i^{th} tray (y_i) with molar fraction of A in the liquid leaving the same tray (x_i)

Equilibrium relations:

$$y_i = \frac{\alpha x_i}{1+(\alpha-1)x_i} \quad (13)$$

In this work the distillation columns have *six* numbers of trays and are numbered from bottom to top.

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For feed tray, the equilibrium relation becomes:

$$y_f = \frac{\alpha x_f}{1+(\alpha-1)x_f} \quad (14)$$

Feed tray is chosen as third tray ($i = f = 3$)

Substitute equation (14) into equation (2) and solve for $\dot{X}_f$ then

$$\dot{X}_3 = \frac{x_2 V_2}{M_3\,(E+(\alpha-1))} + \frac{x_3}{M_3}\left(V_3 - V_2 - F_3 - L_2 - \frac{V_3\,\alpha}{F+(\alpha-1)}\right) + \frac{F_3\,C_3}{M_3} + \frac{L_4 x_4}{M_3} \quad (15)$$

For the case of top tray ($i = N = 6$), the equilibrium relation becomes:

$$y_N = \frac{\alpha x_N}{1+(\alpha-1)x_N} \quad (16)$$

Substitute equation (16) in to equation (4) to obtain $\dot{X}_6$ as:

$$\dot{X}_6 = \frac{x_6}{M_6}\left(V_6 - F_R - V_5 - \frac{V_6\,\alpha}{K+(\alpha-1)}\right) + F_R x_D \frac{1}{M_6} + \frac{V_5\,\alpha x_5}{M_6\,(L+(\alpha-1))} \quad (17)$$

Consider the case of bottom tray ($i = 1$), the equilibrium relation becomes:

$$y_1 = \frac{\alpha x_1}{1+(\alpha-1)x_1} \quad (18)$$

Substitute equation (18) in equation (6) and solve for $\dot{X}_1$

$$\dot{X}_1 = \frac{1}{M_1}\left(V_1 - L_2 - V - \frac{V_1\,\alpha}{A+(\alpha-1)}\right) x_1 + \frac{V\alpha}{M_1\,(B+(\alpha-1))} x_B + \frac{L_2\,\alpha x_2}{M_1} \quad (19)$$

i^{th} Tray (i=2, 4 & 5) the equilibrium relations become y_2, y_4 & y_5 respectively. Substitute corresponding '*y*' values and solve; Then

$$\dot{X}_2 = \frac{1}{M_2}\left(V_2 - V_1 - L_3 - \frac{L_3}{C+(\alpha-1)}\right) x_2 + \frac{L_3 x_3}{M_2} + \frac{V_1\,\alpha x_1}{D+(\alpha-1)} \quad (20)$$

$$\dot{X}_4 = \frac{x_4}{M_4}\left(V_4 - V_3 - L_3 - \frac{V_4\,\alpha}{G+(\alpha-1)}\right) + \frac{V_3\,\alpha x_3}{M_4(H+(\alpha-1))} + \frac{L_5 x_5}{M_4} \quad (21)$$

and

$$\dot{X}_5 = \frac{x_5}{M_5}\left(V_5 - V_4 - L_6 - \frac{V_5\,\alpha}{I+(\alpha-1)}\right) + \frac{L_6\,x_6}{M_5} + \frac{V_4\,x_4\,\alpha}{(J+(\alpha-1))M_5} \quad (22)$$

Reflux drum:

$$\dot{X}_D = \frac{x_D}{M_{RD}}(F_R - V_6 - F_D) + \frac{V_6\,\alpha x_6}{(M+(\alpha-1))M_{RD}} \quad (23)$$

Column base:

$$\dot{X}_B = \frac{x_D}{M_B}\left(V - L_1 + \frac{\alpha}{N+(\alpha-1)}\right) + L_1 \quad (24)$$

where;

F_f = Feed flow

C_f = Feed composition

α = Relative volatility

$M_1, M_2, M_3, M_4, M_5, M_6, M_{RD}, M_B$ are the liquid holdups in each trays and in reflux and reboiler drum respectively.

$x_1, x_2, x_3, x_4, x_5, x_6, x_D, x_B$ are the liquid concentrations in each trays and liquid concentration of the distillate and bottom product respectively.

$V_1, V_2, V_3, V_4, V_5, V_6, V$ are the vapour holdups in the each trays and vapour holdup in the bottom of the column.

$y_1, y_2, y_3, y_4, y_5, y_6, y_D, y_B$: are the vapour concentrations in each tray and vapour concentration of the distillate and bottom product respectively.

Implementing all the above $\dot{X}_i$ using MATLAB/SIMULINK and excited using a step function to obtain composition of distillate and bottom product (bottoms).

TABLE 1 Parameter values

Variables	Corresponding Values
Feed mass rate, F_{mass}	15.4761 tons/hour
Holdup in the column base, M_B	31.11 kmole
Holdup on each tray, M	5.80 kmole
Holdup in reflux drum, M_D	13.07 kmole
Density of feed, d_F	0.670 ton/$meter^3$
Relative volatility, α	5.68
Vapour flow, V	75.9 kmole/hour
Liquid flow, L	8.847 ton/hour
V_{steady} $state$, $\bar{V}$	66.3407 kmole/hour
$L_{steady\,state}$, $\bar{L}$	75.6380 ton/hour
Condenser Holdup, D	92.7597 kmole
Boiler Holdup, B	110.9235 kmole

[*"Modeling and Control Simulation for a Condensate Distillation Column"* Vu Trieu Minhand John Pumwa , Papua New Guinea University of Technology]

C. Model Verification

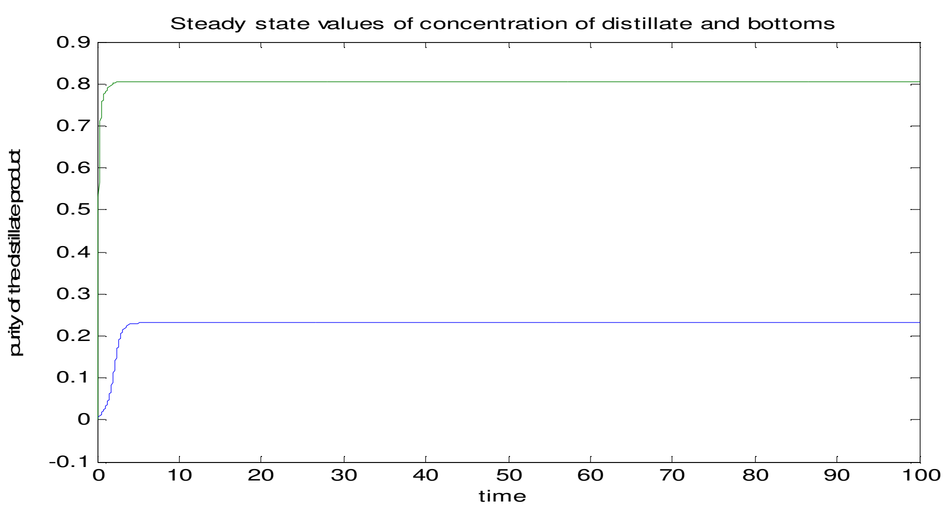

Fig. 5 Output graph representing concentrations on top and bottom tray.

III.CONCLUSIONS

If there is no disturbance in the operating conditions the system is able to achieve steady state purity of the product. From the above response it is clear that it does not achieve the desired purity, this is one of the problem that has to rectify. For this an efficient controlling scheme that can preserve the actual nonlinear characteristics of the practical system is needed.

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