

A
Project Report
On
Simulation and Modelling of Divided Wall Distillation Column
By Programming Design Equations using MATLab.

Submitted by

Abhilash Pati
(Roll No: 110CH0372)

In partial fulfillment of the requirements for the degree in
Bachelor of Technology in chemical Engineering.

Under the guidance of

Dr. BASUDEB MUNSHI



Department of Chemical Engineering
National Institute of Technology Rourkela
May, 2014



CERTIFICATE

*This is certified that the work contained in the thesis entitled “Simulation and design of Divided Wall Distillation Column by modelling and programming design equations,” Submitted by **Abhilash Pati (110CH0372)**, has been carried out under my supervision and this Work has not been submitted elsewhere for a degree.*

Date:

Place: Rourkela

(Thesis supervisor)

Dr. BASUDEB MUNSHI
PROFESSOR
Chemical Engineering,
NIT Rourkela

Acknowledgements

First and the foremost, I would like to offer my sincere gratitude to my thesis supervisor, **Dr. BASUDEB MUNSHI** for his immense interest and enthusiasm on the project. His technical prowess and vast knowledge on diverse fields left quite an impression on me. He was always accessible and worked for hours with me. Although the journey was beset with complexities but I always found his helping hand. He has been a constant source of inspiration for me.

I am also thankful to all faculties and support staff of Department of Chemical Engineering, National Institute of Technology Rourkela, for their constant help and extending the departmental facilities for carrying out my project work.

I would like to extend my sincere thanks to my friends and colleagues. Last but not the least, I wish to profoundly acknowledge my parents for their constant support.

(Abhilash Pati)

110CH0372

ABSTRACT

The thesis describes about the simulation and design study of divided wall distillation columns using various mathematical models. Since all of us are aware, that distillation is the fundamental aspect of separation processes in the Chemical industries. In the current thesis, simulation studies of the divided wall distillation column using various mathematical models are presented. Steady state simulations are being performed using Thomas mathematical model supported by rigorous programming using combination of MATLAB which is the fundamental programming language. In the steady state simulation we have tried to see the effect of changing the number of plates on the component mole fraction, vapor flow rate, liquid flow rate, Temperature etc., which gives an idea about the optimum number of plates in the divided wall distillation column. The basic input variables used are tear variables i.e. temperature and vapor flow rate. Firstly, MESH equations has been written for an equilibrium stage in a multi-component vapor liquid cascade. Those equilibrium stages can be combined to form a counter-current cascade of N equilibrium stages that can be used to model divided wall distillation column. Then the mathematical model of tri-diagonal matrix algorithm has been applied to solve the MESH equations. And then rigorously solving countercurrent-flow, multi-equilibrium stage, multi-component separation system with the help of Thomas algorithm and with the help of a process simulator. And thereby by rigorous programming and continuous simulation it predicts optimum number of plates alongside implementation of controllability factors could be implemented for feasible operation of divided wall distillation column. Thus, designing of divided wall distillation column must be encouraged in chemical industries reducing two important parameters cost and energy to a great extent thereby enhancing profitability of the industries to a great extent.

Keywords: MATLAB, Steady state simulation, Cascade control, Composition, Temperature, Divided wall distillation column, Vapor flow rate.

CONTENTS

	PAGE NO
CERTIFICATE	2
ACKNOWLEDGEMENT	3
ABSTRACT	4
LIST OF FIGURES AND TABLES	7
CHAPTER 1: INTRODUCTION	9
1.1: GENERAL	10
1.2: OBJECTIVES OF CONTROL	11
1.3: CONTROL STRATEGIES	11
CHAPTER 2 : LITERATURE REVIEW	12
2.1: BRIEF REVIEW	13
2.2: SALIENT FEATURES OF DWC	13
2.3: REVIEW OF VARIOUS MATHEMATICAL MODEL	14
CHAPTER 3 : DESIGNING OF DWC	16
3.1: APPLICATION OF MAIN MATHEMATICAL MODEL	17
3.2: DESIGNING OF DWC BY MESH EQUATIONS.	19
CHAPTER 4 : SIMULATION AND CONTROL OF DWC	21
4.1: SIMULATION ALGORITHM	22
4.2: BUBBLE POINT CALCULATION	24
4.3: STEADY STATE EQUATIONS	25
4.4: PROGRAMMING ANALYSIS	29
CHAPTER 5: PROGRAMMING RESULTS	30

CHAPTER 6: CONCLUSIONS AND SCOPE FOR FUTURE 42

CHAPTER 7: REFERENCES 44

CHAPTER 8: APPENDIX 46

List of Figures and symbols.

List of symbols:

- U: Liquid side stream flow rate.
- W: Vapor side stream flow rate.
- Wa: Vapor flow rate from divided section.
- Uz: Liquid flow rate from divided section.
- K: Phase equilibrium ratio.
- F: Molar feed flow rate.
- V: Molar vapor flow rate.
- L: Molar liquid flow rate.
- Z_f: Feed composition.
- N: Number of stages
- C: Number of components.
- γ: Activity Coefficient.
- P^S: Vapor pressure.
- A,B,C: Antoine Coefficients.
- Del: Solubility parameter.
- MV: Liquid molar volume.
- H_F: Molar feed enthalpy.
- H_L: Liquid molar enthalpy.
- H_v: Vapor Molar enthalpy.
- R: Reflux Flow rate.
- .

List of Figures:

FIGURE NO	TITLE OF FIGURE	PAGE NO
1	Temperature versus Pressure for propane by BPC Method.	33
2	Temperature versus Pressure for butane by BPC Method.	33
3	Temperature versus Pressure for pentane by BPC Method.	34
4	Vapour flow rate versus number of stages by BPC analysis	34
5	Temperature versus number of stages by BPC analysis	35
6	Vapour flow rate versus number of stages by DWC analysis	37
7	Temperature versus number of stages by DWC analysis	38
8	Equilibrium phase ratio versus number of stages by DWC analysis .	38
9	Liquid phase mole fraction versus number of stages for propane by DWC	39
10	Liquid phase mole fraction versus number of stages for butane by DWC.	39
11	Liquid phase mole fraction versus number of stages for pentane by DWC	40
12	Liquid Mixture Enthalpy versus number of stages by DWC analysis	40
13	Vapour Mixture Enthalpy versus number of stages by DWC analysis.	41
14	Liquid flow rate versus number of stages for multi-component mixture by DWC.	42

CHAPTER 1

INTRODUCTION

INTRODUCTION

1.1 GENERAL: Distillation is costly and energy consuming process. It is the most common separation process in the chemical industries. Distillation is predominantly used in refinery and petrochemical industries. Various fractionation process for instance extractive distillation for hydrocarbons has been developed.

Distillation is a thermal separation process. It will remain the most preferable alternative among all processes deployed in chemical industries. At present there are 40000 columns operating around the world. The single drawback is the considerable high demand of energy since it would account for more than half of the total plant operating cost.

A ternary mixture can be separated in three different ways. The first alternative is direct process most volatile component would be separated first. Second alternative is indirect process when the most heaviest component would be separated first. The last alternative is distributed sequence when there will be a mid split comprising of two to three distillation columns. This kind of separation has led to petlyuk column system comprising of two fully thermally coupled distillation column. Ultimately it has led to the concept of divided wall column that integrates two column of petlyuk column to one column shell. Divided wall column derived its name since its middle part is divided by a wall. Multi-component mixture is fed to one side of the column. Deflected by the wall the lightest component moves upward and recovered as top distillate. While the heaviest component moves down and recovered as the bottom product. Intermediate component that initially moves up and down with both upward as well as downward stream subsequently separate out from top as well as bottom and recovered as side stream.

Use of divided wall column require a match between operating condition of two stand alone column in a direct or indirect sequence. Divided wall column is very demanding as it can separate three or more components in a single column. Thus it eliminates the need for second unit saving the cost of building two columns and minimizing operating costs by use of single condenser and re-boiler. Use of divided wall column saves thirty percent in the capital investment and forty percent in the energy cost. The leading companies are MONTZ and BASF. In divided wall distillation column it has got high purity for all streams reached in the single column. Due to reduced remixing effects it has got high thermodynamic efficiency. Due to integrated design it has got lower capital investment. It requires low energy in comparison to conventional separation process. Due to reduced number of equipment units it has got small footprint. It is more advantageous when divided wall column is added with reactive distillation leading to more integrated design. Direct sequence consisting of two columns used for separation of ternary mixture. Other two column have lower cost and energy requirements. They used to feature main column and second column. Pre-fractionator have separate re-boiler and condenser in the two column and it can split vapor and liquid streams between the column by use of single re-boiler and condenser. The significant application of petlyuk column is the divided wall column that separate middle section into two sections by a

wall at appropriate position. Feed is being fed to pre-fractionator and sidestream is removed recovered from other side primarily being the intermediate component. The divided wall restricts the lateral combination of vapor and liquid. Dividing wall is vertical partition made up of flat metal sheet. Sheet welded to the column consisting of flexible thin metal sheet slacked together. Wall flow must be reduced as it lower the quality of product as well as purity. Construction is encouraged by self-centering packed element. They can balance the poor tolerance of column.

1.2 OBJECTIVE OF CONTROL:

No fundamental differences has been applied to usual column sequence.

No control of the internal separation of gas and liquid but if required special parts can be implemented.

Dynamic simulation role is significant and quite important.

Model prediction control needs to be tested.

Application:

Separation sequence has to be separated in sequence for multi component.

Petlyuk design is feasible with flow rate of component need to be comparable.

1.3 CONTROL STRATEGIES:

Parameters which should be taken to consideration:

Reflux ratio.

Number of theoretical stages in divided wall column.

Liquid distribution, vapor distribution and specification of feed as well as product.

.

CHAPTER 2

LITERATURE REVIEW

2.1 BRIEF REVIEW.

Divided wall distillation column has been known 50 years back. It has huge potential to make huge savings in energy and capital in distillation. One of the major fear is uncertainty in control and operation of the arrangement. As a result of which operation and control of the dividing wall column need to be investigated. Dynamic modeling of dividing wall column is used to detect optimum startup. It minimizes time required to reach steady state. Problem is settled by transformation of dynamic model in system of differential equation. Algebraic calculation avoided by use of iterative dynamic programming to minimize startup time. The main idea is the optimum design of thermally coupled distillation column. Divided wall column uses column model and mathematical optimization. Column model is capable to describe conventional as well as thermally coupled column. The focus has been shifted to rationalize degree of freedom analysis of Divide wall distillation column for steady state simulation. That is possible by using detailed Mathematical model consisting of MESH equations. In Divided wall distillation column pressure difference used to detect vapor and liquid flow in different trays. Divided wall distillation column operating in steady state with feed and condenser pressure has degrees of freedom as four in contrast to conventional column which have three degrees of freedom by having three product streams. This can be used to mention liquid split but no degree of freedom left to mention vapor split.

2.2 SALIENT FEATURES OF DWC.

Divided wall distillation column is not a new concept. It was designed way back in 1949. Due to lack of reliability and speculation about the operation and control of the column have resulted in the minimization of use. Dividing wall column are process equipment having the capacity to reduce both capital and operation cost in comparison to conventional column. Distillation column comprising of two dividing walls have proved to lower energy and cost requirement in comparison to a single divided wall. But the integration of two columns into single shell brings about the change in the operation mode and the controllability of the system. The divided wall distillation column brings a major change in the field of science and technology by considerably lowering the energy requirements and cost requirements. Divided wall distillation column are intensified process equipment. They have the tendency to lower both investment capital as well as the cost of operation. The addition of reactive column along with a divided wall column gives rise to reactive divided wall column. Different configurations of two dividing wall column system are enquired for the desired separation of a multi component mixture. As a result of which rigorous model is generated allowing the motionless and motional simulation of the process. Steady optimization is being performed to design the column system and to select the configuration so as to minimize the total cost. The main focus is to enquire about the process involved in executing the divided wall column technology to treat the petrochemical fractions.

Special tools used for simulation have been designed to process the overall column configuration and a modern algorithm is developed to find the optimal column design on the basis of total annual cost. Operation is tested on laboratory scale with special set of divided wall column processed as variable unit construction. Enriching experiences along with a clear cut economical advantage led to industrial realization of new concept in various commercial plant. Column need to satisfy energy requirement, yield of product and purity.

2.3 REVIEW OF VARIOUS MATHEMATICAL MODEL.

The basic use of reactive divided wall column is process of hydrolysis of methyl acetate. The optimum method of fully coupled distillation for ternary system is being applied. The thermally coupled phenomena can be processed in the form of original petlyuk configuration. This kind of approach use shortcut design method allowing the system to be modeled in the form of a non linear program.

Work has also been carried out to observe the pattern flow of fluid mixture in the divided wall distillation column particularly from view point of controllability. It include different area like design, modeling and control. On the basis of various publications and patent it tries to give an idea. Approaches for shortcut, rigorous simulation, optimization and proper control are being focused particularly on column internals and dimensioning have been provided.

SHORTCUT MODEL FOR OPTIMUM DESIGN OF DWC AND PETLYUK SYSTEM.

There are three sections. In the first section the process of recovery of the lightest as well as heaviest component in the overhead stream are mentioned from the analysis of degrees of freedom and an extra parameter is required for recovering the intermediate component as a variable.

For multi-component mixture under-wood basic equation provides the following:

$$\sum \alpha_i x_i F / (\alpha_i - \theta) = 1 - q \quad i=1 \text{ to } 3$$

The minimum reflux can be achieved through the proper substitution of roots:

$$L_{\min} = \max_j [F_i \theta_j^{1} r_i / (\alpha_i - \theta_j^{1})]$$

Main column design:

For minimum reflux ratio for the second section:

$$Q_D = L^1 / (V^1 - L^1) = -R^2$$

For minimum reflux ratio for the third section:

$$Q_W = L^1 / (L^1 - V^1)$$

Choosing the most dominant section for the main column:

$$R_{\min} = \max \{ L_{\min}/D, L_{\min} + S - (D \cdot Q_D/D) \}$$

Design value for R above the minimum value can be set:

$$L_2 = R \cdot D_2$$

Composition can be determined for interconnecting streams:

In multi-component mixture composition of saturated stream can be determined considered equivalent to non saturated feed which correspond to the composition approximately of the interconnecting stream which can be estimated with the help of feed line and operating line.

$$Y_i = (q/(q-1)) \cdot X_i - X \cdot D_I / (q-1)$$

$$Y_I = (R/(R+1)) \cdot X_{I+} + X \cdot D_I / (R+1)$$

$$Y_I = (R \cdot Z_i + q \cdot X_{Di}) / (R+q)$$

DYNAMIC DISTILLATION MODEL

The advantage and primitive of the following model underlies in the fact that iterative algebraic equations are being avoided. The main portion of the model comprises of the following system of ordinary differential equation.

Total mass balance around plate:

$$dN_j/dt = L_{j-1} - L_j + V_{j+1} - V_j + F_{L,j} - F_{V,j}$$

component mass balance around plate j for component i:

$$d(N_j \cdot X_{ij})/dt = L_{j-1} \cdot X_{i,j-1} + V_{j+1} \cdot Y_{i,j+1} - V_j \cdot Y_{i,j} - L_j \cdot X_{i,j} + F_{L,j} \cdot X_{F,i,j} - F_{V,j} \cdot Y_{F,i,j}$$

The total pressure varies during each time integration step much smaller in comparison to the variation of composition and temperature. The vapor pressure in each plate is considered constant in each of the time integration step but it will be again recalculated at the starting of new time step. Tray pressure drop is calculated on hydraulic correlations. vapor flow rate V_j can be estimated from total energy balance and composition is calculated in accordance to murphee efficiency. Liquid flow rate L_j can be estimated on the basis of francis correlation.

CHAPTER 3

DESIGNING OF DWC

3.1 APPLICATION OF MAIN MATHEMATICAL MODEL.

Simple Distillation Column

A complete mathematical analysis is being carried out to describe material, energy and momentum balance equation for each individual tray of the entire distillation column subject to condition of thermodynamic constraints of vapor liquid equilibrium.

These modeling equations are called as Material-balance-vapor liquid equilibrium summation and enthalpy balance equations.

Model equations which are used in the present formula gives rise to $N*(2*C+1)$ number of independent equations for simple column with 1 feed and two product streams where C is the number of components and N is the number of stages including condenser and re-boiler.

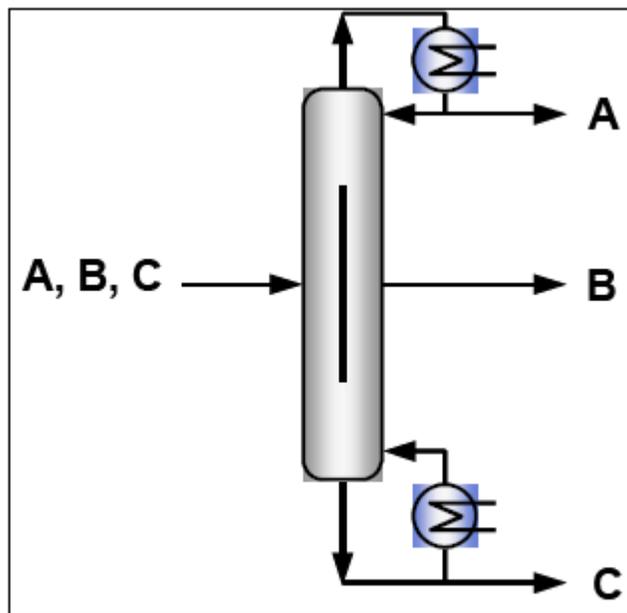


Figure 4. Dividing Wall Columns – Separation of a 3-Component Mixture

Component material balance equation for all $j=1$ to N .

$$V_{2,j} - V_{1,j} - L_{1,j} = 0 \quad (\text{for condenser } i=1)$$

$$V_{i+1,j} - V_{i,j} + L_{i-1,j} - L_{i,j} = 0 \quad (\text{for } i=2 \text{ to } N-1)$$

$$V_{f+1,j} + L_{f-1,j} - L_{f,j} - V_{f,j} + F_j = 0 \quad (\text{for feed plate } i=f)$$

$$L_{N-1,j} - L_{N,j} - V_{N,j} = 0 \text{ (for re-boiler } i=N)$$

Overall summation equation:

$$L_i = \sum l_{i,j} \text{ (for } i=1 \text{ to } N)$$

$$V_i = \sum v_{i,j} \text{ (for } i=1 \text{ to } N)$$

Equilibrium Relation:

$$Y_{i,j} = K_{i,j} * X_{i,j}$$

Where equilibrium constant is dependent variable

$$K_{i,j} = K(T_i, P_i, L_{i,j}, V_{i,j})$$

Enthalpy balance equation:

$$V_2 H_2 - (L_1 + V_1) * h_i - Q_C = 0 \text{ (for condenser } i=1)$$

$$L_{i-1} * h_{i-1} + V_{i+1} * H_{i+1} - L_i * h_i - V_i * H_i = 0$$

$$L_{f-1} * h_{f-1} - L_f * h_f + V_{f+1} * H_{f+1} - V_f * H_f + H_f \sum F_j = 0$$

$$L_{N-1} * h_{N-1} - L_N * h_N + Q_B - V_N * H_N = 0 \text{ (for re-boiler } i=N)$$

Vapor and Liquid phase enthalpies are obtained through integration of heat capacity of individual components with respect to a fixed reference temperature in distillation column.



A divided wall distillation column comprise of $N-2$ full size trays among which N_1+1 to N_2 are splitted into two parts. The trays are numbered sequentially from top to bottom including of the feed tray and all the divided trays of section 1.

Thus the condenser is numbered as stage 1. The re-boiler is stage number N. Top most tray of the divided wall section 1 is N_1+1 . The last tray of the divided section 1 is N_2 . The re-boiler is stage number N. From top numbering of second column starts from N_3+1 and continues till N_T that is last divided tray in section 2. Tray numbered 2 to N_1 are full size trays and tray below N_1 till N_2 are splitted into two parts. The first tray in first half in section 1 that is N_1 is labeled as N_1+1 and on the other hand second half of the same section tray in section 2 is labeled as N_3+1 .

Liquid stream coming out from N_1 is partitioned as two parts L_{N1} and S_1^L . L_{N1} goes to N_1+1 of section 1 and S_1^L goes to N_3+1 that is to uppermost tray of section 2 in a divided wall distillation column. Similarly vapor stream coming out from N_2 is splitted into two parts V_{N2} and S_2^V which in turn goes to the bottom stage of section 2. Main column has two side draws S_1^L coming out from N_1 and S_2^V coming out from N_2 and secondary stream S_3 is taken out from second half of the divided section.

3.2 DESIGNING BY MESH EQUATIONS:

Component Material balance equation:

$$L_{N1-1,j} + V_{N1+1,j} - V_{N1,j} - L_{N1,j} - L_{N1,j} * (S_1^L / L_{N1}) + V_{N3+1,j} = 0$$

$$L_{N2-1,j} + V_{N2+1,j} - L_{N2,j} - V_{N2,j} * (S_2^V / V_{N2}) + L_{NT,j} = 0$$

Enthalpy balance equation:

$$L_{N1-1} * h_{N1-1} + V_{N1+1} * H_{N1+1} - L_{N1} * h_{N1} - V_{N1} * H_{N1} - R_1 * L_{N1} * h_{N1} + V * H_{N+1} = 0$$

Where $R_1 = S_1^L / L_{N1}$

$$L_{N2-1} * h_{N2-1} + V_{N2+1} * H_{N2+1} - L_{N2} * h_{N2} - V_{N2} * H_{N2} - R_2 * V_{N2} * H_{N2} + L * h_{N2} = 0$$

Pressure balance equation:

$$(P_2 - P_1) - (P_X - P_Y) = 0$$

Since the number of trays in divided wall distillation column is N. 1 to N_1 is rectifying section. N_1 to N_3 is divided wall section in between feed stage at N_2 . N_3 to N is stripping section.

Normal steady state equations could be applied:

Top tray:

$$R + V_2 - L_1 - V_1 = 0$$

$$R * X_D - L_1 * X_1 - V_1 * Y_1 + V_2 * Y_2 = 0$$

$$R \cdot H_D^L + V_2 \cdot H_2^V - V_1 \cdot H_1^V - L_1 \cdot H_1^V = 0$$

$$L_1 + V_3 - L_2 - V_2 = 0$$

$$L_1 \cdot X_1 + V_3 \cdot Y_3 - L_2 \cdot X_2 - V_2 \cdot Y_2 = 0$$

$$L_1 \cdot H_1^L + V_3 \cdot H_3^V - L_2 \cdot H_2^L - V_2 \cdot H_2^V = 0$$

At the dividing section:

$$L_{N1-1} - L_{N1} + V_{N1+1} + V - V_{N1} - L_{N1} \cdot (S_1^L/m) = 0$$

CHAPTER 4

SIMULATION AND CONTROL OF DWC

4.1 SIMULATION ALGORITHM:

Thomas Algorithm:

Specify all F_j , $Z_{i,j}$, Feed conditions (T_{Fj}, P_{Fj} , or h_{Fj}), P_j , U_j , W_j , all Q_j except Q_1 and Q_N .

Set $K=1$ to begin first iteration.

STEP 1: Initialize tear variables T_j , V_j .

STEP 2: Calculate X by Thomas Method.

STEP 3: Normalize $X_{i,j}$ for each step.

STEP 4: Calculate New T_j from bubble point equation and Y .

STEP 5: Calculate Q_1 and Q_N .

STEP 6: Calculate New V_j and L_j .

STEP 7: Is $T < 0.01N$

If yes then it would be converged and it would exit.

If No then it would adjust tear variables and then it would go to STEP 2 and

It would again recalculate till it converge and exit from the loop.

Since the Algorithm is based on tri-diagonal matrix equations it would involve the evaluation of one component at a time.

STEP 4-6 are sequential evaluation equations.

Usually, the process of distillation involve the component covering a narrow range of K values. The effective process is being suggested by Friday and Smith and importantly being called as bubble point method since a new temperature is being computed from each iteration and equations are being separated and in sequence process these equations are being solved except M equations being solved for each component by tri-diagonal matrix technique.

Final design of multi-component mixture separation demands rigorous calculation of Temperature, Pressure, Steam flow rates, Stream compositions by rigorously solving material, energy balance and equilibrium relations for each stage. As a result of which mathematical model for an equilibrium stage for efficient contacting of vapor and liquid needs to be developed. These equations when collected and interconnected together in a cascade of vapor and liquid are

termed as MESH equations. Bubble point method is being most suitable for those components in feed having a narrower boiling range and it is confined to ideal and mixtures.

Some critical assumptions are being made:

Phase equilibrium is reached at each stage. No chemical reaction at each stage takes place. And most importantly entrainment of liquid drops in vapor and occlusion of vapor bubbles in liquid are generally neglected.

$$K_{i,j} = K_{i,j}(T_j, P_j, X_j, Y_j) \quad h_{Vj} = h_{Vj}(T_j, P_j, Y_j) \quad h_{Lj} = h_{Lj}(T_j, P_j, X_j)$$

A single or multi-phase feed entering stage J with a flow rate of F_j having total composition of component I possessing mole fraction Z_i , having a temperature of T_{Fj} and a pressure of P_{Fj} and having a overall molar enthalpy of h_{Fj} . The difference between feed pressure and stage pressure is reduced to zero.

Each equilibrium stage is described by $(2 \cdot C + 3)$ mesh equations and system is having N components and countercurrent stage is described by $N \cdot (2 \cdot C + 3)$ equations. The system is specified by $F_j, T_{Fj}, Z_{i,j}, P_{Fj}, U_j, W_j, Q_j$ and the model is described by $N \cdot (2 \cdot C + 3)$ simultaneous equations.

In a multi-component mixture comprising of components having a narrow boiling range bubble point method is most useful. The most important aspect in bubble point method is the tri-diagonal matrix and the material balance equation are obtained by elimination of vapor phase mole fraction. The equation used for calculation of vapor phase mole fraction are separated from other equation. The design of column involving multi-component mixture in multi stage column demands the involvement of determination of temperature, pressure, steam flow rate, stream composition, heat transfer rate in each stage of the column by solving material balance and equilibrium relation in each stage of the divided wall distillation column but the relation are highly complicated and require vigorous programming by the use of digital computer making the availability of solution readily available. Those equation when assembled together for countercurrent flow are termed as MESH equations. The main criteria for the application of bubble point method is involvement of components having a narrower boiling point range and restricted to ideal mixture.

The most important aspect of the bubble point method is the tri-diagonal matrix resulting from the modified form of the material balance equation when separated from other equations by selection of T_j and V_j as the tear variables leading to the modified material equations in the unknown liquid mole fraction. And K values are composition independent as a result of which constants B_j and C_j for component is a function of tear variables temperature and pressure.

4.2 BUBBLE POINT CALCULATION.

In distillation components having a comparatively narrower range of K values. And the most efficient process for the divided wall distillation column was suggested by Friday and Smith and designed in detail by Wang and Henke. Known as bubble point method since new set of stage temperature is being calculated from bubble point equation during successive iteration. And equations are being separated out and solved in a systematic procedure except material balance equation which are being computed separately for the tri-diagonal matrix. Inputs are feed location, pressure, side-stream flow rate, total number of stages, bubble point, heat transfer rate for all stages except for the first and last stage, reflux flow rate and vapor distillate flow rate. To begin the computing process values of tear variables are being assumed. V_j and T_j are being assumed. Initial T_j value can be received by calculating the bubble point temperature of the bottom product and dew temperature of the distillate and thereby using interpolation to compute the stage temperature. New temperature can be obtained for each of the stage by using bubble point calculation and henceforth using normalized values. Since temperature is not sensitive to composition bubble point method is convenient for components having narrower range of boiling point. Component having low K value changes rapidly with temperature in contrast to component having a high K value.

ALGORITHM:

STEP 1: Input Liquid composition and pressure.

STEP 2: Output are vapor composition and temperature.

STEP 3: Assume Temperature.

STEP 4: Calculation of activity coefficient for multi-component mixture by the application of Hildebrand model.

STEP 5: Calculation of vapor pressure that is P_1^S and P_2^S by employing Antoine equation.

STEP 6: Calculation of equilibrium vapor composition Y_i according to the following:

$$Y_i = \gamma_i \cdot P_i^S \cdot X_i / P_t$$

STEP 7: Check if the value of $\sum Y_i - 1 \leq \text{Tolerance limit}$.

STEP 8: If Yes the temperature should be noted down and also the vapor composition.

STEP 9: Calculate $F_t = \sum Y_i - 1$ and $\text{deriv}(F_t) = \sum B_i \cdot Y_i / (T + C_i)^2$

STEP 10: Calculation of T for the next time using iterative equation:

$$T_{t+1} = T_t - (F_t / \text{derive}(F_t))$$

And proceed to STEP 3 for further processing.

STEP 11: Stop.

HILDEBRAND MODEL:

For a multicomponent mixture involving liquid hydrocarbons frequently uses the model. Regular answer are co-related by the excessive entropy reduced to zero. Heat of the solution contributes to the non ideality.

$$\gamma_i = \exp(V_i^*(\delta_i - \delta_{avg})/R*T)$$

$$\delta_{avg} = (\sum X_i^*V_i^*\delta_i / \sum X_i^*V_i)$$

Hildebrand model demands two parameters for each component that is solubility δ_{avg} parameter and liquid molar volume. The average value of the solubility is denoted by the following code.

4.3 STEADY STATE EQUATIONS.

Firstly we need to construct a tri-diagonal matrix involving equations used primarily for the purpose of divided wall distillation column designing. It involves three matrices that is a square matrix and two column matrices. Out of two column matrices one is the output matrix and the other one is matrix involving constants. Firstly we have to find out the composition variation along with number of stages and then we have to calculate the vapor and liquid flow rate along with number of stages.

Divided wall distillation column is consisting of plates numbered from 1 to N. Out of which plate numbered 1 to N_1 is enriching section. N_1 to N_3 is divided section of the column which is being divided at plate numbered N_1 and N_3 respectively. N_2 is the feed plate located in between N_1 and N_3 and the divided wall distillation column are being divided at N_1 and N_3 respectively. Lastly, N_3 to N is stripping section.

Now we have to design divided wall distillation column by designing steady state equations for separate section that is from 1 to N_1 and from N_1 to N_3 and lastly from N_3 to N.

Primarily we have to use material balance equation, phase equilibrium relation, Mole fraction summation equation and Energy balance equation.

At each of the stage there is feed which is fed to each of the plate of the divided wall distillation column. And also there is vapor and liquid side-streams from plates which are being numbered from 1 to N. And most importantly Reflux flow rate is being fed to the first stage of the divided wall distillation column and at the divided stage that is N_2 there is vapor fed to the main column which in turn coming out from the divided section. Then feed is being fed in the intermediate stage that is feed stage located between N_1 and N_3 . Liquid coming out from divided section is

again fed back to the main column. Then heavy stream of vapor is being fed to the last stage of the divide wall distillation column coming out from re-boiler.

Material balance equation:

$$M_{i,j} = L_{j-1} * X_{i,j-1} + V_{j+1} * Y_{i,j+1} - L_j * X_{i,j} - V_j * Y_{i,j} = 0$$

Phase equilibrium relation:

$$E_{i,j} = Y_{i,j} - K_{i,j} * X_{i,j} = 0$$

Mole fraction summation equation:

$$S_{Yj} = \sum Y_{i,j} - 1 = 0 \quad i \text{ is varying from } 1 \text{ to } C.$$

$$S_{Xj} = \sum X_{i,j} - 1 = 0 \quad i \text{ is varying from } 1 \text{ to } C.$$

Energy balance equation:

$$H_j = L_{j-1} * h_{L,j-1} + V_{j+1} * h_{V,j+1} - L_j * h_{L,j} - V_j * h_{V,j} - Q_j = 0$$

In order to eliminate L and Y from material balance equations involving Liquid flow rate, Vapor flow rate, Vapor composition and Liquid composition. For elimination of vapor composition we need to equilibrium phase relationship and the Liquid flow rate can be eliminated by use of successive iteration using the iterative relationship between Liquid Flow rate and Vapor Flow rate. Since it involves liquid and vapor side-stream in each of the stage it would lead to change in material and energy balance equation. It would also lead to change iterative equation involving vapor and Liquid flow rate.

MODIFIED EQUATIONS:

Material balance equation:

$$L_{j-j-1} + V_{j+1} * 1 * X_i, Y_{i,j+1} - (L_j + U_j) * X_{i,j} - (V_j + W_j) * Y_{i,j} + F_j * Z_{i,j} = 0$$

Energy balance equations:

$$H_j = L_{j-1} * h_{L,j-1} + V_{j+1} * h_{V,j+1} - (L_j + U_j) * h_{L,j} - (V_j + W_j) * h_{V,j} - Q_j = 0$$

Iterative equation:

$$L_j = V_{j+1} - V_1 + \sum F_m - U_m - W_m \quad m \text{ is varying from } 1 \text{ to } j.$$

Then we have to create the main matrix:

Main matrix involves coefficients A_i , B_i , C_i and the column matrix involves D_i .

Coefficient of A_i , B_i , C_i and D_i are being provided by the following iterative relations:

$A_i = V_j - V_1 + \sum F_m - U_m - W_m$ whereas m is varying from 1 to $j-1$ and j is varying from 2 to N .

$B_i = -V_{j+1} + V_1 - U_j - (V_j + W_j) * K_{i,j} - \sum F_m - U_m - W_m$ whereas m is varying from 1 to j and j is varying 1 to N .

$C_i = V_{j+1} * K_{i,j+1}$ and j is varying from 1 to $N-1$ throughout the column except at the dividing section.

$D_i = -F_j * Z_{i,j}$ j is varying from 1 to N throughout the column except at the dividing section of DWC.

Then we have to normalize X for each of the stage that is component mole fraction.

Applying the bubble point equation to find out the Temperature of the main column and vapor phase mole fraction.

Most importantly by use of enthalpy balance equation we have to find out the vapor flow rate in each stage and thereby by use of iterative equation we have to find out the Liquid flow rate as well. To find out the vapor flow rate we have to construct matrix having coefficients involving enthalpy terms. The coefficients can be obtained through iterations whose coefficients are stated as:

$$A_j = h_{L,j-1} - h_{V,j}$$

$$B_j = h_{V,j+1} - h_{L,j}$$

$$C_j = [(F_m - U_m - W_m) - V_1] * (h_{L,j} - h_{L,j-1}) + F_j * (h_{L,j} - h_{F,j}) + Q_j + W_j * (h_{V,j} - h_{L,j})$$

After evaluating the coefficients we can evaluate the vapor flow rate in each of the stage and by using the iterative equation we can evaluate the liquid flow rate in each stage of the column.

The iterative formula is given by for each stage as:

$$L_j = V_{j+1} - V_1 + (F_m - U_m - W_m) \quad m \text{ is varying from } 1 \text{ to } j.$$

After that rigorous programming has to be implemented so as to give the desired output and in order to evaluate a comparative analysis.

Main Programming equations:

$$A * X_{i,j-1} + B * X_{i,j} + C * X_{i,j+1} = D$$

The coefficient of D is (-R) for the very first stage and at the divided section is $(-W_A * K_A * X_A)$ and $(-U_Z * X_Z)$ and for the remaining section it is $(-F * Z_f)$ and for the last stage it is (-B).

Coefficients of A, B and C are varying according to the stages of the divided wall distillation column. From stage 1 to stage N_1 the coefficients are as follows:

$$\begin{aligned} A &= V_j - V_1 + \sum F_m - U_m - W_m \\ B &= -(V_{j+1} - V_1) - K_{i,j} * (V_j + W_j) - U_j - \sum F_m - U_m - W_m \\ C &= K_{i,j+1} * V_{j+1} \end{aligned}$$

From stage N_1 to N_3 including the feed stage the coefficients of A, B and C are given as:

$$\begin{aligned} A &= V_j - V_1 - U_2 \\ B &= -(V_{j+1} - V_1 - U_2) - K_{i,j} * V_j \\ C &= K_{i,j+1} * V_{j+1} \end{aligned}$$

From stage to N_3 to the last stage there are separate set of coefficients excluding the stage N_3 .

$$\begin{aligned} A &= V_j + L_N + \sum F_m - U_m - W_m \\ B &= -(V_{j+1} + L_N) - K_{i,j} * (V_j + W_j) - U_j - \sum F_m - U_m - W_m \\ C &= K_{i,j+1} * V_{j+1} \end{aligned}$$

But at N_3 the following change is being made in the coefficients of A, B and C.

$$\begin{aligned} A &= V_j + L_N + W_3 \\ B &= -(V_{j+1} + W_3) * K_{i,j} - (V_{j+1} + W_3 + L_N) \\ C &= K_{i,j+1} * V_{j+1} \end{aligned}$$

After the material balance analysis has been carried out Energy balance need to be carried out:

$$\theta_j * V_j + \beta_j * V_{j+1} = T_j$$

$$\theta_j = h_{L,j-1} - h_{V,j}$$

$$\beta_j = h_{V,j+1} - h_{L,j}$$

$$T_j = [(F_m - U_m - W_m) - V_1] * (h_{L,j} - h_{L,j-1}) + F_j * (h_{L,j} - h_{F,j}) + Q_j + W_j * (h_{V,j} - h_{L,j})$$

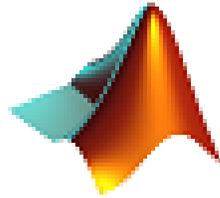
Likewise Material Analysis there is a variation in the coefficient of constant which is not a function of the vapor flow rate there is variation in the first stage and at the divided section and at the last stage of the divided wall distillation column.

4.4 PROGRAMMING ANALYSIS

Rigorous program is being performed by the application of programming language MATLAB so as to simulate the divide wall distillation column. It is very important to have an important introduction about the programming language MATLAB.

MATLAB or otherwise known as matrix laboratory is a language. It is a program so that as per input desired output can be produced. It is a language belonging to the fourth generation and is being developed by math-work. Since it includes the processing of an algorithm so that as per input output can be achieved, to plot a graph involving functions and various data. It is being primarily used to compute numerically. Most importantly Simulink helps in implementing multiple simulations and help us in designing systems on the basis of a model. MATLAB is being implemented on a large scale across different domain of engineering, in the field of science and in the field of economics. Various technical universities, Institutions of pure academic research and across various industrial enterprises. It has huge number of users in the year 2004 about more than one lacs. MATLAB was developed in the year 1984.

MATLAB has got excellent graphical interface and is very much user-friendly. Much rigorous and complex programs could also be executed with much ease. Since we have to rigorously execute the program to design the divided wall column system MATLAB is convenient and it involves the generation of matrix and taking the inverse of it to provide liquid phase mole fraction, vapor flow rate and liquid flow rate across different stages in a divided wall distillation column. And to draw a comparative analysis of the divided wall distillation column with respect to purity of distillate and bottom product and helping us to conclude the advantages in implementing the divided wall distillation column with respect to energy as well as cost requirement.



CHAPTER 5

SAMPLE PROGRAMMING RESULTS

BUBBLE POINT ANALYSIS:

enter the number of stages 3 number of components 3 number of iterations 10

enter pressure of the column 13680 R =1.9870

enter F(j) 1xN matrix with no. of elements= [100 100 100 100 100]

enter Tf(j) 1xN matrix with no. of elements= [320 320 320 320 320]

enter Zf(i,j) cxN matrix with no. of elements= [1 0 0;0 1 0;0 0 1]

Temperature in each stage of the divided wall distillation column.

327.0572 384.5535 432.5269

Vapor phase mole fraction in each stage of DWC.

1.0000 0 0
0 1.0000 0
0 0 1.0000

Equilibrium phase constant in each stage of the DWC.

1.0000 0 0
0 1.0000 0
0 0 1.0000

enter the number of stages 3 number of components 3 number of iterations 10

enter pressure of the column 15200 R =1.9870

enter F(j) 1xN matrix with no. of elements= [100 100 100]

enter Tf(j) 1xN matrix with no. of elements= [320 320 320]

enter Zf(i,j) cxN matrix with no. of elements= [1 0 0;0 1 0;0 0 1]

Temperature in each stage of the divided wall distillation column.

332.2742 390.6519 439.193

Vapor phase mole fraction in each stage of DWC.

```
1.0000  0  0
      0 1.0000  0
      0  0  1.0000
```

Equilibrium phase constant in each stage of the DWC.

```
1.0000  0  0
      0 1.0000  0
      0  0  1.0000
```

enter the number of stages 3 number of components 3 number of iterations 10

enter pressure of the column 16720 R =1.9870

enter F(j) 1xN matrix with no. of elements= [100 100 100]

enter Tf(j) 1xN matrix with no. of elements= [320 320 320]

enter Zf(i,j) cxN matrix with no. of elements= [1 0 0;0 1 0;0 0 1]

Temperature in each stage of the divided wall distillation column.

```
337.1514 396.3545 445.4230
```

Vapor phase mole fraction in each stage of DWC.

```
1.0000  0  0
      0 1.0000  0
      0  0  1.0000
```

Equilibrium phase constant in each stage of the DWC.

```
1.0000  0  0
      0 1.0000  0
      0  0  1.0000
```

Fig 1: TEMPERATURE AND PRESSURE PROFILE OF PROPANE .

X AXIS-PRESSURE IN mm Hg and Y AXIS-TEMPERATURE IN k.

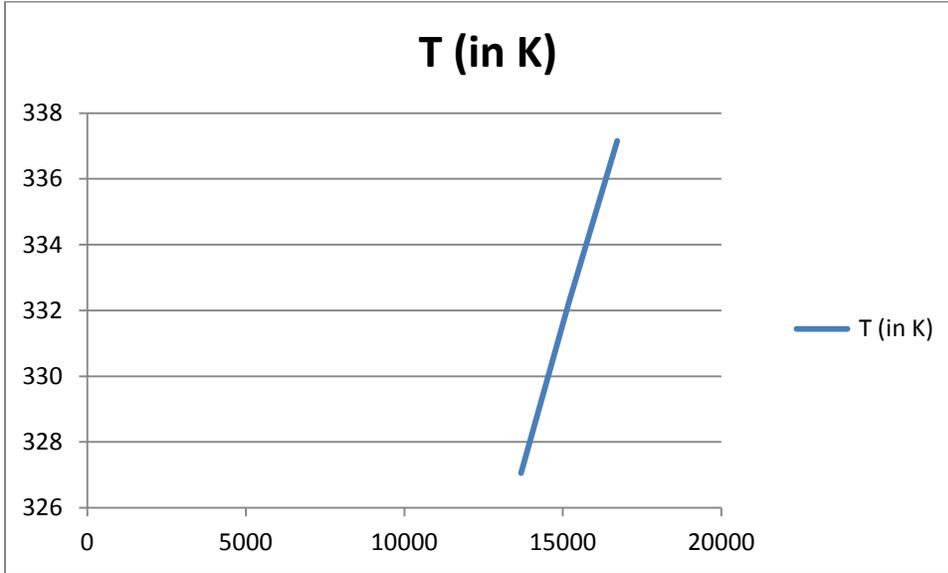


Fig 2: TEMPERATURE AND PRESSURE PROFILE OF BUTANE .

X AXIS-PRESSURE IN mm Hg and Y AXIS-TEMPERATURE IN k.

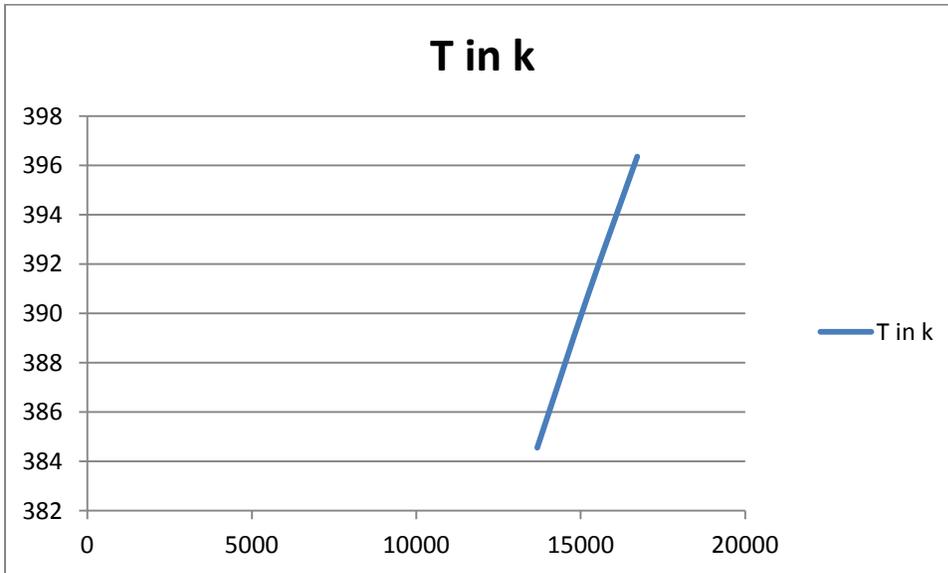


Fig 3: TEMPERATURE AND PRESSURE PROFILE OF PENTANE .

X AXIS-PRESSURE IN mm Hg and Y AXIS-TEMPERATURE IN k.

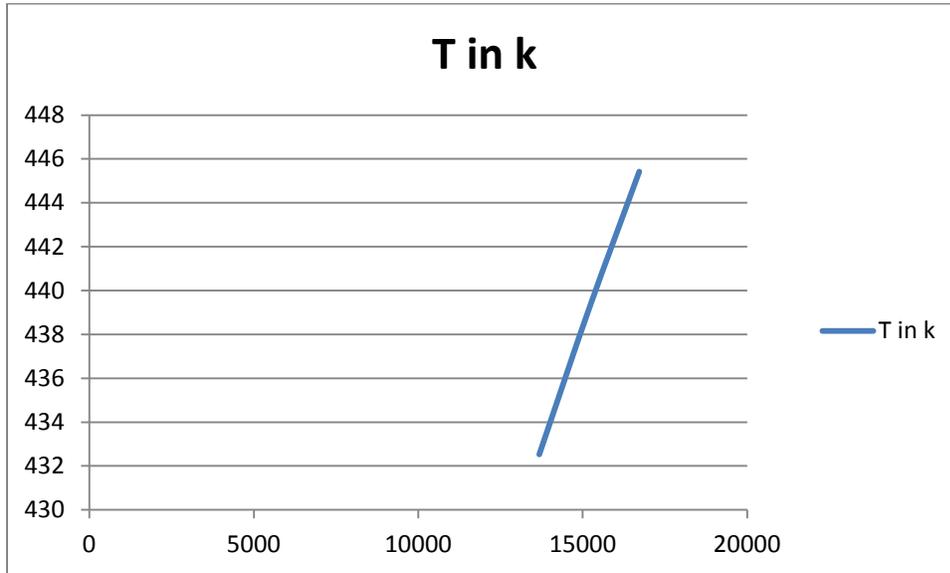


Figure 4:

VARIATION OF VAPOUR PHASE MOLE FRACTION OF A MULTICOMPONENT MIXTURE ALONG WITH NUMBER OF STAGES AT A PRESSURE OF 18 KILOPASCAL.

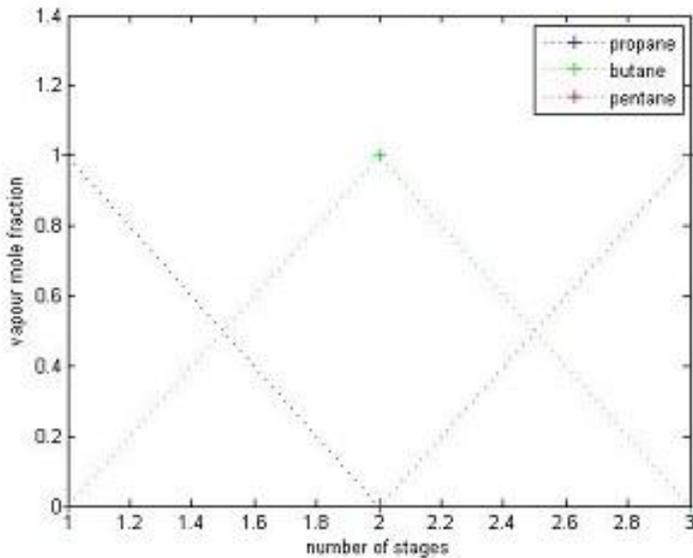
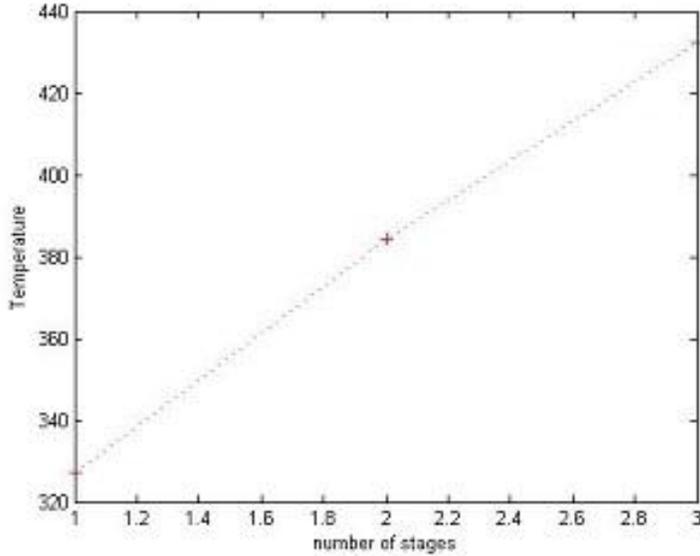


Figure 5:

VARIATION OF TEMPERATURE OF INDIVIDUAL COMPONENT IN THE MIXTURE AT PRESSURE OF 18 KILOPASCAL ALONG WITH NUMBER OF STAGES.



DETAILED ANALYSIS OF DWC:

enter the number of stages 5 number of components 3 number of iterations 10

enter pressure of the column 13680

enter N1- 2 enter N2- 3 enter N3- 4

enter hF(j) 1xN matrix with no. of elements= [100 100 100 100 100]

enter hU2 100 enter hWa 100

enter liquid side-stream flow rate- 20 enter vapour side stream flow rate- 20

enter Wa 20 enter Uz 20

enter Ka(i) cx1 matrix with no. of elements= [2.56;1.28;0.64]

enter Xa(i) cx1 matrix with no. of elements= [0.1;0.2;0.3]

enter Xz(i) cx1 matrix with no. of elements= [0.2;0.4;0.6]

enter U(j) 1xN matrix with no. of elements= [20 20 20 20 20]

enter W(j) 1xN matrix with no. of elements= [10 10 10 10 10]

enter $Q(j)$ $1 \times (N-2)$ matrix with no. of elements= [0 0 0]

enter reflux rate= 10 enter vapor distillate rate= 10

enter Liquid flow rate of last stage= 10 enter Vapor flow rate of second stage= 10

$R = 1.9870$

enter $F(j)$ $1 \times N$ matrix with no. of elements= [100 100 100 100 100]

enter $Tf(j)$ $1 \times N$ matrix with no. of elements= [320 320 320 320 320]

enter $Zf(i,j)$ $c \times N$ matrix with no. of elements= [0.1 0.2 0.3 0.4 0.5; 0.6 0.1 0.3 0.2 0.3; 0.3 0.7 0.4 0.4 0.2]

Temperature in each stage of the divided wall column

384.5256 387.8886 369.2988 361.7220 351.5209

Vapour phase mole fraction in each stage of the DWC

Propane- 0.2744 0.5813 0.6531 0.7689 0.8022

Butane- 0.6001 0.1064 0.2267 0.1302 0.1581

Pentane- 0.1255 0.3123 0.1202 0.1009 0.0396

Equilibrium phase constant in each stage of the DWC

Propane- 2.7442 2.9067 2.1768 1.9221 1.6044

Butane- 1.0002 1.0637 0.7558 0.6510 0.5271

Pentane- 0.4183 0.4461 0.3005 0.2524 0.1982

enter -R 5 enter -B 5

enter $V(j)_{10}$ enter $V(j)_{10}$ enter $V(j)_{10}$ enter $V(j)_{10}$

MOLE FRACTION OF LIQUID 1-Propane

0.1297 0.2625 0.5212 0.0835 0.0031

enter -R 10 enter -B 10

enter $V(j)_{20}$ enter $V(j)_{20}$ enter $V(j)_{20}$ enter $V(j)_{20}$

MOLE FRACTION OF LIQUID 2-Butane

0.1757 0.2970 0.4585 0.0638 0.0050

MOLE FRACTION OF LIQUID 3-Pentane

0.6946 0.4404 0.0203 0.8527 0.9919

enter pressure of the column 13680

enter Tf1(j) 1xN matrix with no. of elements= [330 330 330 330 330]

330 330 330 330 330

0.2744 0.5813 0.6531 0.7689 0.8022

0.6001 0.1064 0.2267 0.1302 0.1581

0.1255 0.3123 0.1202 0.1009 0.0396

2.1165 2.2145 1.2530 9.2034 25.1491

3.4150 0.3581 0.4946 2.0421 31.5338

0.1806 0.7090 5.9099 0.1184 0.0400

Enthalpy of Liquid Mixture

5.5773e+04 5.2389e+04 4.1855e+04 5.3475e+04 5.3770e+04

Enthalpy of Vapor Mixture

1.8902e+05 3.0534e+05 4.8315e+05 1.4029e+05 7.9010e+04

vapor flow rate

10 20 0 0 123.3716

liquid flow rate 80 59.9954 0 153.716

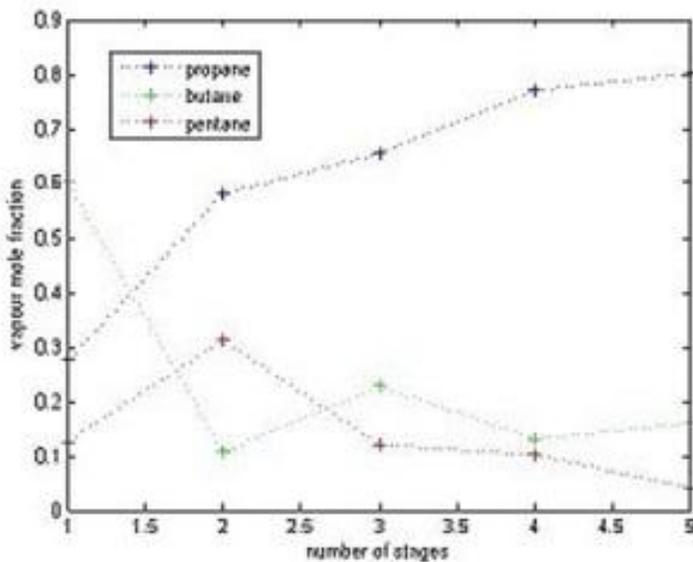


Figure 7:

VARIATION OF TEMPERATURE ALONG WITH NUMBER OF STAGES IN DWC.

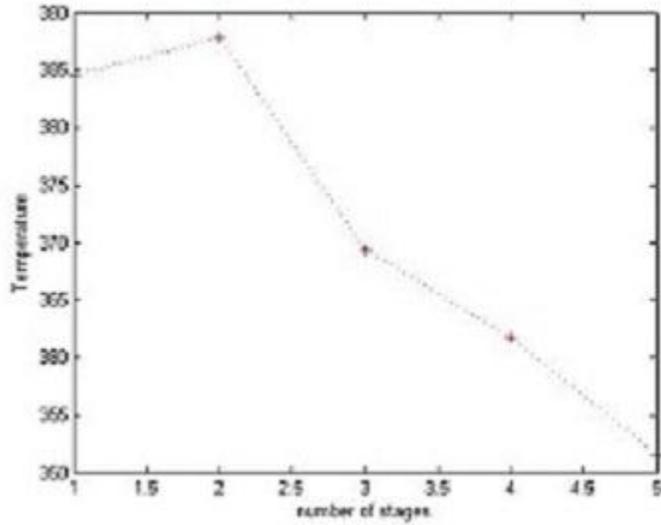


Figure 8:

VARIATION OF PHASE EQUILIBRIUM RATIO OF INDIVIDUAL COMPONENTS IN A MULTI-COMPONENT MIXTURE ALONG WITH NUMBER OF STAGES IN DWC.

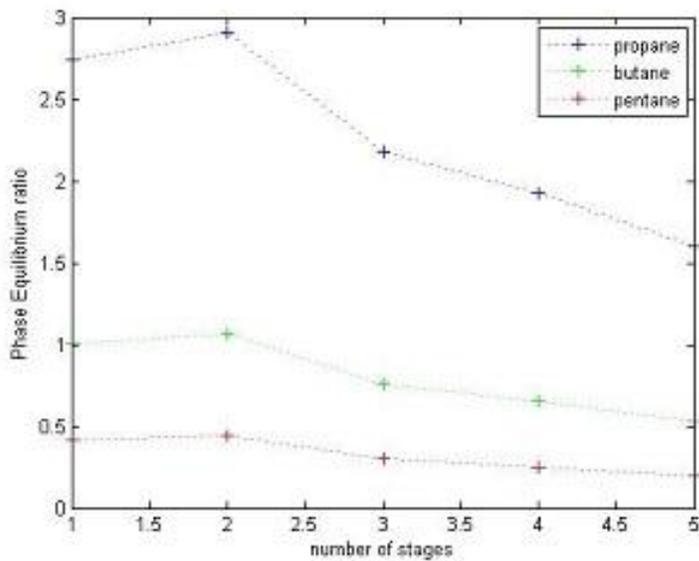


Figure 9:

VARIATION OF LIQUID PHASE MOLE FRACTION OF PROPANE ALONG WITH NUMBER OF STAGES IN DIVIDED WALL COLUMN.

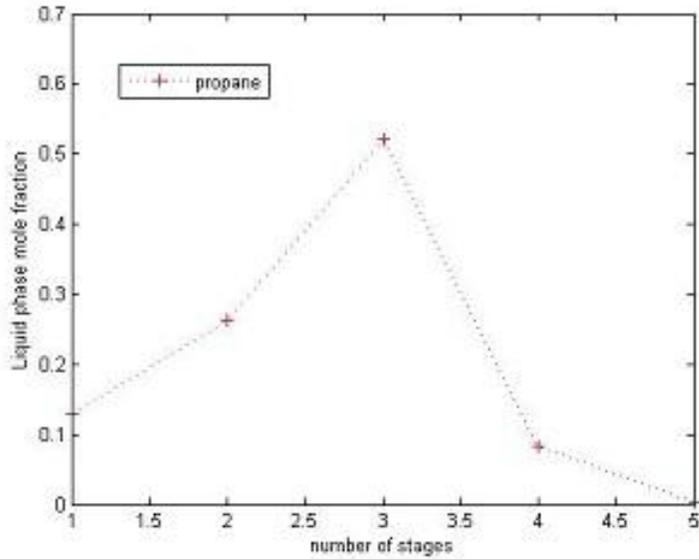


Figure 10:

VARIATION OF LIQUID PHASE MOLE FRACTION OF BUTANE ALONG WITH NUMBER OF STAGES IN DIVIDED WALL COLUMN.

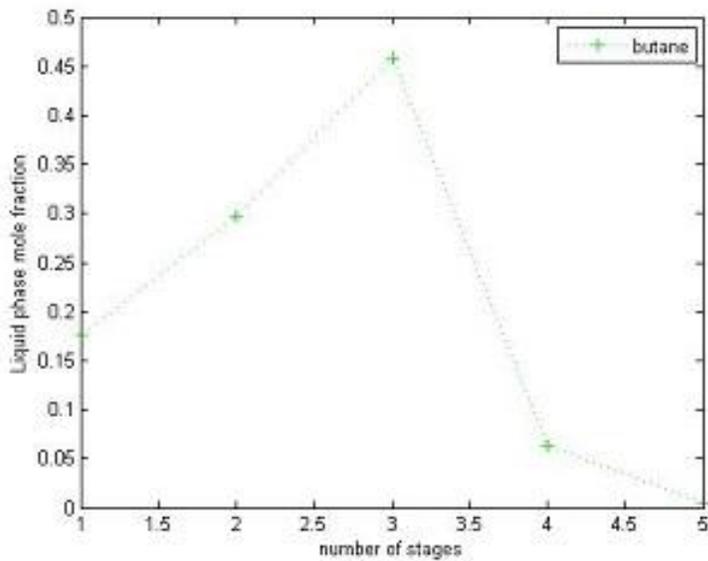


Figure 11:

VARIATION OF LIQUID PHASE MOLE FRACTION OF PENTANE ALONG WITH NUMBER OF STAGES IN DIVIDED WALL COLUMN.

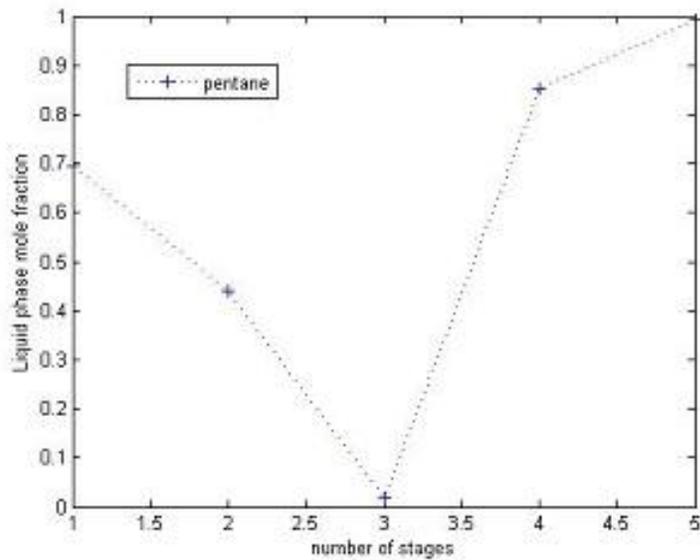


Figure 12:

VARIATION OF ENTHALPY OF LIQUID MIXTURE ALONG WITH NUMBER OF STAGES IN DWC.

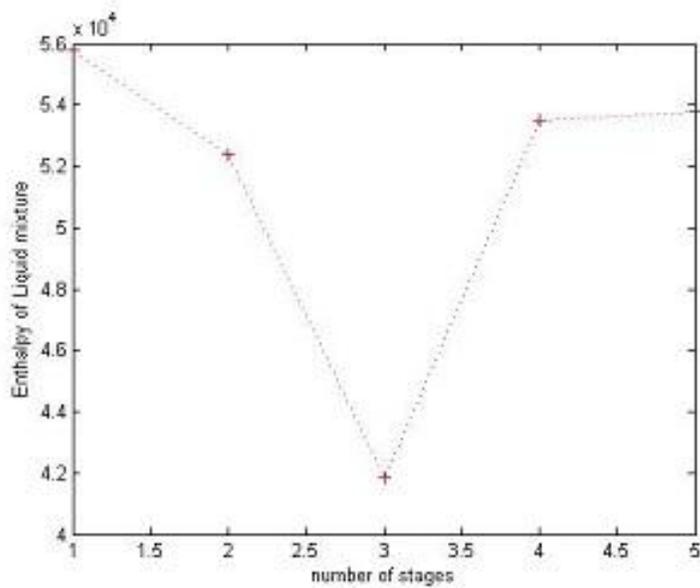


Figure 13:

VARIATION OF ENTHALPY OF VAPOUR MIXTURE ALONG WITH NUMBER OF STAGES IN DWC.

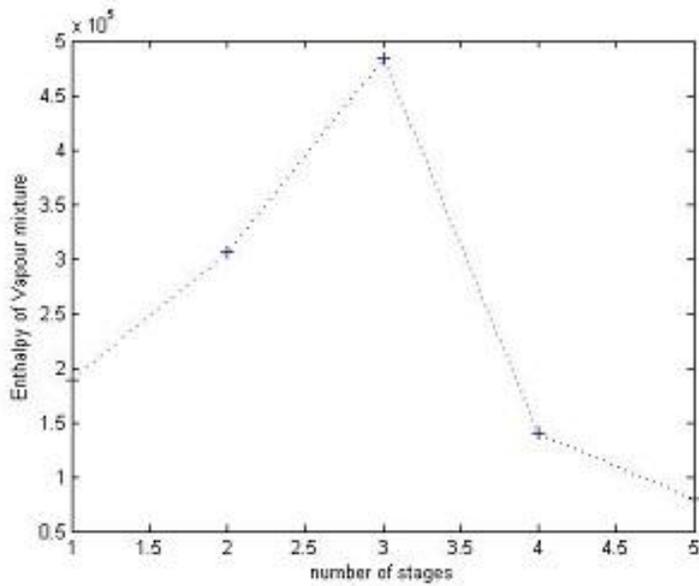
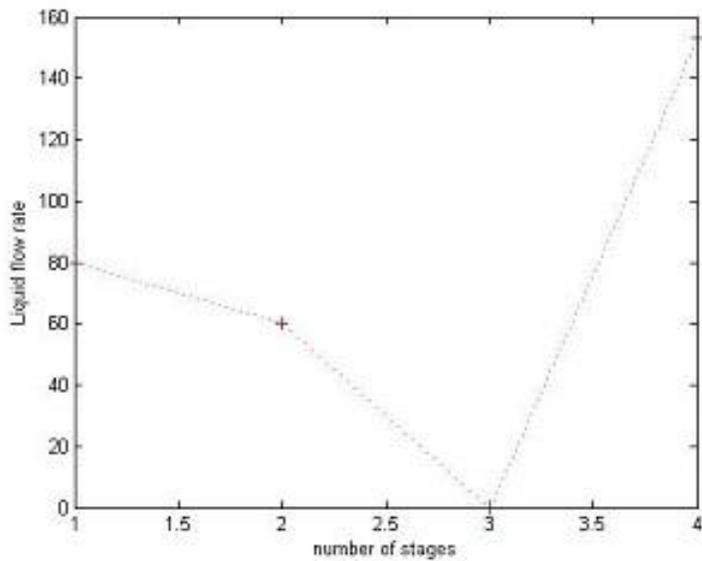


Figure 14:

VARIATION OF LIQUID FLOW RATE ALONG WITH NUMBER OF STAGES IN DWC UNDER INPUT CONDITIONS:



CHAPTER 6

CONCLUSION AND SCOPE FOR FUTURE WORK

6.1 CONCLUSIONS:

Rigorous Programming is done using mathematical model with the help of MATLAB to find out the liquid, vapor molar flow rate, Liquid phase mole fraction, Temperature, Enthalpy of Liquid and Vapor across all stages so as to investigate the controllability aspect of the divided wall distillation column. A multi-component mixture comprising of propane, butane and pentane is taken as feed and sequentially solved once at a time to find out the variation of Temperature along with pressure which linearly increases to investigate the optimal control Temperature. From the graphical analysis Liquid phase mole fraction of Light and intermediate increases with increase in number of stages and start to decrease in stripping section whereas reverse process occur in case of heavy component. In the divided wall distillation column there are four degrees of freedom in contrast to conventional column having three degrees of freedom and the extra one is used to specify either Liquid split or vapor split. From the analysis due to better remixing of Liquid and Vapor and enough Liquid and Vapor split provides purity of product to a great extent with minimal Temperature and Energy consumption. Energy consumption analysis is being studied from enthalpy of vapor and Liquid mixture. And most importantly by studying the graphical analysis obtained by rigorous programming simulation analysis we can conclude that in a three component mixture the intermediate would one be moving upward as well as downward along-with the lightest and heaviest component in the multi-component mixture. And the lightest being most volatile would be removed as the distillate and the heaviest component being withdrawn as the bottom product and the intermediate would be removed as side-stream product. The total analysis of divided wall column is highly feasible for separation process with reduced energy requirements as well as cost requirements with the cost being compensated in the construction of a single column shell instead of two column shell. Thus it must be implemented in industrial practice with the suitable application of design procedures. And the constraint doesn't make it suitable for every separation process.

6.2 SCOPE FOR FUTURE WORK.

There is a huge scope to work like there is wide range of boiling point among component, operating pressure, operating height and hydraulic imbalance due to small size of component in the side-stream are among the constraints making it incompatible. And most importantly dynamic simulation could also be carried out throughout the divided wall distillation column with the parameters would be varying with time as composition, temperature profile being variable along with time as a result of which rigorous simulation can be carried out for more reactive distillation column by proper interface of Aspen dynamics with MATLAB. Lastly, If dynamic simulation is carried out extending its operation across all domains.

CHAPTER 7

REFERENCES

7. REFERENCES.

- [1]- Smith J. M., Van Ness H. C., Abbott M M, "Introduction to Chemical Engineering Thermo-dynamics", McGraw Hill, 2005.
- [2]- Petlyuk FB, Platonov VM, Slavinskii DM. Thermodynamically optimal method for separating multi-component mixtures. *Int. Chem. Eng.* 1965; 5(3):555-561.
- [3]- Dejanović I, Matijašević L, Olujić Ž. Dividing wall column—A breakthrough towards sustainable distilling. *Chem. Eng. Proc.: Proc. Int.* 2010; 49(6):559-580.
- [4]- Separation process and principles in chemical and bio-chemical operations by seader, Henley and Roper-3rd edition.
- [5]- Analysis of multi loop control structure of divided wall distillation column using fundamental of divided wall distillation column by Salvador Tututi-avila^{1,2}, Arturo Jiménez-Gutiérrez² and Juergen Hahn¹
- [6]-. Mutalib, M.I. A.; Smith, R. Operation and control of dividing wall distillation columns: Part 1: Degrees of freedom and dynamic simulation. *Chem. Eng. Res. Des.* **1998**, 76, 308–318.
- [7]- Segovia-Hernández, J.G.; Hernández-Vargas, E.A.; Márquez-Muñoz, J.A. Control properties of thermally coupled distillation sequences for different operating conditions. *Comput. Chem. Eng.* **2007**, 31, 867–874.
- [8]-Process Parametric Optimization of a Divided Wall Distillation Column by vikas k sangal¹, vineet kumar², and indra mani mishra².
- [9]-Designing 4 product dividing wall column for separation of a multi-component mixture by I.Dejanovic^a, Lj Matijasevic^a, I.J Halvorsen^b, B.Kaibel^d, S.Skogestad^c, H.jansen^d, Z. Olujić^e.
- [10]-Reduced cost with dividing wall column by Michael A Schultz, Douglas G Stewart, James M Harris, Steven P Rosenblum, Mohammed S Shakur, Dennis E Obrien.
- [11]-Dividing wall column-which wall separates dutch industry from application by-Dr.Hartmut schoenmakers Technische Universität Dortmund Fakultät Bio- und Chemieingenieurwesen Lehrstuhl für Fluidverfahrenstechnik Germany

CHAPTER 8

APPENDIX

BUBBLE POINT ANALYSIS OF THE DIVIDED WALL DISTILLATION COLUMN.

```
clc

clear all

close all

N=input('enter the number of stages');

c=input('number of components');

M=input('number of iterations');

P=input('enter pressure of the column');

% A(i),B(i),C(i)=Antoine constants for component i;
% del(i)=solubility parameter of component i;
% delavg=average value of del;
% gama(i)=Activity coefficient of component i;
% p=column pressure of the column in mm Hg;
% ps(i)=vapour pressure of component i in mm Hg;
% R=universal gas constant in cal/(gmol)(K);
% Tf=Tray temperature in K;
% V(i)=Liquid molar volume of component i in ml/gmol;
% X(i)=Mole fraction of component i in the liquid phase.
% Y(i)=Mole fraction of component i in the vapour phase.
% '1' denotes for propane;
% '2' denotes for n-butane;
% '3' denotes for n-pentane;
A(1)=15.7260;
B(1)=1872.46;
C(1)=-25.16;
A(2)=15.6782;
B(2)=2154.90;
C(2)=-34.42;
A(3)=15.8333;
B(3)=2477.07;
C(3)=-39.94;
del(1)=6.40;
del(2)=6.73;
del(3)=7.02;
V(1)=84;
V(2)=101.4;
V(3)=116.1;
R=1.987
F=input('enter F(j) 1xN matrix with no. of elements= ' ');
```

```

Tf=input('enter Tf(j) 1xN matrix with no. of elements= ');
Zf=input('enter Zf(i,j) cxN matrix with no. of elements= ');
T=Tf;
x=Zf;
for j=1:N
TT=T(j);
for k=1:M
sum1=0;
sum2=0;
sumy=0;
for i=1:c
sum1=sum1+x(i,j)*V(i)*del(i);
sum2=sum2+x(i,j)*V(i);
end
for i=1:c
delav=(sum1)/(sum2);
gamma(i,j)=exp((V(i)*(del(i)-delav)^2)/(R*TT));
PS(i,j)=exp(A(i)-(B(i)/(TT+C(i))));
Y(i,j)=(gamma(i,j)*PS(i,j)*x(i,j)/(P));
sumy=sumy+Y(i,j)
end
err(j)=abs(sumy-1);
if err(j)>0.00001
sumff=0;
Ftder=0;
for i=1:c
sumff=sumff+((gamma(i,j)*x(i,j)*PS(i,j))/(P));
Ftder=Ftder+((B(i)*Y(i,j))/(TT+C(i))^2);
end
Ft=sumff-1;
TT=TT-(Ft/Ftder);
end
T(j)=TT;
end
end
for j=1:N
for i=1:c
K(i,j)=0;
end
end
for j=1:N
for i=1:c
if x(i,j)>0
K(i,j)=(Y(i,j))/(x(i,j));
end
end
end

```

```

end
disp(T);
disp(Y);
disp(K);

```

SIMULATION PROGRAM FOR ANALYSIS OF DIVIDED WALL DISTILLATION COLUMN BY DESIGNING PROGRAM IN ACCORDANCE WITH THE GIVEN MATHEMATICAL MODEL.

```

clc
clear all
close all
N= input('enter the number of stages');
c= input('number of components');
M= input('number of iterations');
P= input('enter pressure of the column');
N1= input('enter N1- ');
N2= input('enter N2- ');
N3= input('enter N3- ');
hF= input('enter hF(j) 1xN matrix with no. of elements= ');
hU2= input('enter hU2');
hWa= input('enter hWa');
U2 = input('enter reflux rate= ');
V1= input('enter liquid side-stream flow rate- ');
W3= input('enter vapour side stream flow rate- ');
Wa= input('enter Wa');
Uz= input('enter Uz');
Ka= input('enter Ka(i) cx1 matrix with no. of elements= ');
Xa= input('enter Xa(i) cx1 matrix with no. of elements= ');
Xz= input('enter Xz(i) cx1 matrix with no. of elements= ');
U= input('enter U(j) 1xN matrix with no. of elements= ');
W= input('enter W(j) 1xN matrix with no. of elements= ');
Q= input('enter Q(j) 1x(N-2) matrix with no. of elements= ');
L1= input('enter vapor distillate rate= ');
LN= input('enter Liquid flow rate of last stage= ');
V2= input('enter Vapour flow rate of second stage= ');
% A(i),B(i),C(i)=Antoine constants for component i;
% del(i)=solubility parameter of component i;
% delavg=average value of del;
% gama(i)=Activity coefficient of component i;
% p=column pressure of the column in mm Hg;
% ps(i)=vapour pressure of component i in mm Hg;
% R=universal gas constant in cal/(gmol)(K);
% Tf=Tray temperature in K;
% V(i)=Liquid molar volume of component i in ml/gmol;
% X(i)=Mole fraction of component i in the liquid phase.

```

% Y(i)=Mole fraction of component i in the vapour phase.

% '1' denotes for propane;

% '2' denotes for n-butane;

% '3' denotes for n-pentane;

A(1)=15.7260;

B(1)=1872.46;

C(1)=-25.16;

A(2)=15.6782;

B(2)=2154.90;

C(2)=-34.42;

A(3)=15.8333;

B(3)=2477.07;

C(3)=-39.94;

del(1)=6.40;

del(2)=6.73;

del(3)=7.02;

V(1)=84;

V(2)=101.4;

V(3)=116.1;

R=1.987

p(1)=0;

q(1)=60.79;

r(1)=0.22371;

s(1)=-8.941*(10⁻⁴);

t(1)=1.561*(10⁻⁶);

p(2)=0;

q(2)=108.36;

r(2)=6.82*(10⁻²);

s(2)=-3.49*(10⁻⁴);

t(2)=8.06*(10⁻⁷);

p(3)=0;

q(3)=164.21;

r(3)=-0.16044;

s(3)=3.68*(10⁻⁴);

t(3)=1.89*(10⁻¹²);

l(1)=27268.64;

m(1)=36.93;

n(1)=611*(10⁻²);

o(1)=-2.513*(10⁻⁵);

g(1)=-2.0349*(10⁻⁷);

l(2)=29573.990;

m(2)=146.91;

n(2)=-0.444;

o(2)=1.184*(10⁻³);

g(2)=-1.11*(10⁻⁶);

l(3)=38772.71;

```

m(3)=138.06;
n(3)=-0.2318;
o(3)=5.41*(10^(-4));
g(3)=-3.458*(10^(-7));
F= input('enter F(j) 1xN matrix with no. of elements= ');
Tf=input('enter Tf(j) 1xN matrix with no. of elements= ');
Zf=input('enter Zf(i,j) cxN matrix with no. of elements= ');
T=Tf;
x=Zf;
for j=1:N
TT=T(j);
for k=1:M
sum1=0;
sum2=0;
sumy=0;
for i=1:c
sum1=sum1+x(i,j)*V(i)*del(i);
sum2=sum2+x(i,j)*V(i);
end
for i=1:c
delav=(sum1)/(sum2);
gamma(i,j)=exp((V(i)*(del(i)-delav)^2)/(R*TT));
PS(i,j)=exp(A(i)-(B(i)/(TT+C(i))));
Y(i,j)=(gamma(i,j)*PS(i,j)*x(i,j)/(P));
sumy=sumy+Y(i,j);
end
err(j)=abs(sumy-1);
if err(j)>0.00001
sumff=0;
Ftder=0;
for i=1:c
sumff=sumff+((gamma(i,j)*x(i,j)*PS(i,j))/(P));
Ftder=Ftder+((B(i)*Y(i,j))/(TT+C(i))^2);
end
Ft=sumff-1;
TT=TT-(Ft/Ftder);
end
T(j)=TT;
end
end
for j=1:N
for i=1:c
K(i,j)=0;
end
end
for j=1:N

```

```

for i=1:c
if x(i,j)>0
K(i,j)=(Y(i,j))/(x(i,j));
end
end
end
disp('Temperature in each stage of the divided wall column');
disp(T);
disp('Vapour phase mole fraction in each stage of the DWC');
disp(Y);
disp('Equilibrium phase constant in each stage of the DWC');
disp(K);
SS=zeros(1,N);
SS(1,1)=input('enter -R ');
for j=2:N-1
SS(1,j)=-F(j)*Zf(1,j);
end
SS(1,N1)= -Wa*Ka(1)*Xa(1);
SS(1,N3)= -Uz*Xz(1);
SS(1,N)=input('enter -B ');
A=[];B=[];C=[];
for j=1:N-1
V(j)=input('enter V(j)');
end
V=[V1 V 0];
for j=1:N1
abc(j)=F(j)-U(j)-W(j);
end
for j=N3+1:N
def(j)=F(j)-U(j)-W(j);
end
for j=2:N1-1
gh(j)=F(j)-U(j)-W(j);
end
for j=N3+1:N-1
mnp(j)=F(j)-U(j)-W(j);
end
for j=1:N
if j<=N1
A(j)=V(j)-V(1)+abc(j);
B(j)=-((V(j+1)-V(1))-K(1,j)*(V(j)+W(j)))-U(j)-abc(j);
C(j)=K(1,j+1)*V(j+1);
elseif j>N1 && j<N3
A(j)=V(j)-V(1)-U2;
B(j)=-((V(j+1)-V(1))-U2)-K(1,j)*V(j);
C(j)=K(1,j+1)*V(j+1);

```

```

elseif j==N3
A(j)=V(j)+W3+LN;
B(j)=-(V(j)+W3)*K(1,j)-(V(j+1)+LN+W3);
C(j)=K(1,j+1)*V(j+1);
elseif j>N3
A(j)=V(j)+LN+def(j);
B(j)=-(V(j+1)+LN)-K(1,j)*(V(j)+W(j))-U(j)-def(j);
C(j)=K(1,j)*V(j+1);
end
end
M=zeros(N,N);
for i=1:N
for j=1:N
if i == j
M(i,j)=B(i);
elseif i==j+1
M(i,j)=C(i);
elseif i==j-1
M(i,j)=A(i);
end
end
end
SS=reshape(SS,N,1);
XX1=inv(M)*SS;
for j=1:N
XXnorm1(j)=XX1(j)/(sum(XX1));
end
for j=1:N
if XXnorm1(j)<0
XXnorm1(j)=0;
end
end
disp('MOLE FRACTION OF LIQUID 1');
for j=1:N
disp(XXnorm1(j));
end
SS=zeros(1,N);
SS(1,1)=input('enter -R ');
for j=2:N-1
SS(1,j)=-F(j)*Zf(2,j);
end
SS(1,N1)= -Wa*Ka(2)*Xa(2);
SS(1,N3)= -Uz*Xz(2);
SS(1,N)=input('enter -B ');
A=[];B=[];C=[];
for j=1:N-1

```

```

V(j)=input('enter V(j)');
end
V=[V1 V 0];
for j=1:N1
abc(j)=F(j)-U(j)-W(j);
end
for j=N3+1:N
def(j)=F(j)-U(j)-W(j);
end
for j=2:N1-1
gh(j)=F(j)-U(j)-W(j);
end
for j=N3+1:N-1
mnp(j)=F(j)-U(j)-W(j);
end
for j=1:N
if j<=N1
A(j)=V(j)-V(1)+abc(j);
B(j)=- (V(j+1)-V(1))-K(2,j)*(V(j)+W(j))-U(j)-abc(j);
C(j)=K(2,j+1)*V(j+1);
elseif j>N1 && j<N3
A(j)=V(j)-V(1)-U2;
B(j)=- (V(j+1)-V(1)-U2)-K(2,j)*V(j);
C(j)=K(2,j+1)*V(j+1);
elseif j==N3
A(j)=V(j)+W3+LN;
B(j)=- (V(j)+W3)*K(2,j)-(V(j+1)+LN+W3);
C(j)=K(2,j+1)*V(j+1);
elseif j>N3
A(j)=V(j)+LN+def(j);
B(j)=- (V(j+1)+LN)-K(2,j)*(V(j)+W(j))-U(j)-def(j);
C(j)=K(2,j)*V(j+1);
end
end
M=zeros(N,N);
for i=1:N
for j=1:N
if i == j
M(i,j)=B(i);
elseif i==j+1
M(i,j)=C(i);
elseif i==j-1
M(i,j)=A(i);
end
end
end
end

```

```

SS=reshape(SS,N,1);
XX2=inv(M)*SS;
for j=1:N
XXnorm2(j)=XX2(j)/(sum(XX2));
end
for j=1:N
if XXnorm2(j)<0
XXnorm2(j)=0;
end
end
disp('MOLE FRACTION OF LIQUID 2');
for j=1:N
disp(XXnorm2(j));
end
for j=1:N
XXnorm3(j)=1-XXnorm1(j)-XXnorm2(j);
end
disp('MOLE FRACTION OF LIQUID 3');
for j=1:N
disp(XXnorm3(j));
end
for j=1:N
for i=1:c
if i==1
XX(i,j)=XXnorm1(j);
elseif i>1 && i<c
XX(i,j)=XXnorm2(j);
elseif i==c
XX(i,j)=XXnorm3(j);
end
end
end
P1=input('enter pressure of the column');
Tf1=input('enter Tf1(j) 1xN matrix with no. of elements= ');
T1=Tf1;
for j=1:N
TT1=T1(j);
for k=1:M
sum1=0;
sum2=0;
sumy=0;
for i=1:c
sum1=sum1+XX(i,j)*V(i)*del(i);
sum2=sum2+XX(i,j)*V(i);
end
for i=1:c

```

```

delav=(sum1)/(sum2);
gamma(i,j)=exp((V(i)*(del(i)-delav)^2)/(R*TT1));
PS(i,j)=exp(A(i)-(B(i)/(TT1+C(i))));
Y(i,j)=(gamma(i,j)*PS(i,j)*XX(i,j)/(P1));
sumy=sumy+Y(i,j);
end
err(j)=abs(sumy-1);
if err(j)>0.00001
sumff=0;
Ftder=0;
for i=1:c
sumff=sumff+((gamma(i,j)*XX(i,j)*PS(i,j))/(P1));
Ftder=Ftder+((B(i)*Y(i,j))/(TT1+C(i))^2);
end
Ft=sumff-1;
TT=TT-(Ft/Ftder);
end
T1(j)=TT1;
end
end
for j=1:N
for i=1:c
K1(i,j)=0;
end
end
for j=1:N
for i=1:c
if XX(i,j)>0
K1(i,j)=(Y(i,j))/(XX(i,j));
end
end
end
disp(T1);
disp(Y);
disp(K1);
for i=1:c
for j=1:N
hLp(i,j)=p(i)+(q(i)*T(j))+(r(i)*(T(j)^2))+(s(i)*(T(j)^3))+(t(i)*(T(j)^4));
hVp(i,j)=l(i)+(m(i)*T(j))+(n(i)*(T(j)^2))+(o(i)*(T(j)^3))+(g(i)*(T(j)^4));
end
end
for j=1:N
for i=1:c
if i==1
hL1(j)=hLp(i,j)*XXnorm1(j);
hV1(j)=hVp(i,j)*XXnorm1(j);

```

```

elseif i>1 && i<c
hL2(j)=hLp(i,j)*XXnorm2(j);
hV2(j)=hVp(i,j)*XXnorm2(j);
elseif i==c
hL3(j)=hLp(i,j)*XXnorm3(j);
hV3(j)=hVp(i,j)*XXnorm3(j);
end
end
end
for j=1:N
hL(j)=(hL1(j)+hL2(j)+hL3(j));
hV(j)=(hV1(j)+hV2(j)+hV3(j));
end
disp('Enthalpy of Liquid Mixture');
for j=1:N
disp(hL(j));
end
disp('Enthalpy of Vapour Mixture');
for j=1:N
disp(hV(j));
end
for j=3:N-1
alpha(j)=hL(j-1)-hV(j);
end
for j=2:N-1
beta(j)=hV(j+1)-hL(j);
end
for j=2:N1-1
gamma(j)=V(1)*(hL(j-1)-hL(j))+gh(j)*(hL(j)-hL(j-1))+F(j)*(hL(j)-hF(j))+W(j)*(hV(j)-hL(j));
end
gamma(N1)=gamma(N1)-Wa*hWa;
for j=N1+1:N2-1
gamma(j)=(V(1)+U2)*(hL(j-1)-hL(j));
end
gamma(N3)=(LN+W3)*(hL(N3)-hL(N3-1))+W3*hV(N3)-U2*hU2;
for j=N3+1:N-1
gamma(j)=LN*(hL(j)-hL(j-1))+mnp(i)*(hL(j)-hL(j-1))+F(j)*(hL(j)-hF(j))+W(j)*(hV(j)-hL(j));
V(3)=(gamma(2)-alpha(2)*V2)/(beta(2));
for j=4:N
V(j)=(gamma(j-1)-alpha(j-1)*V(j-1))/(beta(j-1));
for j=1:N1
L(j)=V(j+1)-V(1)+abc(j);
for j=N1+1:N3-1
L(j)=V(j+1)-V(1)-U2;
L(N3)=V(N3+1)+LN+W3;
for j=N3+1:N-1

```

```
L(j)=V(j+1)+LN+mdp(j);  
for j=3:N  
if V(j)<0  
V(j)=0;  
for j=1:N-1  
if L(j)<0  
L(j)=0;  
disp('vapour flow rate');  
for j=1:N  
disp(V(j));  
end  
disp('liquid flow rate');  
for j=1:N-1  
disp(L(j));  
end
```