

Mathematical Modeling Of Multi Component Batch Extractive Distillation

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Abstract

A dynamic model has been developed to study the dynamic behavior of multi component batch extractive distillation column. The set of equations governing (material balance, heat balance, summation of mole and equilibrium equations) which represent the dynamic model are solved to give the temperature and composition profile. Eigenvalue method was used to integrate the stiff ordinary differential equations.

Matrix method was used to solve many equations simultaneously to redefine the column parameters during program run. Newtons algorithm was used to calculate the plate temperatures on each tray.

The calculations and simulations in this paper were obtained by using MATLAB environment, version 6. The result of the proposed model are compared with experimental result taken under the same operating conditions. This model shows good agreement with experimental results and explains features of the batch extractive distillation process.

Keywords: Extractive Distillation, Azeotropic, Batch Distillation, Dynamic Simulation.

الموديل الرياضي لبرج التقطير الاستخلاصي بالدفعه الواحدة

الخلاصة

في هذا البحث تم تطوير النموذج الديناميكي لدراسة سلوك برج التقطير الاستخلاصي بالدفعه الواحدة. تم حل مجموعة المعادلات اللاخطية غير المستقرة لعمود التقطير الاستخلاصي باستعمال طريقة تكامل (Eigenvalue method) وذلك لحساب التراكيز خلال البرج مع الزمن.

الموديل الرياضي يتضمن حل اربعة انواع من المعادلات مع الزمن وهذه المعادلات تعبر عن (موازنة المادة , موازنة الطاقة , مجموع التراكيز , التوازن البخاري). استخدمت طريقة نيوتن والتي تعتمد على طريقة الفرضية والحساب وذلك لتقييم درجات الحرارة خلال البرج. وكذلك تم استخدام طريقة المصفوفات لحساب معدلات الجريان للبخار والسائل لكل الصواني الموجودة في برج التقطير .

كل الحسابات والمعالجات الرياضية في هذا البحث قد تمت باستعمال برنامج (Matlab 6). في النهاية تمت مقارنة النتائج النظرية المستنتجة من هذا الموديل الرياضي مع نتائج عملية مأخوذة بنفس الظروف , ظهر ان هنالك توافقا كبيرا بين النتائج العملية والنظرية. لذلك يمكن استخدام هذا الموديل الرياضي مستقبلا لوصف كل من التركيز ودرجة الحرارة ومعدل الجريان في أي نقطة من نقاط جهاز التقطير الاستخلاصي.

Symbol	Definition	Units
D	: distillate molar flowrate	mol/hr
E	: entrainer feed flow rate	mol/hr
h	: enthalpy of a liquid mixture	kJ/kmol
H	: enthalpy of a vapor mixture	kJ/kmol
K	: equilibrium coefficient	-
L_j	: molar flow rate of liquid leaving j tray	mol/hr
M_j	: molar holdup of j tray	mol
n	: number of trays	-
N_C	: number of components of a mixture	-
Q	: reboiler heat duty	Watt
R	reflux ratio	-
T	: temperature	°C
t	: time	hr
V_j	: vapor flow rate leaving a tray or still	mol/hr
x_{ij}	: liquid mole fraction of i component in j th tray	mol/mol
y_{ij}	: vapor mole fraction of i component in j th tray	mol/mol

1.Introduction

In Greek the term azeotrope means nonboiling by any way (a-non, zeo-boil, tropos-way), and denotes a mixture of two or more components where the equilibrium compositions of the vapor and liquid are equal at a given pressure and temperature⁽¹⁾.

In thermodynamic view, an azeotropic mixture behaves as non-ideal mixture, therefore, the distillation becomes impossible in conventional column if the feed is azeotropic mixture.

Extractive distillation method is one of the must known methods used to separate Azeotropic mixtures. In a batch extractive distillation column,

the azeotropic mixture to be separated is initially added to the reboiler, and during distillation a higher boiling point solvent fed to the column and changes the relative volatility of the azeotropic mixture. According to the new VLE the component having the greater volatility is taken as the first distillate cut, and then the component having second greater volatility is fed as the second distillation cut, finally the solvent can be separated as last distillation cut or as the residual in the reboiler

2. Conventional Batch Distillation Dynamics

Basualdo and Gomes ⁽²⁾ proposed commercial software named HYSYS with MATLAB 5.1 program to simulate dynamic behavior of multicomponent batch distillation. This model was valid by using operational condition of the real systems.

Klingberg ⁽³⁾ in her thesis made a detailed dynamic modeling, simulation and optimization of a batch distillation process. Simulations were performed by using gPROMS modeling tool, and proved that the model gives a very accurate description of the process behavior.

Costa et al. ⁽⁴⁾ made dynamic simulation on batch distillation. They found that dynamic modeling of batch distillation columns frequently leads to a mixed system of differential and algebraic equations. The resulting system was solved by using numerical integration method.

3. Batch Extractive Distillation Dynamics

Yatim et al. ^(5, 6, 7) simulated batch extractive distillation column used to separate azeotropic mixture and then they compared their simulation results with experimental results.

Yatim et al. ⁽⁵⁾ used water as extractive agent to separate acetone-methanol mixture, and they recovered approximately 82% by mole acetone. The distillate that was obtained was approximately 96% acetone.

Yatim et al. ⁽⁷⁾ extended the work of Yatim et al. ⁽⁵⁾ for batch extractive distillation using a batch rectifier by investigating different operational policies for the reflux ratio and entrainer flow rate, then they

compared the recoveries of these policies.

Parton et al. ⁽⁸⁾ used ethylene glycol as extractive agent to separate methanol-propanol mixture in batch extractive distillation column. They computed the concentration profiles and they proved that the control of temperature profile is necessary for each studied system to find satisfactory operating conditions.

Milani ⁽⁹⁾ studied batch extractive distillation of acetone-methanol mixture by using water as entrainer. In their study the water was charged directly to the reboiler, also large quantities of water was needed in order to achieve high purity acetone in the distillate.

Hilmen and Skogestad ⁽¹⁾ obtained an expensive result on batch extractive distillation column by using ethanol-water-ethylene glycol system. They observed, that in conventional batch extractive distillation column, the semi-continuous operation has two main disadvantages due to accumulation of the extractive agent: (1) filling of the reboiler, and (2) degradation of the composition profile in the column. The first may cause operational problems and the latter decreases the efficiency of the separation.

Gomez and Basualdo ⁽¹⁰⁾ used a methodology for the identification of nonlinear models of multicomponent batch distillation columns. The proposed method consist in generating enough data for identification, by performing a simulation of a rigorous model (based on first principles) of the column implemented in the HYSYS environment. This model was validated by using the operational conditions of the real system.

Zaidoon ⁽¹¹⁾ in his PhD thesis

makes detailed model to simulate the batch extractive distillation column and then he compared the model result for various parameters with experimental results. He found that there is a good agreement between them. Finally he used the proposed model to find the optimum conditions to operate the column.

4. Experiment Description

The experiments were carried out using laboratory scale batch distillation column as shown in picture of Figure (1).

The distillation column was manufactured of QVF glass and fitted with ten bubble cup trays.

The upper part of the main column contains double coil condenser with reflux ratio control valve (magnetic valve). The main column consists of two parts. Each part contains 5 bubble cup trays with 30 cm³ holdup for each tray. At the lower part of the column there was an 18 liters spherical glass vessel, with three openings. The vessel was placed in the reboiler and Glycerin was used as heating oil in the reboiler.

Each two parts of this plant were connected using a flange with teflon gasket. To reduce the heat losses to minimum value, the column parts were insulated with a mineral wool. The column has several small openings which allow us to measure the temperatures inside of the column as well as taking samples.

The solvent feed tank is supported in upper part of the plant. The solvent feed temperature is setup before experiment runs and kept constant. The solvent feed flow rate is measured and controlled by using a flow meter .

The system used in this study is

the ethanol-water mixture, and ethylene glycol is added to the mixture as an extractive solvent.

The initial feed compositions are calculated depending on the residue curve map of the system. A 15 liter of ethanol-water mixture was prepared and charged to the vessel. The heating was started and the temperature was increases until the liquid in vessel and on trays start to boil. At the first period there was no feed solvent but all condensate were returned to the column (total reflux).

In production period the extractive solvent (Ethylene Glycol) was fed continuously at desired rate and temperature at the upper part of the column (stage 8), and pure ethanol started to produce as first distillate cut. The extractive solvent was fed as pure liquid with a temperature equal to the boiling point of the more volatile component (100 C). The reflux ratio was constant during this period. After the ethanol started to deplete, the solvent valve was closed and the second distillate cut become to produce as pure water. And finally the distillate was be only the non-pure water and the heavy solvent remained in the reboiler.

The temperature of the column was read continuously by using six T-type sensors placed in various section of the plant. The temperatures were continuously recorded by a PC which got its information from temperature interface unit. During the experiment run, liquid samples were taken from the bottom vessel and the distillate every (10 minutes). The liquid samples taken from experiments were analyzed using gas-liquid chromatography (type Varian 6000, Vista) connected to an electronic integration unit.

5. Dynamic Model

5.1 Model Assumptions

The proposed model includes the following assumptions.

1. Constant tray efficiency.
2. Neglect of vapor holdup.
3. Perfect mixing on all trays and in all vessels (condenser and reboiler).
4. Total condensation.
5. Ideal vapor phase for all components in mixture.

5.2 Model Equations

In this column, there is vapor liquid equilibrium in the reboiler and condenser, therefore each of reboiler and condenser can be assumed as a theoretical stage. Hence by starting from the lower point, the reboiler was numbered as stage one and the first real tray of column was numbered stage 2, then we counted from the bottom to the top. The last tray of the column was thus stage number 11, also the condenser was named stage 12.

Making the total material, component and energy balances on the various sections of the batch extractive distillation column, and by further simplifications of the differential equations lead to the system of equations in Appendix (1).

With the aid of the finite-difference representation, it is useful to evaluate the values of liquid and vapor enthalpy derivatives $\frac{dh}{dt}$ and

$\frac{dH}{dt}$ depending on the values of h and H at previous time steps, by using the following two equations.

$$\frac{dh}{dt} \approx \frac{h(t) - h(t + \Delta t)}{\Delta t} \quad . . (12)$$

$$\frac{dH}{dt} \approx \frac{H(t) - H(t + \Delta t)}{\Delta t} \quad . . (13)$$

These two equations give very good results because the contribution to the energy balance from the change in enthalpy with time is very small. Table (1) contains a polynomial which can be used to evaluate the vapor and liquid enthalpy as a function of temperature.

Also the previous values of molar holdup M which were calculated depending on a given volumetric holdup, could be used to evaluate the value of the total mass derivative $\frac{dM}{dt}$ according to the following equation.

$$\frac{dM}{dt} \approx \frac{M(t) - M(t + \Delta t)}{\Delta t} \quad . . (14)$$

5.3 Dynamic Simulation

This section contains the dynamic simulation of the batch extractive distillation. In simulation, the initial compositions along the column and in the still are assumed equal to that of the original feed mixture. The Ethanol-Water-Ethylene Glycol system was used in simulation of batch extractive distillation. The above model gives a system of ordinary differential equations and algebraic equations, the algebraic equations include physical properties and vapor liquid equilibrium equations, where the differential equations include total material, heat and component balance equations.

The boiling temperatures along the column was evaluated by total and error method (Newton's method).

For non-ideal mixture used in this study, additional variable which is the liquid phase activity coefficient

(γ_i) appears to represent the degree of deviation from ideality.

$$K_i = \frac{\gamma_i \cdot P_i}{P} \quad \dots (15)$$

Wilson method was used to predict the liquid phase activity coefficient. Table(2) contains the system of equations and the required parameters used in this model.

The vapor pressure of each component in this study is calculated by using Antoine equation. Table (3) contains parameters of Antoine equation for all components used in this study.

Figure (2) shows the flowchart of the computer simulation for batch azeotropic distillation. This algorithm can be applied to calculate the temperature, liquid flowrate, vapor flowrate and the composition profiles for a column containing a known number of stages.

Initially, the vapor and liquid flowrates are equal to the still vapor flowrate. The input parameters needed in simulation program were: reflux ratio, number of plates, heat duty in reboiler, initial charge in reboiler, hold-up on plates, hold-up in condenser, and the initial concentration on plates and in reboiler.

First of all, by using Newton's method with the aid of the summation equations, the equilibrium equations are solved to predict the equilibrium constants $K_{i,j}$, and the temperatures T in the condenser, plates and reboiler. The values of equilibrium constants $K_{i,j}$ are necessary in integration of the component material balance equations.

The component material balance equations represented in equations (2, 5 and 8) were arranged as

differential Jacobian matrix and then solved to calculate the new compositions $x_{i+1,j}$ for the components in the mixture. The vapor compositions $y_{i+1,j}$ are calculated from the liquid composition and equilibrium constant. This new temperature and compositions were used to compute liquid and vapor specific enthalpies.

The differential matrix contains terms of internal vapor and liquid flowrates, which must be updated during the simulation (every time period). To determine the values of the vapor and liquid flowrate in the column, the set of total material balance Eqns. (1, 4 and 7) and energy balance Eqns. (3 and 6) were combined with the finite difference Eqns. (12, 13 and 14) and then arranged as 23×23 matrix, and then solved by using Gauss elimination method.

At this point the time counter is incremented by one and the above sequences of calculation are repeated based on the new values of model variables.

The term of solvent feed flow rate remains zero in the startup period. Then when production period is started a step change in reflux ratio and solvent flow rate imposed. The reflux ratio changed from infinity to a desired reflux and the solvent flow rate was changed from zero to a desired flow rate.

The sequence of calculations for the production period is exactly the same as that given for the start-up period. Production period may be continued for any specified period of time or until a desired still pot liquid composition achieved. The simulation provide complete concentration and temperature

profiles throughout the column, as well as still, plates and condenser molar holdups as a function of time.

The step time (Δt) was taken as (10 sec) because it gives an accurate prediction. Every time interval (Δt), the change in composition and temperature on each tray cause a change in liquid phase activity coefficient and hence a change in equilibrium constant, K value.

6. Comparison between Experimental and Simulation Results

Figures (3, 4) represent a comparison between the experimental and simulation results for the distillate and still composition profiles respectively. The experimental composition profiles are represented by dotted lines while the simulated results represented by solid lines.

At the start of the production period, the distillate was enriched in the most volatile component (ethanol). As the amount of ethanol present in the still is depleted, the intermediate component (water) is distilled as a pure component at the top and then the more volatile component (ethylene glycol) is distilled. The distillate compositions approach either pure ethanol, water, or ethylene glycol. Since the ethanol was continuously removed, the composition of the ethylene glycol increased monotonically in the still and tends towards 100% purity. The composition of ethanol decreased because it removed as top product and the composition of water increased up to the moment when it started to be removed and then decreased to zero.

These two figures show that, there is a significant deviation between

simulated and experimental results, especially in the distillate compositions, but the same behavior was recognized in both experimental and simulated results. This lag between the results was due to the accumulated time delay in column behavior.

The mean absolute deviation between experimental and simulated results for the composition profiles in the distillate and in the still was calculated and tabulated as in Table (4). In this table the mean absolute deviation of the distillate compositions is higher than that of the bottom compositions, and this is because the distillate composition changes from minimum values to maximum values and reverse in relatively small time period.

The water composition profile shows mean absolute deviation higher than that for ethanol and ethylene glycol in distillate. On the other hand the ethylene glycol shows mean absolute deviation higher than the other two components in the still.

As shown in this section, it is clear that there is a reasonable agreement between the experimental and simulated results.

7. Model Results

Figures (5, 6 and 7) represent the model results for ethanol, water and ethylene glycol composition profiles in several locations along the column.

Figure (5) shows the change in the ethanol composition with time in condenser, tray 10, tray 5, tray 1 and the reboiler. In this figure the compositions start at feed composition and during startup period they increase until they reached a constant value.

In production period, it is recognized that the ethanol composition above solvent feed tray (tray 8) starts to increase until it reached approximately 100% ethanol. While below the solvent feed tray the ethanol composition decreases in the same time, this reveals that the vapor composition was rich in ethanol while the liquid composition was rich in water and ethylene glycol.

Figure (7) shows the change of ethylene glycol composition with time along the column. In the startup period all the compositions along the column were zero before starting of solvent feed.

In production period the solvent feed was started, and the ethylene glycol composition increased linearly in the still. The composition on plates below the solvent feed tray was approximately constant until the solvent flow was stopped, then the composition decreased to zero. And then after a period of time it increased to be approximately 100% due to depletion of ethanol and water in the column.

The ethylene glycol composition on trays above the solvent feed tray remains zero in solvent feed period because the relative volatility between ethanol and ethylene glycol and between water and ethylene glycol was large, finally it raises to be approximately 100% due to depletion of ethanol and water in the column.

Figures (8 and 9) represent the model results for liquid and vapor flowrate profiles in three places along the column. It can be seen that the overhead vapor flowrate reached a maximum and then begins to decrease. This two figures reveal how the vapor and liquid flowrates

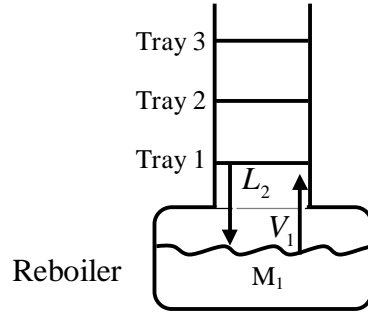
vary with time during the production period. The liquid flowrates were constant at the startup period and at the end of the production period, this is because the compositions were approximately constant in these two period of time. So for the same reason the vapor flowrates was constant at the startup period and at the end of the production period.

Figure (10) shows the molar holdup at different points in the column with respect to time. This figure shows that the holdup was constant in the startup period and then in the production period the still holdup was increased in a linear manner until the solvent flowrate stopped then the still holdup decreased linearly due to production of ethylene glycol in distillate.

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Appendix (1) Column model equations**Reboiler****a. Total Material Balance.**

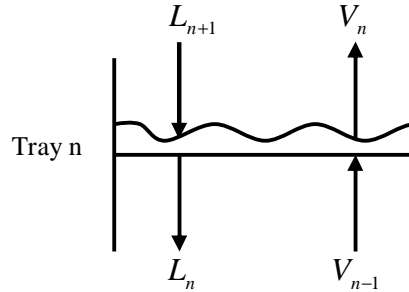
$$\frac{dM_1}{dt} = L_2 - V_1 \quad \dots (1)$$

b. Component Material Balance

$$\frac{dx_{1,i}}{dt} = \frac{(V_1 - L_2)}{M_1} \cdot x_{1,i} + \frac{L_2}{M_1} \cdot x_{2,i} - \frac{V_1}{M_1} \cdot y_{1,i} \quad \dots (2)$$

c. Heat Balance

$$\frac{dh_1}{dt} = \frac{(V_1 - L_2)}{M_1} \cdot h_1 + \frac{L_2}{M_1} \cdot h_2 - \frac{V_1}{M_1} \cdot H_1 + \frac{Q}{M_1} \quad \dots (3)$$

General Tray n**a. Total Material Balance**

$$\frac{dM_n}{dt} = L_{n+1} + V_{n-1} - L_n - V_n \quad \dots (4)$$

b. Component Material Balance

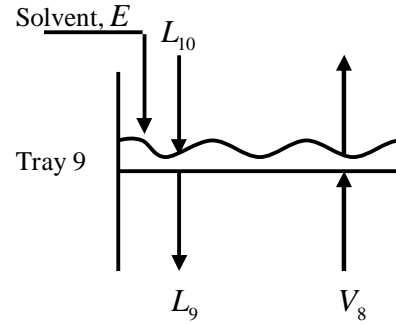
$$\frac{dx_{n,i}}{dt} = \frac{(V_n - L_{n+1} - V_{n-1})}{M_n} \cdot x_{n,i} + \frac{L_{n+1}}{M_n} \cdot x_{n+1,i} + \frac{V_{n-1}}{M_n} \cdot y_{n-1,i} - \frac{V_n}{M_n} \cdot y_{n,i} \quad \dots (5)$$

c. Heat Balance

$$\frac{dh_n}{dt} = \frac{(V_n - L_{n+1} - V_{n-1})}{M_n} \cdot h_n + \frac{L_{n+1}}{M_n} \cdot h_{n+1} + \frac{V_{n-1}}{M_n} \cdot H_{n-1} - \frac{V_n}{M_n} \cdot H_n \quad \dots (6)$$

Solvent Feed Tray

The extractive solvent was fed as a pure liquid.

**a. Total Material Balance**

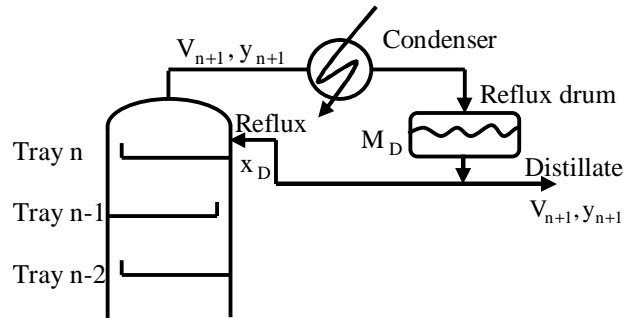
$$\frac{dM_9}{dt} = L_{10} + V_8 + E - L_9 - V_9 \quad \dots (7)$$

b. Component Material Balance

$$\frac{dx_{9,i}}{dt} = \frac{V_8}{M_9} \cdot y_{8,i} - \frac{V_9}{M_9} \cdot y_{9,i} - \frac{(L_{10} + V_8 + E - V_9)}{M_9} \cdot x_{9,i} + \frac{L_{10}}{M_9} \cdot x_{10,i} + \frac{E}{M_9} \cdot x_{E,i} \quad (8)$$

c. Heat Balance

$$\frac{dh_9}{dt} = \frac{(V_9 - L_{10} - V_8 - E)}{M_9} \cdot h_9 + \frac{L_{10}}{M_9} \cdot h_{10} + \frac{V_8}{M_9} \cdot H_8 - \frac{V_9}{M_9} \cdot H_9 + \frac{E}{M_9} \cdot h_E \quad \dots (9)$$

Reflux Drum**a. Total Material Balance on Condenser**

$$\frac{dM_D}{dt} = V_{11} - L_{12} - D \quad \dots (10)$$

b. Component Material Balance

$$\frac{dx_{D,i}}{dt} = \frac{V_{11}}{M_D} \cdot y_{11,i} - \frac{V_{11}}{M_D} x_{D,i} \quad \dots (11)$$

Table (1) Vapor and Liquid Enthalpy Calculation

$$h = h_0 + c_1(T - T_0) + c_2(T^2 - T_0^2)/2 + c_3(T^3 - T_0^3)/3 + c_4(T^4 - T_0^4)/4$$

h in J/gmol $T_0 = 298\text{ K}$

Liquid Enthalpy					
Component	h_0	c_1	c_2	$c_3 \times 10^3$	$c_4 \times 10^5$
Ethanol	0	-67.4908	1.8438	-7.3027	10.5296
Water	0	50.8300	0.2130	-0.6312	0.6486
Ethylene Glycol	0	-31.800	0.5174	-1.3419	.13426
Vapor Enthalpy					
Component	h_0	c_1	c_2	$c_3 \times 10^4$	$c_4 \times 10^8$
Ethanol	43713.9	1.0006	26.0838	-1.5935	3.9649
Water	44529.3	33.9130	-0.3014	0.1520	-0.4857
Ethylene Glycol	52544.0	35.697	0.2483	- 1.497	3.010

Table(2) Binary Location Parameters an Molar Volumes of Wilson Equation

Ethanol(1)- Water(2)- Ethylene glycol(3)		
$A_{11}=\lambda_{11}-\lambda_{11}=0$	$A_{12}=\lambda_{21}-\lambda_{11}=393.1971$	$A_{13}=\lambda_{31}-\lambda_{12}=-129.2043$
$A_{21}=\lambda_{12}-\lambda_{22}=926.263$	$A_{22}=\lambda_{22}-\lambda_{22}=0$	$A_{23}=\lambda_{32}-\lambda_{22}=1266.0109$
$A_{31}=\lambda_{13}-\lambda_{33}=1539.4142$	$A_{32}=\lambda_{23}-\lambda_{33}=-1265.7398$	$A_{33}=\lambda_{33}-\lambda_{33}=0$
$g_i = 1 - \ln \sum_{j=1}^{N_C} x_j \Lambda_{ij} - \sum_{K=1}^{N_C} \left[\frac{x_k \Lambda_{ki}}{\sum_{k=1}^{N_C} \Lambda_{kj}} \right]$ $\Lambda_{ij} = \frac{v_j^L}{v_i^L} \cdot \exp \left[- \frac{(I_{ij} - I_{ii})}{RT} \right]$ <p>where V_j in $\frac{cm^3}{mol}$ and A_{ij} in $\frac{cal}{mol}$</p>		

Table (3) Constants of Antoine Equation for Ethanol-Water-Ethylene Glycol System

Component	A	B	C
Ethanol	18.5242	3578.91	-50.5
Water	18.3036	3816.44	-46.13
Ethylene Glycol	20.2501	6022.18	-28.25

Antoine Equation

$$\log P^{\circ} = A - \frac{B}{T + C}$$

Where P° : Vapor Pressure in mmHg

T : Temperature in $^{\circ}\text{C}$

Table (4) Mean absolute deviation between experimental and simulated composition profiles in distillate and still for batch Extractive distillation.

<i>Component</i>	Mean absolute deviation for distillate composition (Figure 3)	Mean absolute deviation for still composition (Figure 4)
Ethanol	0.0450	0.0172
Water	0.1223	0.0203
Ethylene Glycol	0.0725	0.0375



Fig. (1) Experimental Plant Picture

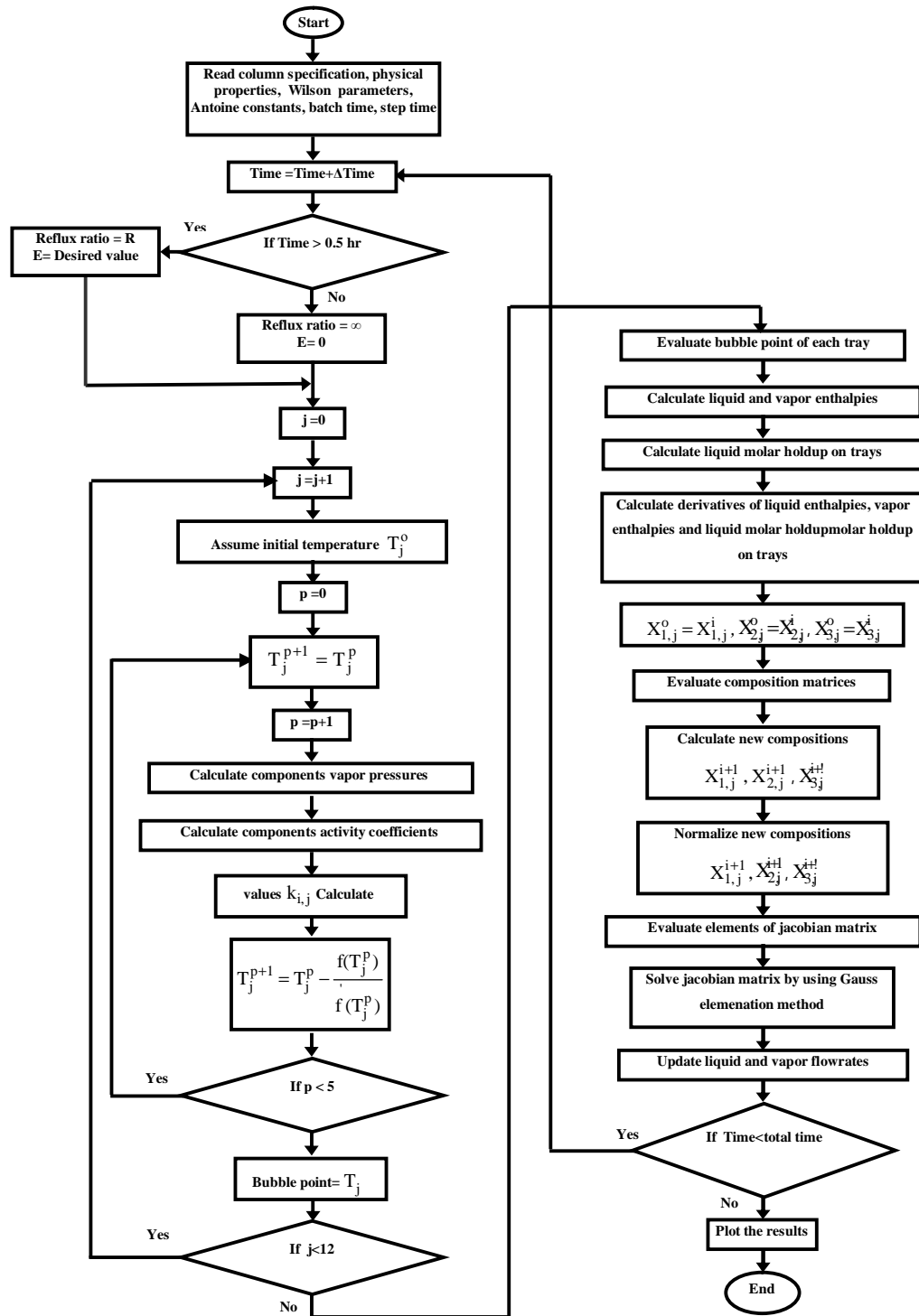


Fig. (2) Flow Chart of Simulation Program for Batch Extractive Distillation

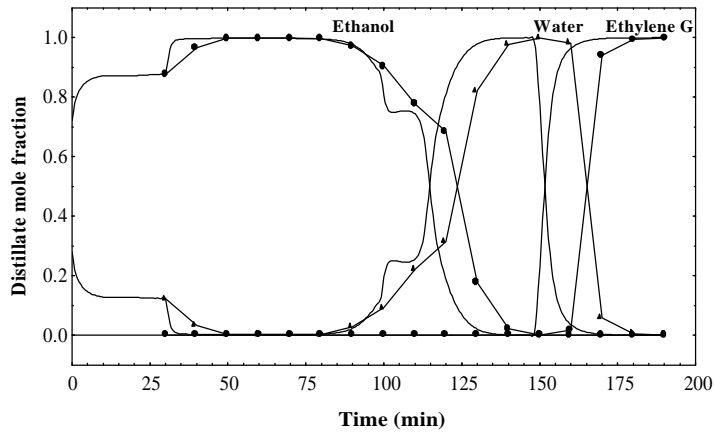


Fig. (3) Experimental and Model Simulation for Distillate Composition Profile

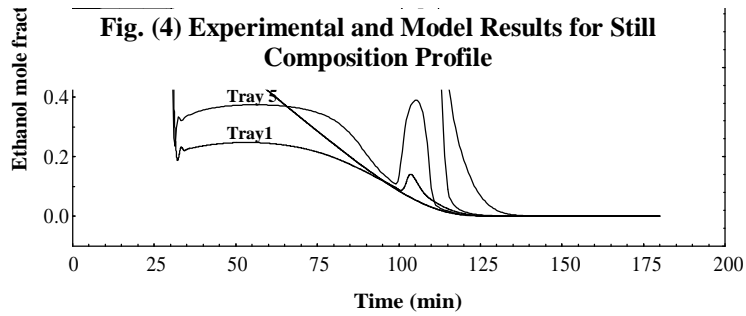
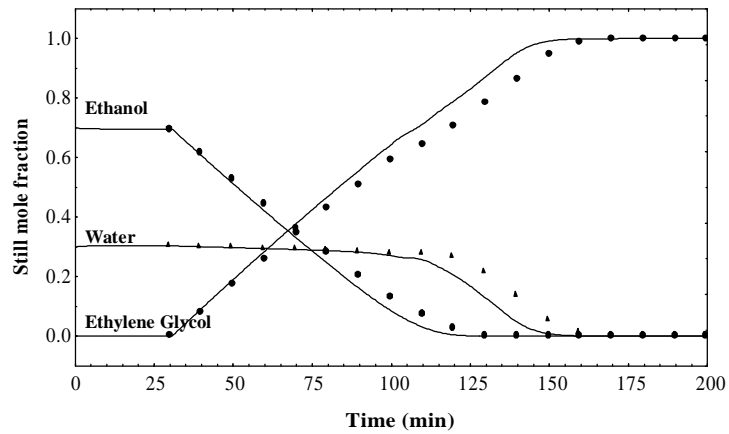


Fig. (4) Experimental and Model Results for Still Composition Profile

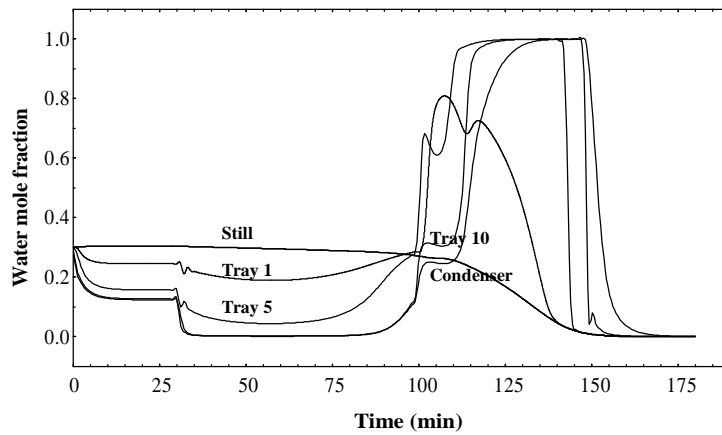


Fig.(6) Model Results for Water Composition Profile on Plates

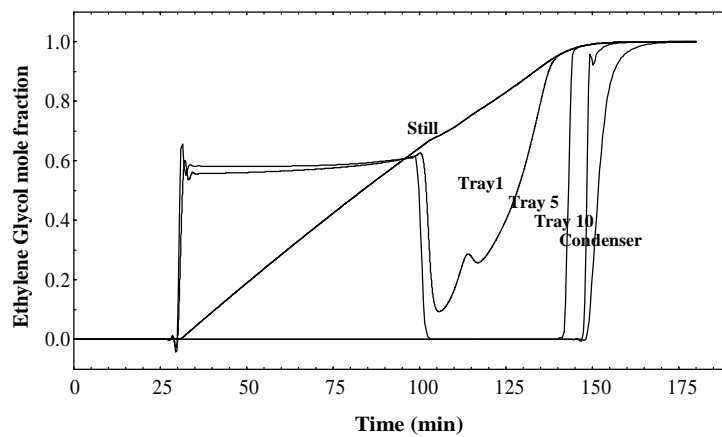


Fig. (7) Model Results for Ethylene Glycol Composition Profile on plates

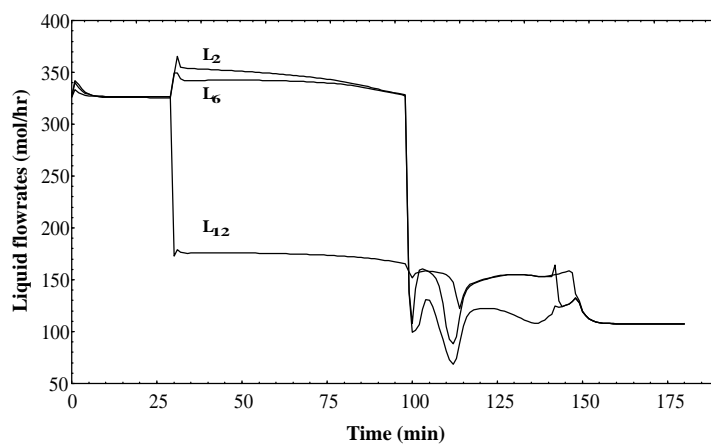


Fig. (8) Model Results for Liquid Flow Rate Profile in Column

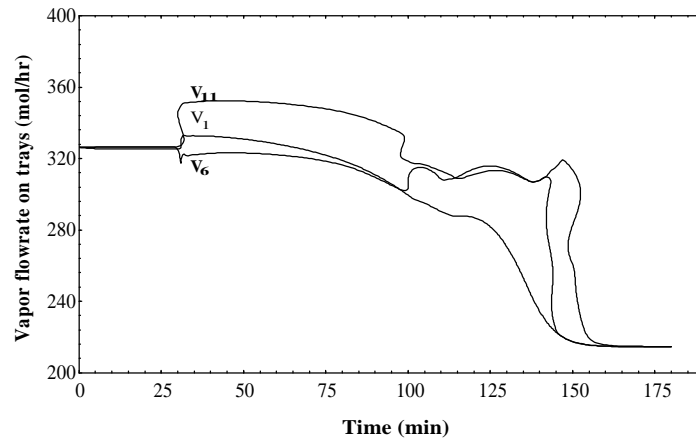


Fig. (9) Model Results for Vapor Flow Rate Profile in Column

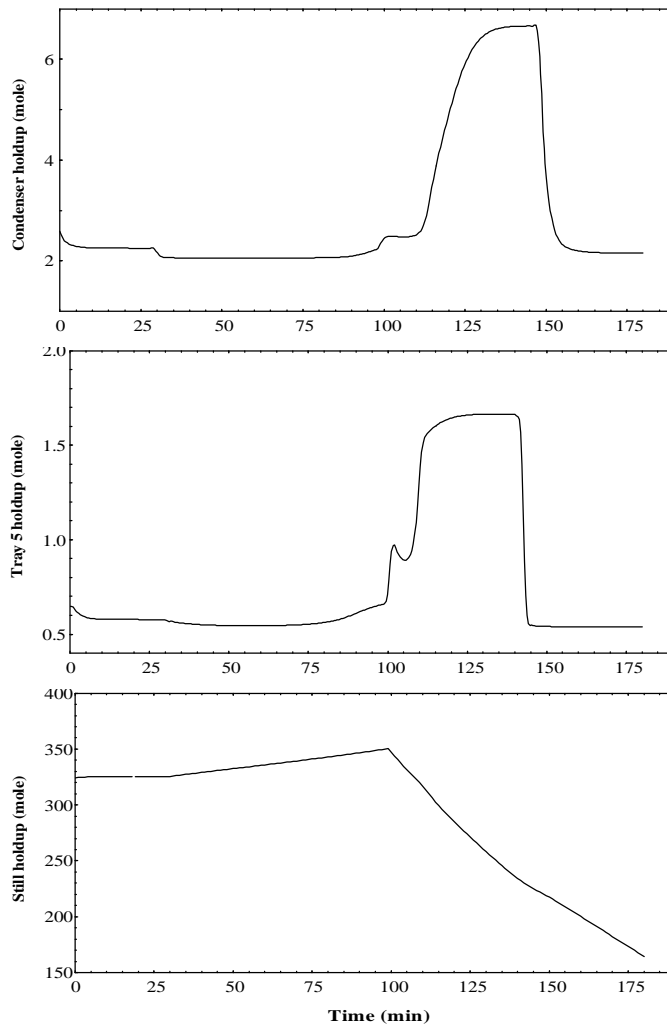


Fig. (10) Model Results for Molar Holdup on Condenser, Tray 5 and Still