DEVELOPMENT OF AN ESTIMATOR FOR BATCH DISTILLATION COLUMN INFERENTIAL CONTROL

A DISSERTATION

Submitted in partial fulfilment of the
requirements for the award of the degree
of
MASTER OF ENGINEERING
in
CHEMICAL ENGINEERING
(With Specialization in Computer Aided Process Plant Design)

By

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CANDIDATE'S DECLARATION

I hereby certify that the work presented in this dissertation entitled **'DEVELOPMENT OF AN ESTIMATOR FOR BATCH DISTILLATION COLUMN INFERENTIAL CONTROL'** in partial fulfillment of the requirements for the award of the degree of **MASTER OF ENGINEERING in CHEMICAL ENGINEERING** with specialization in **COMPUTER AIDED PROCESS PLANT DESIGN** of the University of Roorkee, Roorkee, is an authentic record of my own work carried out during the period from July, 1998 to March, 1999 under the guidance of **Dr. S. N. Sinha**, *Asstt. Professor, Department of Chemical Engineering, University of Roorkee, Roorkee.*

The matter presented in this dissertation has not been submitted by me for any other degree or diploma.

Sunil

Dated: 27th March, 1999 **(SUNIL YADAV)**

This is to certify that the above statement made by the candidate is correct to the best of my knowledge.

27.3.1999

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(SUNIL YADAV)

ABSTRACT

Industrial interest in batch distillation has increased significantly in recent years as more batch processing is being used for low-volume high-value specialty chemicals. The operation and control of the batch distillation column is different particularly in predicting the time of switching from total-reflux operation to producing different product cuts and slopcuts of desired composition. However, in most industrial applications of batch distillation, perfect on-line composition measurements are not available. Due to this fact inferential control system that relies on secondary measurements, e.g., temperature, flow measurements must be used. Models of the batch distillation process can be used to provide estimates of the required compositions.

Many articles dealing with batch distillation have appeared in the literature, but little attention has been paid to the problems of control. The objective of this work was to design an estimator for batch distillation system for inferential control and study the performance of estimator. Earlier some workers have developed estimators based on the steady-state and quasi-dynamic behaviour of the column. In the present work, a more realistic dynamic model of the estimator was studied. Computational technique and computer program were developed. The component material balance equations were written in tridiagonal matrix form. The resulting set of equations alongwith other constitutive equations of total material balance, equilibrium relationship and sum equations were solved by combination of two point implicit method and θ-method of convergence. Recurrence formulas and Newton-Raphson methods were applied to solve tridiagonal matrix and Jacobian matrix forms, respectively. K_b method has been used to update temperature profile. The response of the estimator was studied using the program and compared with actual values reported.

It was observed that the model for estimator is good enough to predict reasonably accurate value of top product compositions of all the components using measured values of the tray temperatures. This estimator being a critical component of the inferential control closed-loop system of a batch distillation column may be further used for the design of the control system.

NOMENCLATURE

A_{ji}	absorption factor for component i and stage j
A_j'	vapor pressure constant for component i
B_i'	vapor pressure constant for component i
B	bottom product, mol
C	total number of components
D	distillate flow rate , mol/h
d_i	distillate flow rate of component i , mol/h
D_1 , D_2	vapor draw off rate and side stream draw off rate, respectively, mol/h
F_f, F_j	feed stream at feed stage and stage j, respectively, mols
F	initial charge to still pot, mol
$\bar{f}_i^L$, $\bar{f}_i^V$	fugacities of component i in the liquid and vapor phases, respectively ; evaluated at the total pressure and temperature of the two-phase system.
f^L_i , f^V_i	fugacities of pure component i in the liquid and vapor phases , respectively;evaluated at the total pressure and temperature of the two-phase system
f	a column vector of functions
$g_j(\theta_0,\ldots, \theta_{N-1})$	the jth function of $\theta_0, \theta_1 ,\ldots\ldots,\theta_{N-1}$
h_j, H_j, H_{Fj}	enthalpies of the liquid stream L_j ,vapor from jth stage V_j and the feed stream F_j, respectively, Btu/mol
$\hat{H}_{ji}$, $\hat{h}_{ji}$	virtual values of the partial molar enthalpies of component i on jth stage for vapour and liquid phases, respectively
J	jacobian matrix
K_{ji}	equilibrium constant for component i at the temperature and pressure of the liquid leaving stage j

K_{jb}	equilibrium constant for the base component evaluated at the temperature of the liquid leaving stage j
L	liquid flow rate , mol/h
L_j	Liquid stream flowing from the jth stage down to the (j+1)th stage, mol/h
l_{ji}	flow rate at which component i in the liquid phase leaves stage j, mol/h
N	total number of trays
P	pressure
P_i, P_1, P_2, P_3	amount of product i, heavy, intermediate and light product, respectively, mol
P^o_i	vapor pressure of pure component i
Q_B ,Q_D	heat duty of reboiler and condenser, respectively
R	reflux flow rate, mol/h
S_i, S_1, S_2	amount of slop cut ,first slop cut and second slop cut, respectively, mol
T_j	temperature at jth stage
t	time in consistent units (t_n is used to denote the time at which the time increment n+1 begins, and $t_n+\Delta t$ the time at which the time increment n+1 ends)
U_N	still pot molar holdup ,mol
U_1 ,U_j	reflux drum molar holdup and tray liquid molar holdup, respectively, mol
U'_j	side stream draft rate, mol/h
u_{ji}^V,u_{ji}^L	vapor and liquid holdups in moles of component i on stage j, respectively
V_j	vapor stream leaving the jth stage to (j -1) th stage above, mol/h
V	vapor boilup, mol/h
v_{ji}	flow rate at which component i in the vapor phase leaves stage j, mol/h
W	bottom draw off rate, mol/h
W_j	vapor side stream from the jth stage, mol/h
X_i	total mole fraction of component i in the feed (regardless of state)
x_{Bi}, x_{Di}	liquid mole fraction of component i in still pot and distillate, respectively
x_{B1}^{spec}	specified purity of heavy component product, component 1
x_{Boi}	initial still pot composition , mole fraction of component i
x_{D2}^{spec},x_{D3}^{spec}	specified purity of intermediate and light component product, respectively
x_{ji}	liquid mole fraction of component i in tray j

x_{pji}	composition of product i (mole fraction of component i)
x_{sij}	composition of slop cut i (mole fraction of component i)
y_{Bi}	vapor mole fraction of component i in still pot
y_{ji}	composition of component i the vapor stream leaving jth stage, mole fraction
Z_i	liquid side stream from jth stage, mol
z_j, z_{ji}	fresh feed composition and feed stream leaving jth stage, respectively

Greek Letters

α_{ji}	relative volatilities of component i at tray j (with respect to heavy component)
γ_{ji}^L , γ_{ji}^V	activity coefficients for component i in the liquid and vapor on stage j, respectively
θ_0	a multiplier associated with the distillate and bottoms
θ_j	a multiplier associated with the stage j
ρ_{ji}	a constant appearing on the central diagonal of the jth row of the coefficient matrix of component material balances
σ	a constant appearing in the component material balances ($\sigma = (1-\phi)/\phi$)
τ_j	dimensionless time factor for stage j ($\tau_j = (U_j/L_j)/(\phi\Delta t)$)
τ_{av}	= $(U_j/L_j)_{av}/(\phi\Delta t)$
ϕ	a weight factor used in the evaluation of an integral in terms of the values of a function at times t_n and $t_n+\Delta t$

Subscripts

av	average value
ca	calculated value
co	corrected value
d	side stream draw off stage number
a	actual value
f	feed stage number

i	component number
j	tray number
n	trial number
N	total number of trays
s	side stream draw off stage number
1,2,3	component number for heaviest, intermediate and lightest components respectively

Superscripts

L	liquid phase
V	vapour phase
spec	specified value
0	values of a variable at the beginning of the time increment under consideration

Mathematical Symbols

$\{\ \}$	set of all values of the variables under consideration
Σ	symbol used for summation
Δ	symbol used for difference

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INTRODUCTION

Batch processing is becoming increasingly important in many chemical industries as the trend to small volume, high value, speciality chemicals continues. Batch distillation columns are frequently an important part of these processes. Batch distillation has the advantage of being able to produce a number of products from a single column. Even though batch distillation typically consumes more energy than continuous distillation, it provides more flexibility and involve less capital investment . A single column can also handle a wide range of feed compositions having a number of components. Since energy costs are not too significant in small volume, high valued products , batch distillation is often attractive for this class of products .

The batch distillation process is characterised by a number of design and operating parameters to be optimised ; such as reflux ratio as a function of time, the number of trays and the size of the initial charge to the still pot.

When constant overhead purity is desired , the automatic operation of the equipment presents challenging control difficulties due to the transient and non linear characteristics of batch distillation process. Different control configurations for batch distillation are as follows:

1.1 FEED BACK CONTROL

In order to control a system the concept of using information about the deviation of system from its desired state is called feed back control. It uses the direct measurement of the controlled variables to adjust the values of the manipulated variables . The objective is to keep the controlled variables at the

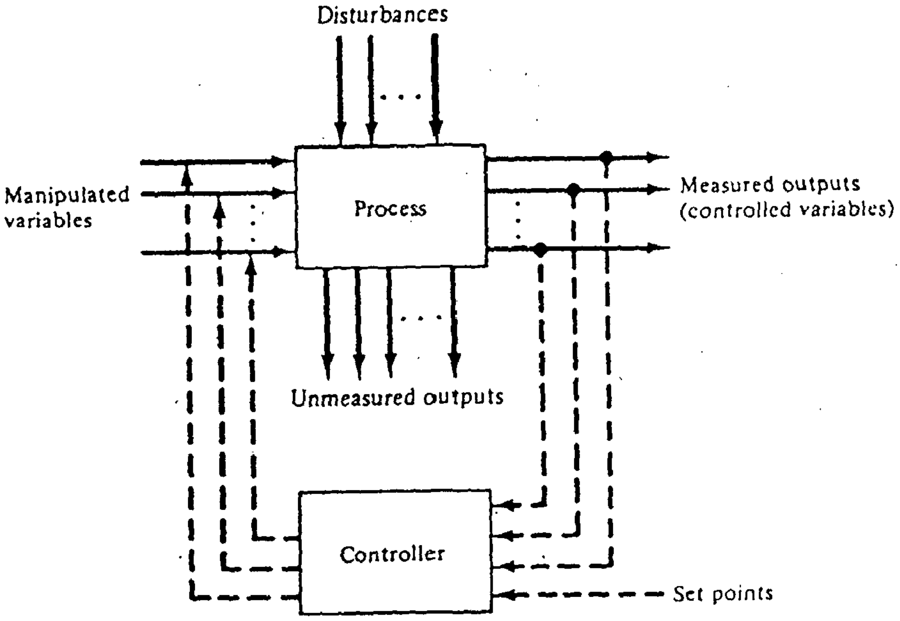


Fig. 1.1 General structure of a Feedback Control Configuration

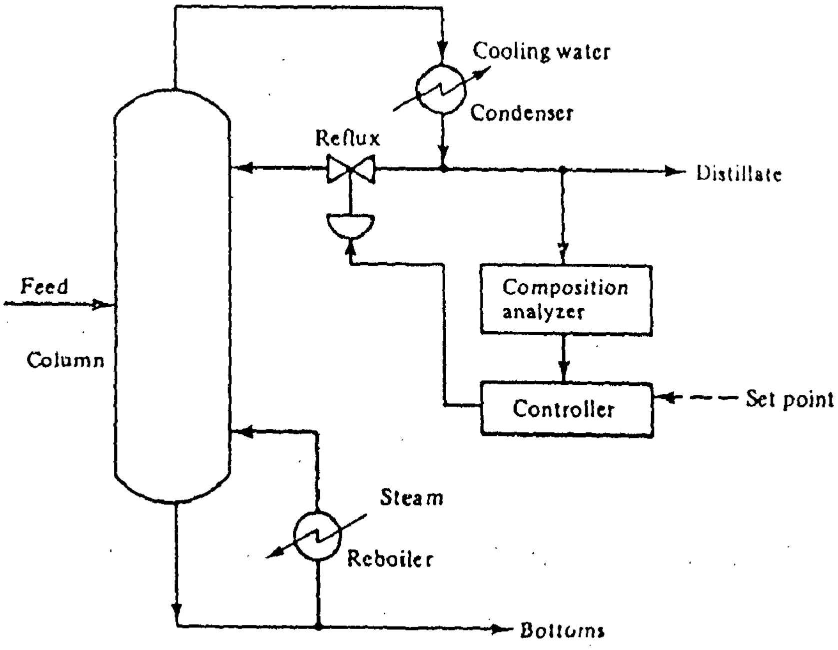
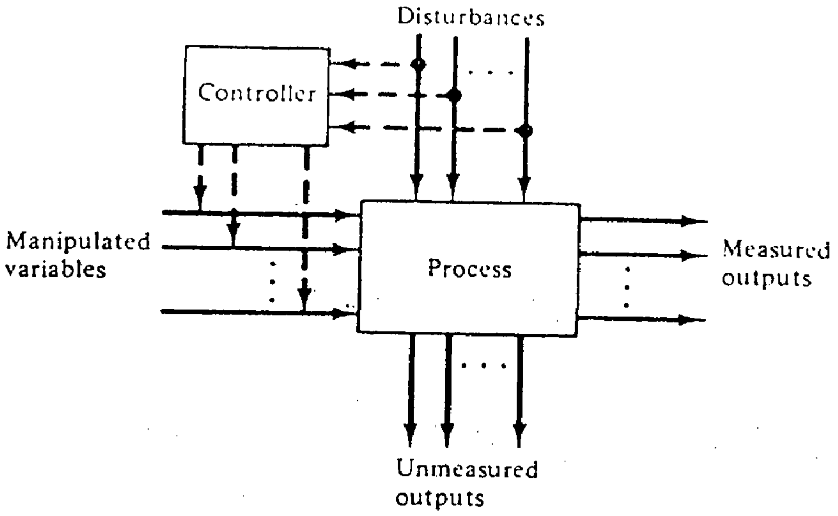


Fig. 1.2 Feedback Control for a Simple Distillation Column



g. 1.3 General structure of a Feed forward Control Configuration

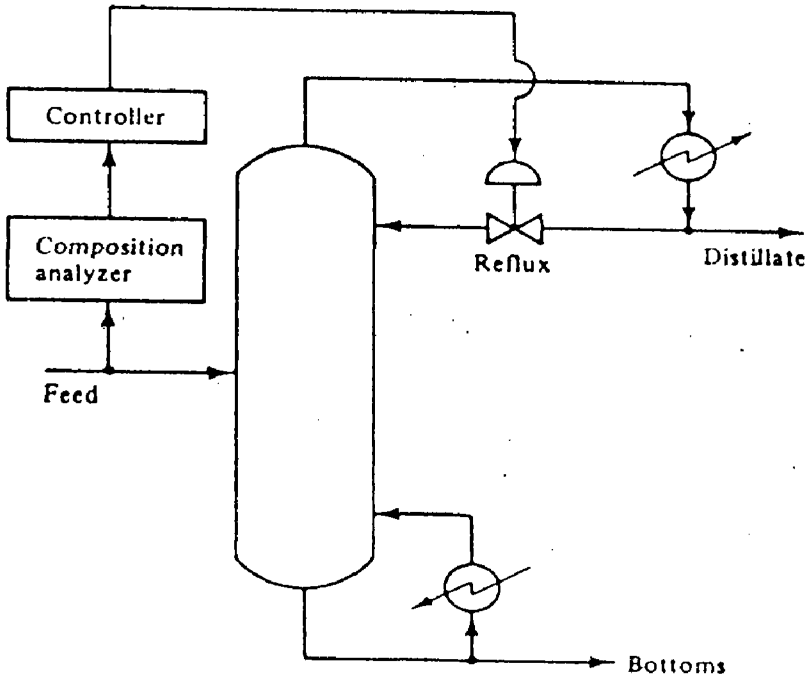


Fig. 1.4 Feed forward Control for a Simple Distillation Colum

desired levels. The general structure of feed back control and feed back control of simple distillation column are shown in Fig. 1.1 and Fig. 1.2 respectively.

1.2 FEED FORWARD CONTROL

The concept of using information fed forward from the source of the load listurbances is called feed forward control. It uses the direct measurement of the listurbances to adjust the values of the manipulated variables. The objective is to eep the controlled variables at the desired levels. The general structure of feed orward control and feed forward control of simple distillation column are shown in Fig. 1.3 and Fig. 1.4 respectively.

1.3 INFERENTIAL CONTROL

In this configuration, secondary measurements are used to adjust the values of the manipulated variables as the controlled variables are not easily measured or not economically viable to measure. The objective is to keep the controlled variables at the desired levels. The general structure of inferential control and inferential control of simple distillation column are shown in Fig. 1.5 and Fig. 1.6 respectively.

Significance for Development of an Estimator

An estimator is used to estimate the values of the unmeasured controlled variables . The estimator uses the values of the available measured outputs, together with material, energy balances and constitutive relations that govern the process. In distillation, secondary measurements like temperatures, flows, pressure etc. are used to infer product composition. The effectiveness of an inferential control scheme depends heavily on the goodness of estimator, which in turn depends on the model that is available for the process. The effectiveness of control can be judged by checking the overhead composition , intermittently. Thus if the

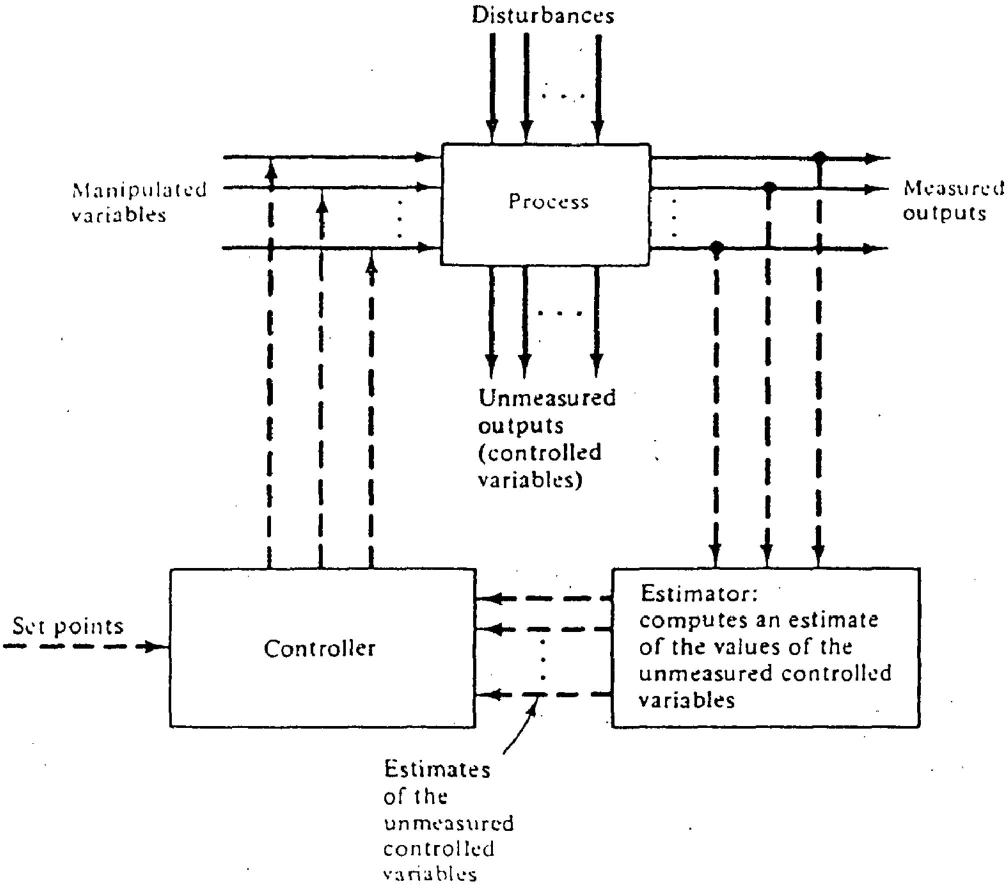


Fig. 1.5 General structure of an Inferential Control Configuration

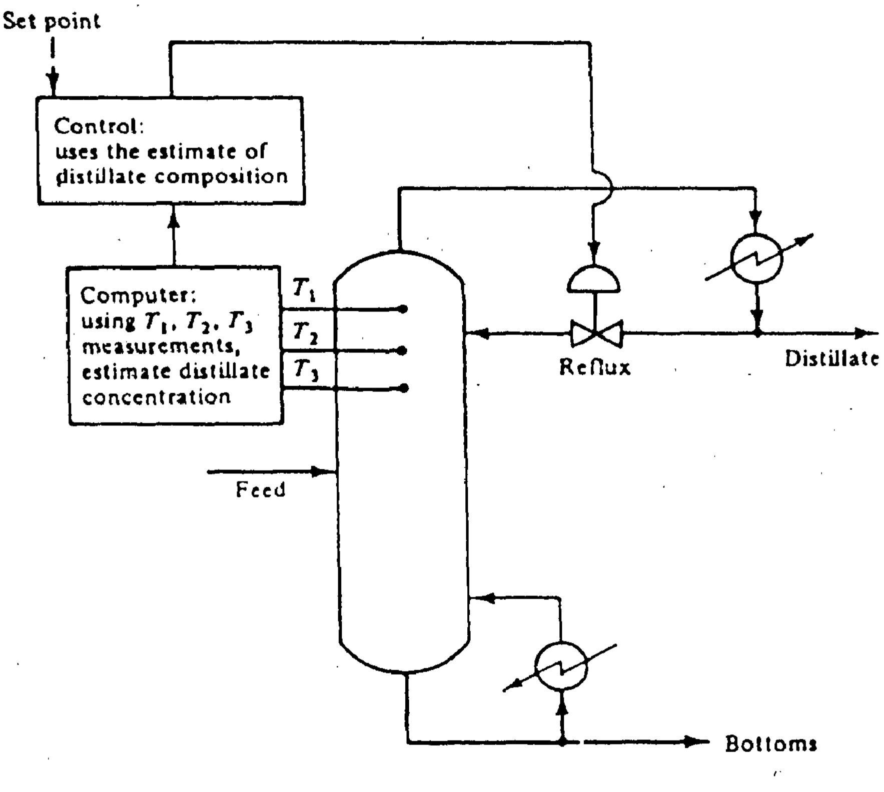


Fig. 1.6 Inferential Control for a Simple Distillation Column

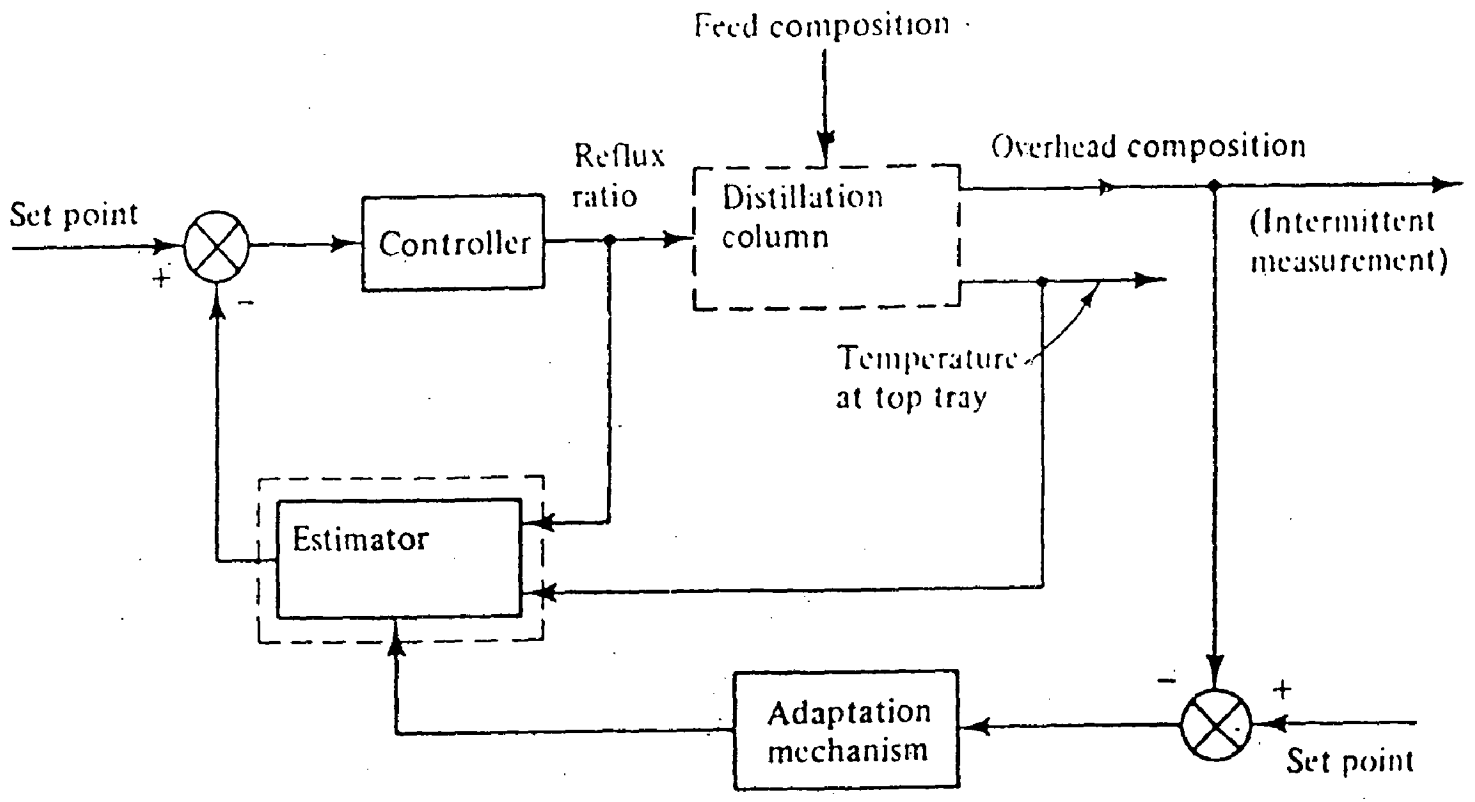


Fig. 1.7 Adaptive Inferential Control for a Distillation Column

measured steady state value of the overhead composition deviates significantly from the desired set point values an adaptive mechanism can be used to correct the estimator with the use of the deviation .

An adaptive inferential control configuration is shown in Fig.1.7.

1.4 PROPOSED STUDY

In view of the literature review done, it was observed that scarcity of information exists in the area of accurate and reliable estimators. It was therefore, thought desirable to develop an estimator for adaptive inferential control of batch distillation column. In view of the above objective following stepwise procedure is proposed for the above study:

i) Study of the model of the batch distillation system.

ii) Development of an estimator for the system.

iii) Development of an algorithm for solution of the model of the estimator.

iv) Development of an efficient computer program in C++.

v) Study of the performance of the estimator developed.

1.5 ORGANIZATION OF THE THESIS

Chapter two gives a review of modelling and control of the continuous distillation column and batch distillation column available in the literature. In chapter three, the operation of batch distillation system is discussed and modelling equations are given. Chapter four explains solution procedure for modelling equations and computational algorithm in detail. On the basis of which an efficient computer program is developed which is given in Appendix-A. Chapter five gives results obtained by the estimator developed. This chapter also includes discussion and comparison of results obtained with actual values. Chapter six gives conclusions and recommendations for future work.

LITERATURE REVIEW

2.1 INTRODUCTION

In the field of batch distillation, most studies have concentrated on the determination of optimum operating strategies : optimum trajectories of reflux ratio and pressure during the batch and processing of the slop cuts that are produced . Little attention has been paid to the problems of automatic control. The control of batch distillation would be straight forward once the optimum policies are available, if instantaneous and perfect chemical composition analysers are available. Since such analysers are not available, therefore, an inferential control system that relies on secondary measurements must be used. The basic objectives and functions of adaptive and inferential control systems may be easily described in a qualitative manner. But practical implementation is rather complicated because of extensive computations required. The digital computers are used for these computations.

The performance of an inferential control system strongly depends on the estimator used. However , before reviewing the literature available on estimators used, it was thought relevant to review the literature available on inferential control that have used such estimators. Since earlier developments in this area was with continuous distillation columns which have been later adopted with modifications for the case of batch distillation columns. It was therefore, thought desirable to review the literature available for modelling and /or inferential control of continuous distillation columns that are as follows:

2.2 MODELLING AND CONTROL OF CONTINUOUS DISTILLATION COLUMN

Multicomponent continuous distillation calculations are performed on a large digital computer by *Amundson and Pontinen (1958)*. Continuous distillation columns are defined as the columns in which the feed (or feeds) enter the column continuously and products are withdrawn continuously. Equations for multicomponent rectification problem were solved simultaneously component by component. The mass balances on each component and the heat balance on each tray will give a set of algebraic equations which may be expressed in matrix form. If the number of components is C and the number of plates is N , including the reboiler but not the partial condenser, the equations for the system will reduce to C matrix equations of order N+1 and one matrix equation of order N, the heat balance. The C matrix equations will contain the compositions as unknowns, while the unknowns in the heat balance matrix will be the vapour rates through out the column. All the matrix contain as a parameter the temperatures that must be fixed on each tray.

Model equations developed for two feeds and a single side stream ;

The overall mass balances are :

$$L_j + D_1 = V_{j+1} \qquad 0 \le j \le d-1$$

$$L_j + D_1 + D_2 = V_{j+1} \qquad d \le j \le f_1 - 1$$

$$L_j + D_1 + D_2 - F_1 = V_{j+1} \qquad f_1 \le j \le f_2 - 1$$

$$L_j - W = V_{j+1} \qquad f_2 \le j \le N-1$$

Mass balances around single trays are:

$$L_0 x_{0i} + D_1 y_{0i} = V_1 y_{1i} \qquad 1 \le j \le d-1$$

$$L_{j-1} x_{j-1,i} - L_j x_{ji} - V_j y_{ji} + V_{j+1} y_{j+1,i} = 0 \qquad d+1 \le j \le f_1-1$$

$$f_1+1 \le j \le f_2-1$$

$$f_2+1 \le j \le N-1$$

$$L_{j-1} x_{j-1,i} - (L_j + D_2) x_{ji} - V_j y_{ji} + V_{j+1} y_{j+1,i} = 0 \qquad j = d$$

$$L_{f_1-1} x_{f_1-1,i} - L_{f_1} x_{f_1,i} - V_{f_1} y_{f_1,i} + V_{f_1+1} y_{f_1+1,i} = -F_1 x_{F_1,i} \qquad j = f1$$

$$L_{f_2-1} x_{f_2-1,i} - L_{f_2} x_{f_2,i} - V_{f_2} y_{f_2,i} + V_{f_2+1} y_{f_2+1,i} = -F_2 x_{F_2,i} \qquad j = f2$$

$$L_{j-1} x_{j-1,i} - W x_{ji} - V_j y_{ji} = 0 \qquad j = N$$

Heat Balance equations around each tray ;

$$(h_0 - H_1) V_1 + (H_2 - h_1) V_2 = D (h_0 - h_1)$$

$$(h_1 - H_2) V_2 + (H_3 - h_2) V_3 = D (h_1 - h_2)$$

$$-$$

$$(h_{f-1} - H_f) V_f + (H_{f+1} - h_f) V_{f+1} = D h_{f-1} + W h_f - F H_f$$

$$-$$

$$(h_{N-2} - H_{N-1}) V_{N-1} + (H_N - h_{N-1}) V_N = W (h_{N-1} - h_{N-2})$$

$$(h_{N-1} - H_N) V_N = W (h_N - h_{N-1}) - Q_W$$

Temperature on each stage must be chosen such that

$$\sum_{i=1}^{C} x_{ji} = 1 = \sum_{i=1}^{C} k_{ji} x_{ji}$$

The method involves simultaneous solution of a large number of equations by an iterative procedure which needs assumption of a column temperature distribution for light hydrocarbon rectification. The corrected temperature distribution is obtained after successive iterations. The number of iterations depends on the precision required but generally four or five iterations are adequate.

Wang and Henke (1966) developed an iterative method for solving problems of Multicomponent distillation in complex columns. This method employs the tridiagonal matrix algorithm for the solution of the linearized material balance equation and uses Muller's method for the convergence of column temperature profile. The material balance is solved simultaneously for each component and therefore no matching is required . Both distributed and non-distributed components are handled with equal ease. The computational procedure is simple, fast and numerically stable, and can be adopted to digital computers of moderate size.

Mathematical Model :

For the convenience of deriving the general working equations, a hypothetical system as shown in Fig.2.1 is considered as the model column. The column has N equilibrium stages including the condenser (partial, total, or compound condenser) and a reboiler.

Each stage in the model column is considered to be an equilibrium stage which is shown in Fig.2.2.

The MESH equation derived for the column are as follows:

(i is for component number and j is for stage number)

M (Material balance) - Equation:

$$M_{ji}(x_{ji,}V_{j,}T_j) = L_{j-1}x_{j-1,i} - (V_j + W_j)y_{ji} - (L_j + U'_j)x_{ji} + V_{j+1}y_{j+1,i} + F_jz_{ji}$$

E (Equilibrium) - Equation:

$$E_j(x_{ji,}V_{j,}T_j) = y_{ji} - K_{ji}x_{ji} = 0$$

S (sum) Equation:

$$S_j(x_{ji,}V_{j,}T_j) = \sum_{i=1}^{C} y_{ji} - 1.0 = 0 \qquad \text{or}$$

$$S_j(x_{ji,}V_{j,}T_j) = \sum_{i=1}^{C} x_{ji} - 1.0 = 0$$

H (Heat Balance) Equation:

$$H_j(x_{ji,}V_{j,}T_j) = L_{j-1}h_{j-1} - (V_j + W_j)H_j - (L_j + U'_j)h_j + V_{j+1}H_{j+1} + FjH_{Fj} - Q_j = 0$$

These equations are combined as functions of V's by an overall material balance of all stages from the condenser through the jth stage.

$$L_j = V_{j+1} + \sum_{k=2}^{j}(F_k - W_k - U'_k) - D \qquad 2 \le j \le N\text{-}1$$

where , $D = V_1 + U'_1$

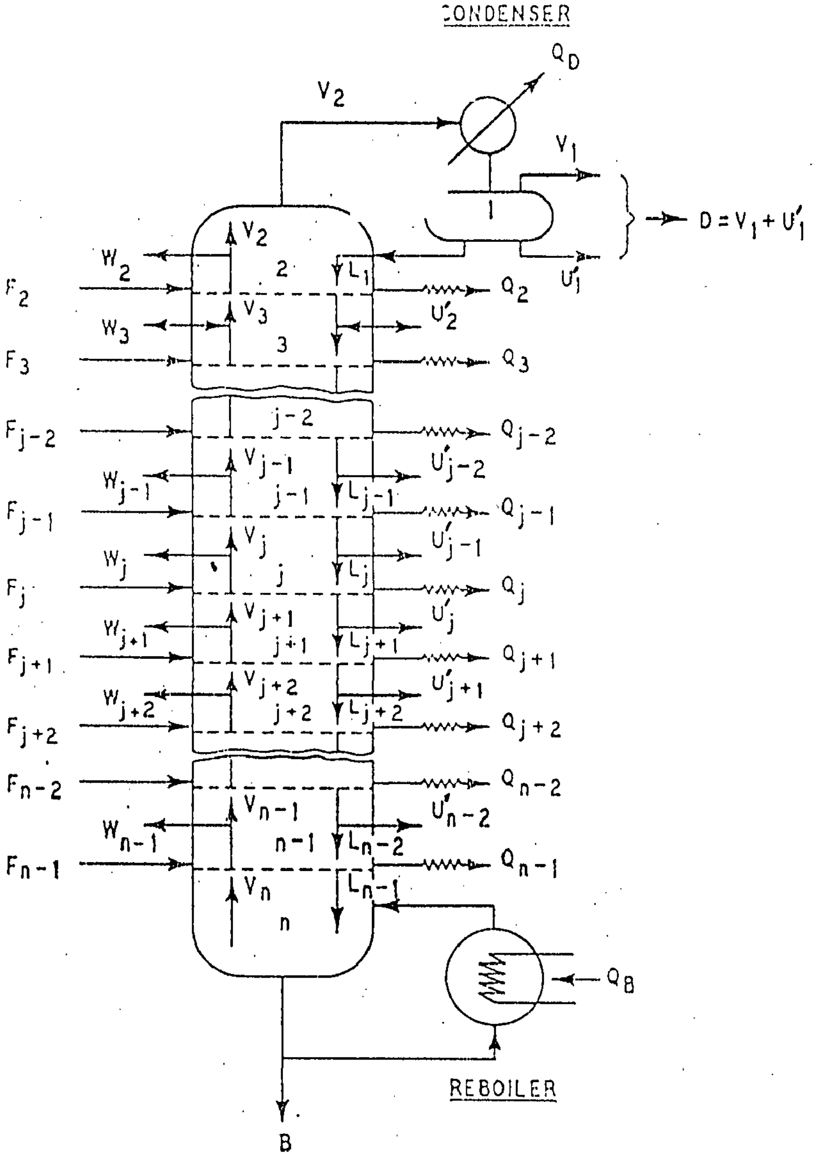


Fig. 2.1 Configuration of a Continuous Distillation Column

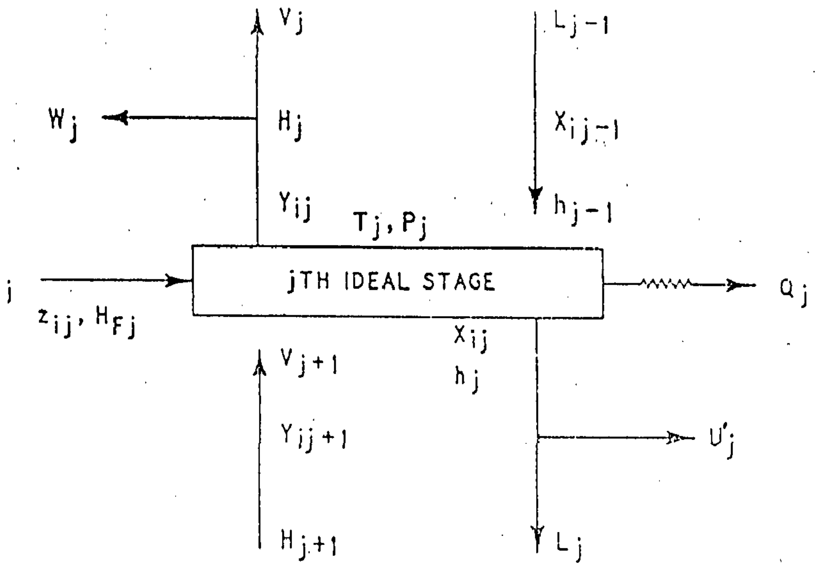


Fig. 2.2 An Ideal Equilibrium Stage

There are N(C+2) independent variables in these N(C+2) equation and therefore this system is consistent. The solution is generally obtained by using some iterative approach. Advantage of this method is greater likelihood success of Muller's method to the Newton - Raphson method and no partial derivatives are required in the Muller's method.

*Holland and Liapis (1983)*described the conventional unsteady state continuous distillation columns. They obtained the equations describing the column which consists of component material balances, the equilibrium relationships and the energy balance.

For a conventional continuous distillation column any stage exclusive of the overhead condenser , the feed stage and the reboiler (j ≠ 1, f, N) is described by the equations presented below. In development of these equations , it is assumed that the vapor and liquid phases are each perfectly mixed.

The component material balance enclosing stage j for each component i is :

$$\int_{t_n}^{t_n+\Delta t}(v_{j+1,i}+l_{j-1,i}-v_{ji}-l_{ji})dt=(u_{ji}^{V}+u_{ji}^{L})\Big|_{t_n+\Delta t}-(u_{ji}^{V}+u_{ji}^{L})\Big|_{t_n}$$

The total material balance for any stage j (j ≠ 1, f, N) is given by

$$\int_{t_n}^{t_n+\Delta t}(V_{j+1}+L_{j-1}-V_j-L_j)dt=(U_j^{V}+U_j^{L})\Big|_{t_n+\Delta t}-(U_j^{V}+U_j^{L})\Big|_{t_n}$$

The enthalpy balance for any stage j (j ≠ 1, f, N) is given by

$$\int_{t_n}^{t_n+\Delta t}\sum_{i=1}^{C}(v_{j+1,i}\hat{H}_{j+1,i}+l_{j-1,i}\hat{h}_{j+1,i}-v_{ji}\hat{H}_{ji}-l_{ji}\hat{h}_{ji})dt=\sum_{i=1}^{C}(u_{ji}^{V}\hat{H}_{ji}+u_{ji}^{L}\hat{h}_{ji})\Big|_{t_n+\Delta t}$$
$$-\sum_{i=1}^{C}(u_{ji}^{V}\hat{H}_{ji}+u_{ji}^{L}\hat{h}_{ji})\Big|_{t_n}$$

The component flow rates are related to the total flow rates as:

$$\sum_{i=1}^{C} l_{ji} - L_j = 0 \qquad (j = 1,2,\ldots\ldots,N)$$

$$\sum_{i=1}^{C} v_{ji} - V_j = 0 \qquad (j = 1,2,\ldots\ldots,N)$$

The component and total hold ups of the vapor and liquid are related as :

$$\sum_{i=1}^{C} u_{ji}^{L} - U_j^{L} = 0 \qquad (j = 1,2,\ldots\ldots,N)$$

$$\sum_{i=1}^{C} u_{ji}^{V} - U_j^{V} = 0 \qquad (j = 1,2,\ldots\ldots,N)$$

The equilibrium relationship for each component j on stage i may expressed as:

$$\frac{\gamma_{ji}^{L} K_{ji} l_{ji}}{\sum_{i=1}^{C} l_{ji}} - \frac{\gamma_{ji}^{V} v_{ji}}{\sum_{i=1}^{C} v_{ji}} = 0 \qquad (j = 1,2,\ldots\ldots,N)\ \&\ (i = 1,2,\ldots\ldots,C)$$

The fundamental relationships may be solved by a number of numerical methods. The component material balance equations are linearized by using two point implicit method and solved with the help of recurrence formulas. The resulting set of equations are solved by use of θ method or 2N Newton-Raphson methods. Calculated results were found to favourably comparable with the experimental results.

In the development of inferential control of a continuous distillation column, *Weber and Brosilow (1972)* presented a method for designing a linear static estimator which predicts product composition by a linear combination of temperatures and flow rates. An important feature of this algorithm is the method of selecting a subset of the available process output measurements which ensures that the resulting estimator is insensitive to modelling error and measurement noise. Once appropriate measurements have been selected, the estimator design can deviate from that presented to include important process non-linearities and dynamic lags. It was found that the composition control achieved, using the estimated product composition is comparable to that achieved with an instantaneous composition measurement and is markedly superior to the composition control achieved by maintaining a constant tray temperature.

Joseph et. al. (1978) presented a strategy for the design of linear inferential control systems for processes which operate about a sequence of steady states. The unmeasurable disturbances are assumed to drift from one mean level to another at a rate such that the process will operate about one or another steady state condition most of the time. Particular attention was paid to the selection of secondary measurements which minimise estimator sensitivity to modelling errors and measurement noise. Application to control the product compositions of simulated multicomponent distillation columns shows that the inferential control systems so designed substantially improve product quality control over that achieved by temperature feed back control.

Shah and Luyben (1979) extended the linear estimator to a rigorous non linear estimator for binary systems, because of the non linear characteristics of distillation columns. Fundamental material and energy balances with rigorous vapour - liquid equilibrium correlations were employed to back calculate compositions throughout the column from measured tray temperatures and flow rates. Experimental work confirmed the practicality of the rigorous estimator . However Shah's estimator was limited to binary columns.

Yu and Luyben (1987) proposed a multiple temperature control of the process . The set point of a conventional temperature controller was reset by using several temperature measurements to detect changes of non key and key components in the feed . This rigorous composition estimator consists of tw

steps:

i) Selection of temperature measurements

ii) Calculation of compositions and temperature on all trays and feed compositions.

The temperature selection criteria based on singular value decomposition was used which was efficient and consistent with engineering judgements. The composition algorithm was a modified *Wang – Henke (1966)*. This rigorous estimator gave better performance in all cases than direct analyser control with typical analyser dead time.

Chapat and Depeyre (1993) had worked in the area of control of continuous distillation column . This paper summarised the past studies in this field and also gave industrial or pilot plant scale developments. Various dynamic models , their identification procedures and some control algorithms were given and compared . Their industrial application was discussed . The trends and limits in advanced process control are also considered.

So far , literature of continuous columns was discussed , however our interest was to study the estimator for batch distillation column so the literature available in the area of batch distillation is presented next.

2.3 MODELLING AND CONTROL OF BATCH DISTILLATION COLUMN

The development of calculational procedures for batch distillation, an inherently unsteady state process , has followed a somewhat different path from that of continuous distillation column. The calculational procedures proposed in the literature for solving batch distillation problems follow closely the development of high computation capability. The early efforts are marked by approximate and graphical procedures. With the advent of high speed computers made it possible to use exact models of the process and application of numerical methods for solving problems of this type.

Luyben (1971) in his work on the practical aspects of optimal batch distillation, presented in his introduction a brief overview of the directions which batch distillation research had taken since 1940's. But most of the work on batch distillation had been limited to the separation of binary mixtures .

Ternary batch distillation was studied by *Stewart et.al.(1973)*, both theoretically and experimentally. They showed the effects of reflux ratio and number of trays on a measure of separation performance called the average product composition.

Holland and Liapis (1983) described the solution of typical batch distillation problems. They divided the description of batch distillation into two parts

i) The Start up Period (D=0, B=0 and F=0)

The complete set of specifications for a batch distillation column for the start up period are as follows : The number of stages , the reboiler duty , the column pressure , the composition and thermal condition of the feed charge, the hold up on each stage of the column , and the operating condition of total reflux D=0 , B=0 and F=0 . At this type of operation , a total condenser and a reboiler (total) are used .

A batch distillation process may be started up in a variety of ways. At the onset, it is assumed that the plates are filled with the liquid to be distilled and this liquid is at its bubble point at the operating pressure . The column is operated at total reflux. The column is operated at these conditions until the steady state is attained or for any specified amount of time.

The equations for start up period consist of the component material balances, total material balances, energy balances and the equilibrium relationships. The basic equations are of the same general form as shown for the continuos distillation column with allowances made for the fact that for start-up period , D=0, B=0, and F=0. The component material balances may be converted to a set of algebraic equations by the use of the two point implicit method. The resulting set of equation along with total material balance and enthalpy balance equations can be solved by θ method of convergence or 2N Newton - Raphson method.

ii) The Product Period (B=0 , D>0)

The product period is that part of the distillation process during which a product is withdrawn from the column. The operating conditions for the column at the initiation of the product period must be known to describe this period. During this part of process, the distillate is removed from the column (D>0) and the bottom rate B = 0. A column may be operated in many ways during this part . Such as two specifications L_1 (or V_2) and D, are made for each time t throughout the product period. These two specifications are used to determine the condenser and reboiler duties. In addition suppose that the liquid hold-ups U_j ($1 \leq j \leq N-1$) are specified. In this mode of operation , the hold up U_N of the reboiler (or still) decreases as the product period progresses. The usual specifications of column pressure, the number of stages , type of condenser (total or partial) , and the conditions existing through out the column at the initiation of the product period have been made.

The equation for product period consist of the component material balances, total material balances, energy balances, and the equilibrium relationships. These equations can be obtained by the equations used for the continuous distillation column by making appropriate changes. Again two point

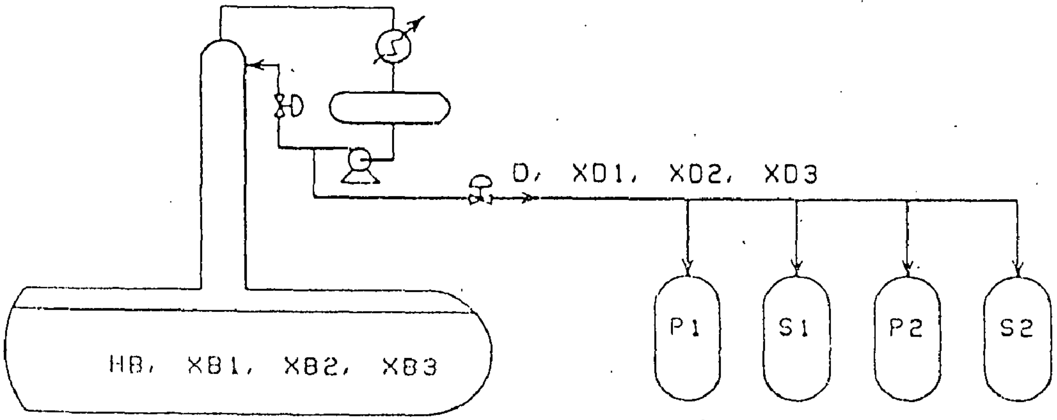


Fig. 2.3 Configuration of a Multicomponent Batch Distillation Column

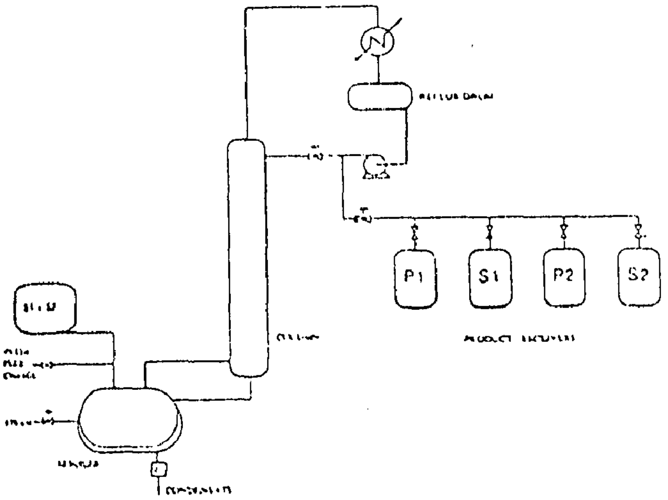


Fig. 2.4 Total Slop Recycle Scheme

implicit method can be used to convert component material balances into algebraic form. The resulting set of equation along with total material balance and enthalpy balance equations can be solved by θ method of convergence or 2N Newton - Raphson method.

Solution of the above equations by use of the two point implicit method and the θ method of convergence was presented for the start up period. The use of the two point implicit method and the θ method of convergence as well as a combination of the two - point implicit method and the 2N Newton - Raphson method , for the product period were presented. The results were compared with experimental results.

All the earlier works in inferential control have been applied to continuous systems. The design of estimators applied to batch distillation appears to be unexplored. Performance of the estimators depends upon the model that describes the process. Therefore while designing the estimator , it is necessary to understand the process.

Luyben (1988) analysed the multi component batch distillation system when the operating strategy was recycle of all slop cuts to the next still pot charge. The effects of both design and operating parameters were explored by using digital simulation : number of trays , reflux ratio (both fixed and variable) , initial still charge, relative volatility and product purity . Results show little difference in capacity between an optimum reflux policy and a variable reflux policy. Capacity increases with increasing number of trays and increasing relative volatility.

Quintero - Marmol and Luyben (1990) presented a paper in which several alternative schemes for handling slop cuts were explored. They considered a ternary batch distillation system as shown in Fig. 2.3. The alternative schemes considered are as follows

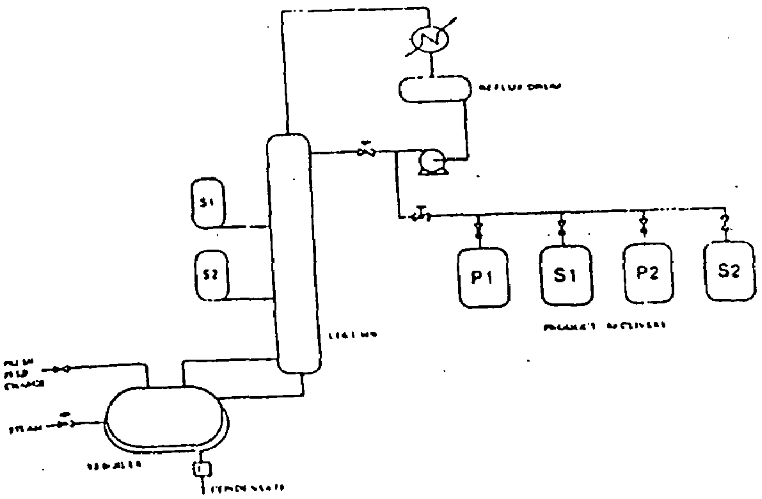


Fig. 2.5 Fed-Batch Distillation

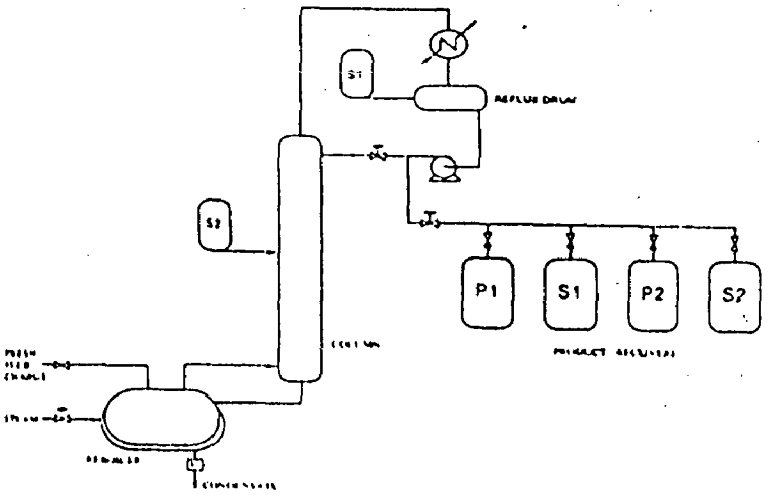


Fig. 2.6 Segregated Initial Charge

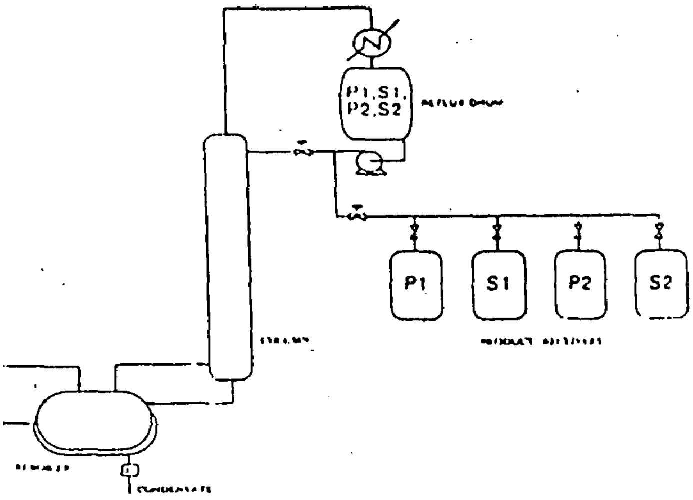


Fig. 2.7 Accumulated Product Strategy

i) Total Slop Recycle :

Total slop cuts of previous batch are collected and recycled by combining it with fresh batch (Fig. 2.4).

ii) Fed Batch Distillation:

The slop cuts are fed into the column at an appropriate time and tray during the next batch distillation.(Fig. 2.5)

iii) Segregated Initial Charge :

The first slop cut is used to fill the reflux drum but if there is enough material then it is fed to the column. The second slop cut is fed to the column.(Fig.2.6)

iv) Intermittent Distillation :

Distillation column is operated at total reflux , when distillate meets product specification , the total amount in the reflux drum is with drawn. The inventory in the reflux drum is built back to its original value.

v) Accumulated Product Strategy :

The total amount of each product or slop cut is collected in the reflux drum then it is discharged to the storage.(Fig. 2.7)

vi) Multicomponent - Binary component Batch Distillation :

Usually the slop cuts are binary , a number of slop cuts stored in segregated tank and after enough material is stored , each slop cut is distilled.(Fig. 2.8)

There is 30-40% increase in capacity factor by segregating the slop cuts and performing binary batch distillation on each slop cut , but total slop recycle is used in common practice because it is simple to handle.

Quintero - Marmol and Luyben (1992) presented model based inferential control for Multicomponent batch distillation systems. Models of the batch distillation system that rely on flow and temperature measurement , can be used to

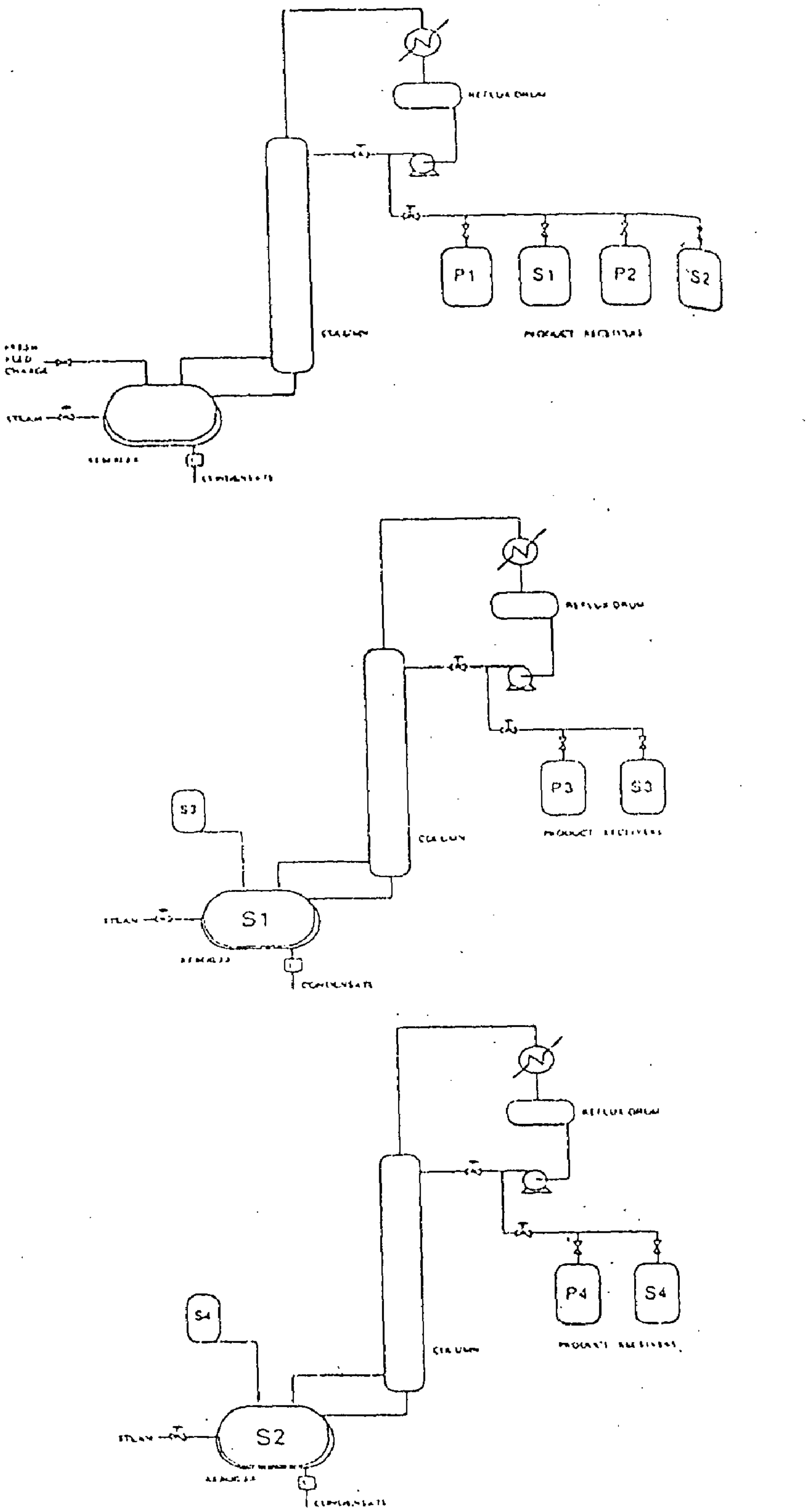


Fig. 2.8 Multicomponent-binary component batch distillation rocessing. (top) The fresh feed. (middle) The first slop cu (bottom) The first slop cut.

provide estimate of the required compositions. This paper presented the results of a study of two types of model based inferential control systems for Multicomponent batch distillation . The models considered were rigorous steady state estimator and a quasi-dynamic non-linear estimator.

In the rigorous steady state estimator, distillate compositions were back calculated from known flow rates and temperatures using rigorous non linear equations. To obtain the compositions , this estimator tried to approximate the batch distillation column as if the whole column and the reflux drum were at steady state at all times , which is true if the hold ups of both were negligible.

In the quasi dynamic non linear estimator , the concept that after the start up period, the composition profile in the upper part of a batch distillation column are essentially binary , independent of the number of components in the initial mixture, is used. Using this approximation and because the pressure is known , the composition on a tray , can be determined by knowing its temperature. With this binary liquid composition , vapour composition can be found that feeds the modelled part of the column over the thermocouple as shown in Fig.2.9. Only that part of the column above the thermocouple is used in the estimation model. The feed to the quasi dynamic model is binary but the model itself is multicomponent with as many components as the actual initial mixture. This permits the model to transition from cut to cut as vapors feeding the top section change over the course of the batch cycle from binary mixtures of components 3 and 2 to mixtures of components 2 and 1 etc.

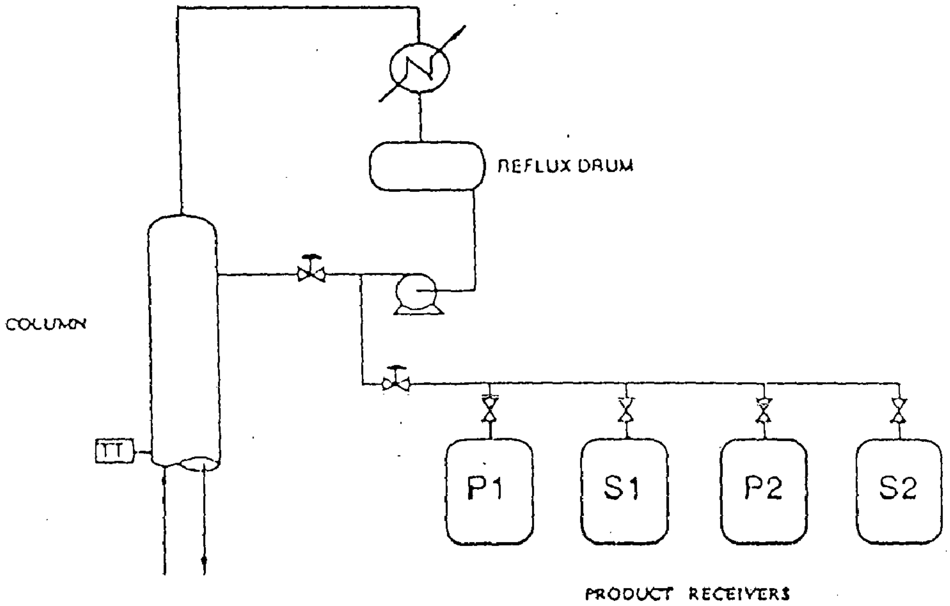


Fig. 2.9 Quasi-dynamic Nonlinear Estimator

DESCRIPTION AND MODELLING OF BATCH DISTILLATION SYSTEM

The successful inferential control requires a good estimator for composition estimation which in turn depends on how well we know the process. If we know the process very well , only then we can describe the process by mathematical model. Once we are able to develop proper mathematical model for the process, we can design a good estimator. Therefore , we present here multicomponent batch distillation system then we will discuss mathematical model.

3.1 DESCRIPTION OF BATCH DISTILLATION SYSTEM

The operation of a batch distillation column is divided into

- Start up at total reflux
- Withdrawl of the lightest product
- Removal of a slop cut , that is reprocessed in the subsequent batch.
- Withdrawl of next heaviest product
- Removal of a second slop cut etc.

If C is number of components , we obtain at most C-1 slop cuts. For a ternary system, we can have only one or two slop cuts and three products . The start up period is the part of the batch cycle when the column operates at total reflux until a distillate of the desired purity in the most volatile component can be with drawn. The initial charge can be assumed to be at its bubble point at the column pressure. Total condenser is used and the reflux is assumed to be saturated liquid. At the beginning of the batch it is assumed the compositions in the reflux drum and on all the trays are equal to the initial charge composition. The system is operated at total reflux until the specification purity for the most volatile component is met, after this system is operated at optimal fixed reflux ratio. The batch is finished when the average composition in the still pot and on the trays meets the product specification purity for the heavy component.

A multicomponent (ternary) batch system is considered . The theoretical trays, equimolal over flow, and constant relative volatilities are assumed. The system is shown in the Fig.2.3.

The total material charged to the column (F moles) can be fresh feed , with compositions X_1, X_2, and X_3, or a mixture of fresh feed and slop cuts. Component 1 and component 3 are heaviest and lightest components respectively. In the still pot, the instantaneous hold up is U_N, and compositions at any time is x_{b1}, x_{b2}, and x_{b3}. Constant tray liquid hold up and constant reflux drum hold up (U_1) are assumed. The vapor boil up rate V (moles/hr) is also constant.

Initially still pot, column trays and reflux drum are filled with material having composition x_{bo1}, x_{bo2} and x_{bo3}. After the vapor boil up is begun , the lightest composition concentration in distillate product is withdrawn at flow rate D and reflux ratio is held constant throughout the batch cycle. The distillate stream initially is withdrawn into a product tank until the average composition of the material remains above specified purity level x_{d3}^{spec}. This is the light component product P_1 . Then the distillate stream is withdrawn as slop cut S_1, into another tank. When the composition of the intermediate component in distillate, x_{d2} reaches its specified purity level x_{d2}^{spec} , the distillate is collected in a third tank as product P_2. Material is collected in this tank until any of following two events occurs:

1) If the composition of product in P_2 tank drops to the specified purity level x_{d2}^{spec} , the distillate stream is diverted into another tank as second slop cut

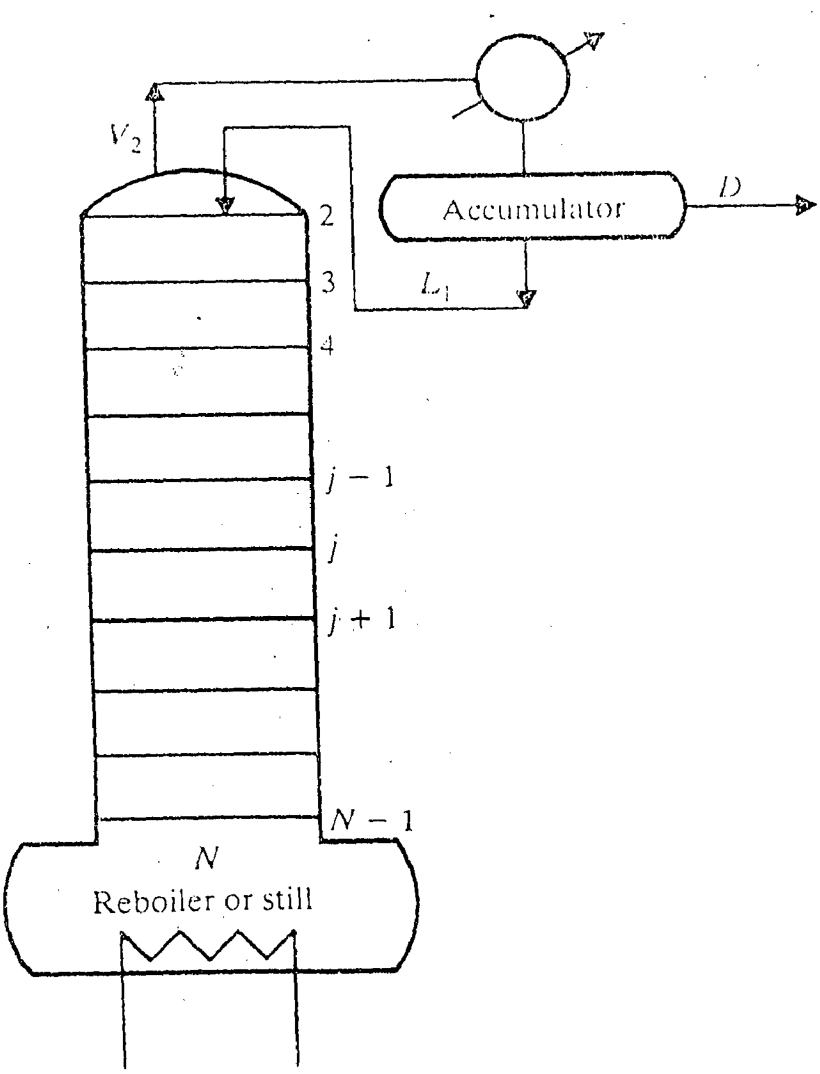


Fig. 3.1 Sketch of Batch Distillation Column

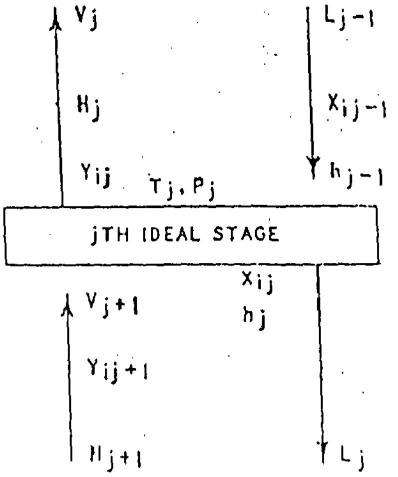


Fig. 3.2 An Ideal Equilibrium Stage for Batch Distillation System

S_2.It is collected until the average composition of material remaining on the trays and in still pot meets the purity level for heavy product P_3, x_{b1}^{spec}. The material along with slop cuts S_1 and S_2 , is recycle back to the next batch feed.

2) The purity of the material in the still pot and on the trays reaches above the heavy product (P_3) purity level x_{b1}^{spec}, then the material in the P_2 tank is above specification. If the average composition in the reflux drum and in the P_2 tank is above x_{d2}^{spec} , both are removed as product P_2. Otherwise, the liquid in reflux drum becomes the slop cut S_2 and is recycled along with the next batch charge. Thus, some batch runs will have two slop cuts and others will have only one.

3.2 MODEL EQUATIONS

The mathematical relations describing the counter current separation processes like distillation, consist of four basic equations, called MESH equations.

- mass balance equations (M)
- equilibrium relations (E)
- sum (or conservation) equations (S)
- enthalpy balance equations (H)

For simplification ,this model is based on the following assumptions:

- Constant tray hold up
- Constant reflux drum hold up
- Equimolal overflow
- Constant relative volatilities
- Constant vapor boil up rate
- Constant reflux ratio

The assumption of equimolal overflow means we do not need to solve the energy balance. Only **MES** equations are required for describing the process. Based on the above assumptions the equations describing the batch distillation system (as shown in Fig. 3.1) are:

Mass balance equations (M) :

The component material balance enclosing stage j for each component i is :

$$\int_{t_n}^{t_n+\Delta t}(v_{j+1,i} + l_{j-1,i} - v_{ji} - l_{ji})dt = (u^V_{ji} + u^L_{ji})\Big|_{t_n+\Delta t} - (u^V_{ji} + u^L_{ji})\Big|_{t_n} \qquad (3.1)$$

The total material balance for any stage j (j ≠ 1, N) is given by

$$\int_{t_n}^{t_n+\Delta t}(V_{j+1} + L_{j-1} - V_j - L_j)dt = (U^V_j + U^L_j)\Big|_{t_n+\Delta t} - (U^V_j + U^L_j)\Big|_{t_n} \qquad (3.2)$$

Equilibrium relations (E)

The equilibrium relationship for each component i on stage j may expressed as:

$$\frac{\gamma^L_{ji} K_{ji} l_{ji}}{\sum_{i=1}^{C} l_{ji}} - \frac{\gamma^V_{ji} v_{ji}}{\sum_{i=1}^{C} v_{ji}} = 0 \qquad (\text{ i} = 1,2,\ldots..,\text{C}) \; \& \; (\text{ j} = 1,2,\ldots..,\text{N}) \qquad (3.3)$$

When the vapor phase forms an ideal solution, $\gamma^V_{ji}=1$ for all i, and when the liquid phase forms an ideal solution $\gamma^L_{ji}=1$ for all i. Thus if both phases form ideal solutions,

Eq.(3.3) reduces to

$$y_{ji} = K_{ji} x_{ji} \qquad (3.4)$$

Sum (or conservation) equations (S) :

The component flow rates are related to the total flow rates as:

$$\sum_{i=1}^{C} l_{ji} - L_j = 0 \qquad (\text{ j} = 1,2,\ldots..,\text{N}) \qquad (3.5)$$

$$\sum_{i=1}^{C} v_{ji} - V_j = 0 \qquad (\text{ j} = 1,2,\ldots..,\text{N}) \qquad (3.6)$$

The component and total hold ups of the vapor and liquid are related as :

$$\sum_{i=1}^{C} u^L_{ji} - U^L_j = 0 \qquad (\text{ j} = 1,2,\ldots..,\text{N}) \qquad (3.7)$$

$$\sum_{i=1}^{C} u^V_{ji} - U^V_j = 0 \qquad (\text{ j} = 1,2,\ldots..,\text{N}) \qquad (3.8)$$

COMPUTATIONAL TECHNIQUE AND COMPUTER PROGRAM

The solution of the time-domain model equations of the estimator requires the use of the two-point implicit and the θ method of convergence for finding the compositions on all trays with time.

In the following discussion, it is supposed that at the beginning of the batch (time $t = 0$) the compositions on all trays are the same as in the still pot. After the start up period (when the column operates at total reflux), we begin to with draw distillate of desired purity.

Computational Algorithm

For the time period from t_n to $t_n + \Delta t$, the steps of the computational algorithm are as follows :

Step 1 : Choose Δt and assume values for the temperatures $\{T_j\}$ and $\{V_j\}$ at time $t_n + \Delta t$, the end of the time period under consideration, as explained subsequently.

Step 2 : Calculate K values for all components on all trays.

Step 3 : Compute $\{v_{j\,i}\}$, $\{l_{j\,i}\}$, $\{u_{j\,i}\}$ by use of component material balances and equilibrium relationships, using a tridiagonal matrix algorithm.

Step 4 : Compute θ_j's ($j = 1, 2, \ldots\ldots, N$) such that $g_0 = g_1 = \ldots\ldots\ldots\ldots g_{n-1} = 0$ by use of the Newton-Raphson method.

Step 5 : Compute the corrected compositions $(x_{j\,i})_{co}$ on all trays.

Step 6 : Compute still composition and still hold up using overall material balance.

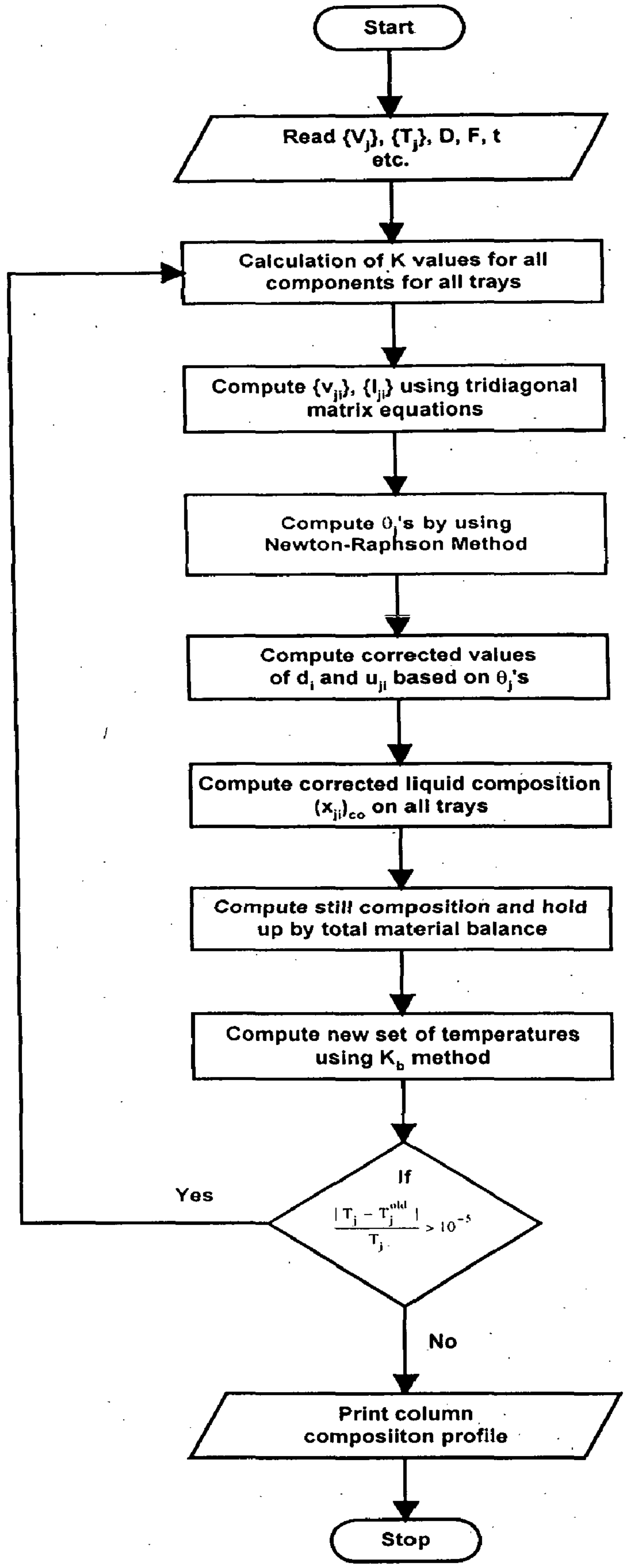


Fig. 4.1 : Flow Chart of the Computer Program for the Estimator

Step 7 : Compute a new set of temperatures by use of K_b method on the basis of the corrected mole fractions.

Step 8 : Repeat steps 2 through 8 until $\frac{|T_j - T_j^{old}|}{T_j} \le 10^{-5}$;

The solution set of the variables at time $t_n + \Delta t$ become the initial set of values of the variables for the next time period. Proceed to the next increment of time period by returning to step 1.

Details of Computational Algorithm

Now we discuss the different steps of estimation algorithm in details :

Step 1 : In order to determine accurate values of the transient variables, small values of Δt are needed for the first few time periods following an upset. The following scheme which is proposed by *Waggoner and Holland (1965)* is recommended. The initial Δt is computed such that $\tau_{av} = 5 / \phi$, where

$$\tau_{av} = \frac{(U_j / L_j)_{av}}{\phi \Delta t} \tag{4.1}$$

and $(U_j / L_j)_{av}$ is the arithmetic average of this ratio over all stages. At the end of every 10 time periods, the value of τ_{av} is halved or Δt is doubled.

For initial values of $\{T_j\}$ and $\{V_j\}$, the values at time $t_n + \Delta t$ may be taken equal to those at time t_n, as a first approximation. As it is an iteration technique, the corrected values of $\{T_j\}$ can be obtained after achieving convergence.

Step 2 : K is the equilibrium constant. For calculation of K, it is necessary to understand the concept of physical equilibrium.

A two-phase multi-component mixture is said to be in equilibrium if the following necessary conditions are satisfied *(Holland, 1975)*.

(a) The temperature T^V of the vapor phase is equal to the temperature T^L of the liquid phase.

(b) The total pressure P^V throughout the vapor phase is equal to the total pressure P^L throughout the liquid phase.

(c) The tendency of each component to escape from the liquid phase to the vapor phase is exactly equal to its tendency to escape from the vapor phase to the liquid phase.

In the following analysis it is supposed that state of equilibrium exists. $T^V = T^L = T$, $P^V = P^L = P$, and the escaping tendencies are equal.

Now consider the special case in which the third condition may be represented by Raoult's law

$$Py_i = P_i^0 x_i \tag{4.2}$$

where, x_i and y_i are the mole fractions of component i in the liquid and vapor phases, respectively, and P_i^0 is the vapor pressure of pure component i at the temperature T of the system, P is the system pressure.

The phase behaviour of many mixtures is not adequately described by Raoult's law. A more precise statement of third condition is that the partial molar free energies are equal from which the following alternate but equivalent statement may be deduced,

$$\bar{f}_i^V = \bar{f}_i^L \tag{4.3}$$

where, $\bar{f}_i^V$ and $= \bar{f}_i^L$ are the fugacties of component i in the vapor and liquid phases, evaluated at the P and T of the system. Equation (4.3) may be restated in the following equivalent form :

$$\gamma_i^V f_i^V y_i = \gamma_i^L f_i^L x_i \tag{4.4}$$

where,

f_i^L, f_i^V = Fugacities of pure component i, in the liquid and vapor states, respectively, evaluated at the total pressure P and temperature T of the system;

x_i, y_i = Mole fractions of component i in the liquid and vapor phases, respectively;

γ_i^L, γ_i^V = Activity coefficients of component i in the liquid and vapor phases, respectively;

$$\gamma_i^L, = \gamma_i^L (P, T, x_1, \ldots\ldots\ldots\ldots, x_C);$$

$$\gamma_i^V = \gamma_i^V (P, T, y_1, \ldots\ldots\ldots\ldots, y_C);$$

If, as is usually the case, the vapor may be assumed to form an ideal solution, then $\gamma_i^V = 1$ for each i, and Eq. (4.4) may be restated as follows :

$$y_i = \gamma_i^L K_i x_i$$

where,

$$K_i = \frac{f_i^L}{f_i^V},$$

The expression given by Eq. (4.5) is recognized as one form of Henry's law. If the liquid phase also forms an ideal solution ($\gamma_i^L = 1$ for all i), then Eq. (4.5) reduces to

$$y_i = K_i x_i \tag{4.6}$$

In some of the literature, the activity coefficient γ_i^L is observed in K_i, that is, the product γ_i^L K_i is called K_i and an equation of the form of Eq. (4.6) is obtained which is applicable to systems described by Eq. (4.5).

If the effect of total pressure on the liquid fugacity is negligible in the neighbourhood of the vapor pressure of pure component i, then

$$f_i^L \Big|_{P,T} \cong f_i^L \Big|_{P_i^0,T} \cong f_i^V \Big|_{P_i^0,T} \tag{4.7}$$

where, P_i^0 is the vapor pressure of pure component i. If in addition to the assumptions required to obtain Eq. (4.6) and (4.7), one also assumes that the vapor phase obeys the perfect gas law (PV=RT), then Eq. (4.6) reduces to Raoult's law, Eq. (4.2). Thus, if we compare Eq. (4.2) and (4.6), we find the following relation

$$K_i = \frac{P_i^0}{P} \tag{4.8}$$

Now, the equilibrium constant K_{ji} is related to the temperature of the system T by the following expression

$$\log_e K_{ji} = \frac{A'_i}{T_j} + B'_i \tag{4.9}$$

where, A'_i and B'_i are constant for component i and for stage j.

From Eq. (4.9), we obtain following relation :

$$K_j = \exp\left[\frac{A'_j}{T} + B'_j\right] \tag{4.10}$$

Thus if constants A'_i and B'_i are known, the value of K can be calculated for any component for any temperature by the Eq. (4.10)

Step 3 : The component-material balance enclosing stage j is as follows for each component i:

$$\int_{t_n}^{t_n+\Delta t} (v_{j+1,i} + l_{j-1,i} - v_{ji} - l_{ji})\,dt = (u_{ji}^V + u_{ji}^L)\Big|_{t_n+\Delta t} - (u_{ji}^V + u_{ji}^L)\Big|_{t_n} \tag{4.11}$$

It may be approximated by use of two-point implicit method as follows :

$$v_{j+1,i} + l_{j-1,i} - v_{ji} - l_{ji} + \sigma(v^{o}_{j+1,i} + l^{o}_{j-1,i} - v^{o}_{ji} - l^{o}_{ji}) = \frac{u_{ji}}{\phi \Delta t} - \frac{u^{o}_{ji}}{\phi \Delta t} \qquad (4.12)$$

where,

$$0 \le \phi \le 1 \quad \text{and} \quad \sigma = (1-\phi)/\phi$$

here the vapor hold up u^{V}_{ji} has been neglected and u^{L}_{ji} has been denoted by u_{ji}.

The two-point implicit method *(Holland and Liapis, 1983)* is shown in Appendix-C.

From equilibrium relationship;

Since $y_{ji} = K_{ji}\, x_{ji}$, $y_{ji} = v_{ji}/V_j$ and $x_{ji} = l_{ji}/L_j$;

Eq. (4.6) may be restated in the form

$$\frac{v_{ji}}{V_j} = K_{ji}\,\frac{l_{ji}}{L_j} \qquad (4.13)$$

$$l_{ji} = A_{ji}\, v_{ji} \qquad (4.14)$$

where,

$$A_{ji} = \frac{L_j}{K_{ji}\, V_j}$$

Since the liquid phase is assumed to be perfectly mixed on each stage, the liquid hold ups may be stated in terms of the vapor flow rates through the use of Eq. (4.14) in the following manner :

$$u_{ji} = U_j\left(\frac{l_{ji}}{L_j}\right) = \frac{U_j}{L_j}\, A_{ji}\, v_{ji} \qquad (4.15)$$

Use of this relationship followed by rearrangement permits Eq. (4.12) to be restated in the following form :

$$A_{j-1,i}\, v_{j-1,i} - \rho_{ji}\, v_{ji} + v_{j+1,i} = -\sigma(l^{o}_{j-1,i} - v^{o}_{ji} - l^{o}_{ji} + v^{o}_{j+1,i}) - \frac{u^{o}_{ji}}{\phi \Delta t} \qquad (j \neq 1, N)$$

(4.16)

In a similar manner, the equations for j = 1, N are developed. The resulting set of equations follows :

$$-\rho_{1i}\, l_{1i} + v_{2i} = -f_{1i} \tag{4.17}$$

$$A_{j-1,i}\, v_{j-1,i} - \rho_{ji}\, v_{ji} + v_{j+1,i} = -f_{ji} \qquad (j = 2, 3, \ldots, N\text{-}1) \tag{4.18}$$

$$A_{N-1,i}\, v_{N-1,i} - \rho_{Ni}\, v_{Ni} = -f_{Ni} \tag{4.19}$$

These equations may be restated in matrix form as follows :

$$A_i\, v_i = -f_i \qquad (i = 1, 2, \ldots\ldots C) \tag{4.20}$$

Where,

$$A_i = \begin{bmatrix} -\rho_{1i} & 1 & 0 & 0 & \cdots & 0 & 0 \\ 1 & -\rho_{2i} & 1 & 0 & \cdots & 0 & 0 \\ 0 & A_{2i} & -\rho_{3i} & 1 & \cdots & 0 & 0 \\ 0 & 0 & A_{3i} & -\rho_{4i} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & \cdots & \cdots & -\rho_{N-1,i} & 1 \\ 0 & 0 & \cdots & \cdots & \cdots & A_{N-1,i} & -\rho_{Ni} \end{bmatrix}$$

$$v_i = [l_{1i}\ v_{2i}\ U_{3i}\ \ldots\ldots\ldots\ldots\ v_{Ni}]^{T}$$

$$f_i = [f_{1i}\ f_{2i}\ \ldots\ldots\ f_{Ni}]^{T}$$

$$\rho_{1i} = 1 + \tau_1\ ;\ \rho_{Ni} = 1 + \frac{U_N / V_N}{Q \Delta t\, K_{Ni}}$$

$$\rho_{ji} = 1 + A_{ji}(1 + \tau_j)\ \ ;\ \ \tau_j = \frac{U_j / L_j}{Q \Delta t} \qquad (j=1,2, \ldots, N\text{-}1)$$

$$= \sigma\{v^{o}_{j+1,i} + l^{o}_{j-1,i} - v^{o}_{ji} - l^{o}_{ji}] + \frac{u^{o}_{ji}}{\phi \Delta t} \qquad (j=2,3,\ldots N\text{-}1)$$

$$f_{1i} = \sigma[v_{2i}^{o} - l_{1i}^{o}] + \frac{u_{1i}^{o}}{\phi\,\Delta t}$$

$$f_{Ni} = \sigma[l_{N-1,i}^{o} - v_{Ni}^{o}] + \frac{u_{Ni}^{o}}{\phi\,\Delta t}$$

The above equations are for start up period. These equations are used for product period also with some modification which are given as follows :

l_{1i} is replaced by $v_{1i} = d_i$

and $f_{1i} = \sigma[v_{2i}^{o} - l_{1i}^{o} - d_i^{o}] + \frac{u_{1i}^{o}}{\phi\,\Delta t}$

This system of simultaneous equations is solved by use of recurrence formula which is also known as Thomas algorithm *(Holland and Liapis, 1983)*. It is a very useful mathematical tool for solving set of equations in tridiagonal form on a digital computer. Brief discussion of this method is given in Appendix D:

Thus this set of simultaneous equations gives us v_{ji}'s $(1 \le j \le N)$.

Step 4 : For each time period, successive approximation of the temperatures at the end of the time period are made until a temperature profile is found such that the component-material balances are satisfied as well as the specifications for the column.

The θ method of convergence is an indirect method for choosing a new set of temperatures. This method alters or corrects the mole fractions. On the basis of these mole fractions which reflect the certainties that each component must be in overall material balance and in agreement with specified values for the total distillate rate and the total holdups (the conditions of constraint), a new set of temperatures is found. Next, θ-method of convergence is discussed separately for the start up period and product period.

i) Start up period

In start up period, θ_j's are defined with respect to u_{1i}, since $d_i = 0$. The composition and boiling point temperature of the initial feed charge, the total holdups U_1, U_2, ... , U_N are specified, which in turn fixes F. Let the N-1 independent θ_j's be defined as follows :

$$\frac{u_{ji}}{u_{1i}} = \theta_j \left(\frac{u_{ji}}{u_{1i}}\right)_{ca} \qquad (j = 2, 3, \dots, N) \tag{4.21}$$

The θ_j's are to be determined such that the corrected u_{ji}'s in overall component-material balance are in agreement with the specified values of U_j's. It follows that

$$\sum_{j=1}^{N} u_{ji} - \sum_{j=1}^{N} u_{ji}^{o} = 0 \tag{4.22}$$

The total moles of each component within the column remain fixed throughout the start up period. Let F X_i denote the total moles of component i in the column at time t = 0, the beginning of the start-up period.

$$F X_i = \sum_{j=1}^{N} u_{ji} = \sum_{j=1}^{N} u_{ji}^{o} \tag{4.23}$$

by relations Eq. (4.21) and Eq. (4.23) it gives;

$$u_{1i} = \frac{F X_i}{1 + \sum_{j=2}^{N} \theta_j \left(\frac{u_{ji}}{u_{1i}}\right)_{ca}} \tag{4.24}$$

The desired set of θ_j's is that set of positive numbers that makes $g_2 = g_3 = \dots = g_N = 0$ simultaneously, where

$$g_{j+1}(\theta_2, \theta_3, \dots\dots, \theta_N) = \sum_{i=1}^{C} u_{ji} - U_j \qquad (1 \le j \le N-1) \tag{4.25}$$

The θ_j's have been found by use of the Newton-Raphson method. These equations have the following matrix representation :

$$J_n h_n = - g_n \tag{4.26}$$

where,

$$J_n = \begin{bmatrix} \dfrac{\partial g_2}{\partial \theta_2} & \cdots & \cdots & \dfrac{\partial g_2}{\partial \theta_N} \\ \vdots & & & \vdots \\ \vdots & & & \vdots \\ \dfrac{\partial g_N}{\partial \theta_2} & \cdots & \cdots & \dfrac{\partial g_N}{\partial \theta_N} \end{bmatrix}$$

$$h_n = [h_2\ h_3\ \ldots\ h_N]^T$$

$$g_n = [g_2\ g_3\ \ldots\ g_N]^T$$

$$h_j = \theta_{j,n+1} - \theta_{jn} \tag{4.27}$$

The desired set of θ_j's is that set of θ_j's ($\theta_j > 0$) that satisfy the Newton-Raphson equations. For the first trial, θ_j is taken equal to 1.0 for all j. Then the system of equations is solved for the h_j's. The θ_j's to be assumed for the next trial solution of Eq. (4.26) are readily computed ($\theta_{j,n+1} = \theta_{j,n} + h_j$). This process is repeated until a set of θ_j's with in the desired degree of accuracy has been found. In the event that one or more of $\theta_{j,n+1}$'s is negative, all of the corrections h_j are reduced successively by factors of ½ until the $\theta_{j,n+1}$'s are all positive. The values of derivatives are evaluated by use of analytical expressions which are given as follows :

for m ≠ j and $2 \le j \le N$;

$$\frac{\partial g_m}{\partial \theta_j} = \sum_{i=1}^{C} \left[-\theta_m \left(\frac{u_{mi}}{u_{li}} \right)_{ca} \frac{(u_{li})^2}{FX_i} \left(\frac{u_{ji}}{u_{li}} \right)_{ca} \right] \tag{4.28}$$

for m = j and $2 \le j \le N$;

$$\frac{\partial g_j}{\partial \theta_j} = \sum_{i=1}^{C} \left[u_{li} \left(\frac{u_{ji}}{u_{li}} \right)_{ca} \left\{ 1 - \frac{\theta_j u_{li}}{FX_i} \left(\frac{u_{ji}}{u_{li}} \right)_{ca} \right\} \right] \tag{4.29}$$

The final θ_j's are used to find the values of corrected u_{1i}'s given by Eq. (4.24) which is used to compute corrected mole fractions.

ii) Product period

In the case of product period, in addition to V_2(or L_1) and D, the molar holdups U_1, U_2, ..., U_{N-1} are specified. The θ_j's are defined as :

$$\frac{u_{Ni}}{d_i} = \theta_o \left(\frac{u_{Ni}}{d_i}\right)_{ca} \tag{4.30}$$

$$\frac{u_{ji}}{d_i} = \theta_j \left(\frac{u_{ji}}{d_i}\right)_{ca} \qquad (j = 1, 2, \ldots\ldots\ldots, N\text{-}1) \tag{4.31}$$

The g functions are given by

$$g_o\,(\theta_o, \theta_1, \theta_2, \ldots\ldots\ldots\ldots, \theta_{N-1}) = \sum_{i=1}^{C} d_i - D \;; \tag{4.32}$$

$$g_j\,(\theta_o, \theta_1, \theta_2, \ldots\ldots\ldots\ldots, \theta_{N-1}) = \sum_{i=1}^{C} u_{ji} - U_j \;; \quad (j = 1, 2, \ldots\ldots., N\text{-}1) \tag{4.33}$$

Again, the desired set of θ_j's is that set of positive numbers that makes $g_o = g_1 = g_2 = \ldots\ldots., g_{N-1} = 0$ simultaneously. These θ_j's are found by use of the Newton-Raphson Method similar to the procedure, as was done for start up period. Here also, the values of derivatives are evaluated by use of analytical expressions which are given as follows :

$$\frac{\partial g_o}{\partial \theta_o} = \sum_{i=1}^{C} \left[\frac{-(d_i)^2 \left(\frac{u_{Ni}}{d_i}\right)_{ca}}{-\sigma \phi \Delta t\, d_i^{\,o} + \sum_{j=1}^{N} u_{ji}^{o}} \right] \tag{4.34}$$

for $1 \le j \le N-1$;

$$\frac{\partial g_j}{\partial \theta_0} = \sum_{i=1}^{C} \left[\frac{-\theta_m \left(\frac{u_{mi}}{d_i} \right)_{ca} \left(\frac{u_{Ni}}{d_i} \right)_{ca} d_i^2}{-\sigma \phi \Delta t d_i^o + \sum_{j=1}^{N} u_{ji}^o} \right] \tag{4.35}$$

for $1 \le j \le N-1,\ 1 \le m \le N-1$ and $m \ne j$;

$$\frac{\partial g_m}{\partial \theta_j} = \sum_{i=1}^{C} \left[\frac{-\left(\frac{u_{mi}}{d_i} \right)_{ca} \left(\frac{u_{ji}}{d_i} \right)_{ca} \theta_m d_i^2}{-\sigma \phi \Delta t d_i^o + \sum_{j=1}^{N} u_{ji}^o} \right] \tag{4.36}$$

for $1 \le j \le N-1,\ 1 \le m \le N-1$ and $m = j$;

$$\frac{\partial g_j}{\partial \theta_j} = \sum_{i=1}^{C} \left(\frac{u_{ji}}{d_i} \right)_{ca} \left[d_i - \frac{\theta_j d_i^2 \left(\frac{u_{ji}}{d_i} \right)_{ca}}{\left[-\sigma \phi \Delta t d_i^o + \sum_{j=1}^{N} u_{ji}^o \right]} \right] \tag{4.37}$$

The final set of θ_j's are used to compute the values of d_i (given in eq.(4.38)), which is used to compute corrected mole fraction.

Corrected value of d_i is obtained by

$$d_i = \frac{-\sigma d_i^o + \left(\frac{1}{\phi \Delta t} \sum_{j=1}^{N} u_{ji}^o \right)}{1 + \frac{1}{\phi \Delta t} \left[\theta_o \left(\frac{u_{Ni}}{d_i} \right)_{ca} + \sum_{j=1}^{N-1} \theta_j \left(\frac{u_{ji}}{d_i} \right)_{ca} \right]} \tag{4.38}$$

Step 5 : Now we calculate corrected compositions profile by the following expressions :

for start up period, for $j = 1, 2, \ldots\ldots, N$

$$x_{ji} = \frac{\left(\frac{u_{ji}}{u_{li}}\right)_{ca} u_{li}}{\sum_{i=1}^{C}\left(\frac{u_{ji}}{u_{li}}\right)_{ca} u_{li}} \tag{4.39}$$

for product period, for j = 1, 2, ..., N

$$x_{ji} = \frac{\left(\frac{u_{ji}}{d_i}\right)_{ca} d_i}{\sum_{i=1}^{C}\left(\frac{u_{ji}}{d_i}\right)_{ca} d_i} \tag{4.40}$$

Step 6 : New value of still hold up (U_N) and still compositions are computed on the basis of total material balance

$$U_N = U_N^o - D\Delta t \tag{4.41}$$

Step 7 : Bubble point temperature calculations are performed to update the tray temperature $\{T_j\}$ in following way

From Eq. (4.2)

$$P_{yj} = P_j^0 x_j$$

From Eq. (4.9)

$$\log K_j = \frac{A'_j}{T} + B'_j$$

Now state of equilibrium for a two-phase (vapor and liquid) system is described by the following equations.

$$y_{ji} = K_{ji} x_{ji}$$

$$\sum_{i=1}^{C} y_{ji} = 1 \tag{4.42}$$

$$\sum_{i=1}^{C} x_{ji} = 1 \qquad (4.43)$$

Here K_{ji} is a function of the total pressure P and the temperature T[K_{ji} = $K_{ji}(P,T)$], but the relative values of the K_{ji}'s are independent of temperature. The expressions given by Eqns. (4.8), (4.42) and (4.43) may be rearranged in a manner such that trial-and-error evaluations are avoided in the determination of bubble point temperature calculations.

The ratio $\frac{K_{ji}}{K_{jb}}$ is called the relative volatility α_{ji} of component i with respect of component b, that is,

$$\alpha_{ji} = \frac{K_{ji}}{K_{jb}} \qquad (4.44)$$

When K_{ji} and K_{jb} are evaluated at the same temperature and pressure, component b may or may not be a member of the given mixture under consideration.

When the x_{ji}'s and the pressure P are given and it is desired to determine the bubble point temperature, the formula needed may be developed by first rewriting the expression of Eq. (4.6) as follows :

$$y_{ji} = \left(\frac{K_{ji}}{K_{jb}}\right) K_{jb}\, x_{ji} \qquad (4.45)$$

$$\Rightarrow \quad y_{ji} = \alpha_{ji}\, K_{jb}\, x_{ji} \qquad (4.46)$$

$$\Rightarrow \quad \sum_{i=1}^{C} y_{ji} = K_{jb} \sum_{i=1}^{C} \alpha_{ji}\, x_{j} \qquad (4.47)$$

$$\Rightarrow \quad 1 = K_{jb} \sum_{i=1}^{C} \alpha_{ji}\, x_{ji} \qquad (4.48)$$

$$K_{jb} = \frac{1}{\sum_{i=1}^{C} \alpha_{ji}\, x_{ji}} \qquad (4.49)$$

From Eq. (4.45) and (4.48)

$$\frac{y_{ji}}{x_{ji}} = \frac{\alpha_{ji}}{\sum_{i=1}^{C} \alpha_{ji}\, x_j} \tag{4.50}$$

Now from Eq. (4.6)

$$y_{ji} = K_{ji}\, x_{ji} \tag{4.6}$$

From Eq. (4.9)

$$\log K_{ji} = \frac{A'_i}{T_j} + \tag{4.9}$$

Combining Eqns. (4.6), (4.7) and (4.

$$T_j = \frac{A'_i}{\log_e \left(\alpha_{ji} / \sum_{i=1}^{C} \alpha_{ji}\, x_{ji} \right) - \bar{B}'_i} \tag{4.51}$$

Tray temperature is updated by the Eq. (4.51).

Step 8 : After updating the tray temperature we obtain the new temperature profile, then we compare this with old temperature profile and check the following convergence criteria.

$$\frac{|T_j - T_j^{old}|}{T_j} \le 10^{-5}$$

If convergence is achieved after some iteration, the latest temperature profile is accepted as corrected temperature profile and corresponding corrected composition profile is accepted as response of estimator.

If convergence is not achieved, we again go to step (2), where we calculate the values of K for updated temperature profile.

On the basis of above computational techniques an efficient computer program was developed in C++ language and listing of program has been attached in Appendix – A.

RESULTS AND DISCUSSIONS

As discussed earlier a good estimator is essential for the design of adaptive inferential control of a batch distillation column system. The estimator for finding the compositions using measured values of tray temperatures was developed, by writing an efficient computer program based on the model given, as discussed earlier. The estimator was tested using actual data reported by *Quintero-Marmol and Luyben (1992).*

The program for the estimator was used to obtain the composition profile of all the components for the distillate as well as for all the trays, including the batch still. While estimating the composition profiles, initially it was supposed that plates were filled with liquid to be distilled. The liquid was assumed to be at its bubble point temperature at the column pressure. Vapor boil up rate was fixed at 100 mol/h. The distillate rate was fixed at 45 mol/h. Tray holdups were specified. The trays were numbered from top to bottom, as shown in Fig. 3.1. The operating conditions and other parameters used in the present study are given in Table 5.1.

The results were obtained for time intervals, from t = 0.0 h to t = 5.25 h till the batch was finished, by withdrawing the last product. Computations were carried out at several small time intervals, for accuracy of estimated results, as mentioned elsewhere in chapter 4 giving the details of computational technique. However, summary of the computed compositions at selected time intervals are being presented in Table 5.2 and Fig. 5.1 for the distillate composition of all the three components. Also, the computed compositions for all the trays at selected ·nes are being presented in Fig. 5.2 – 5.9 and in Appendix B (Table B-1 to B-8).

Table 5.1 Operating Conditions and Other Parameters for Ternary Batch Distillation

1.	Initial Feed to the Still Pot, F		mol	:	300
2.	Initial Feed Composition,	X_{B1}		:	0.4
		X_{B2}		:	0.3
		X_{B3}		:	0.3
3.	Relative Volatility,	α_1		:	1
		α_2		:	3
		α_3		:	9
4.	Tray Holdup, U_n		mol	:	1
5.	Reflux Drum Holdup, U_1		mol	:	10
6.	Distillate Flow Rate, D		mol/h	:	45
7.	Vapor Boilup Rate,V,		mol/h	:	100
8.	Total No. of Trays, N			:	40
9.	Top Temperature, T_1,		K	:	322 - 370
10.	Still Temperature, T_N,		K	:	344 - 390
11.	System Pressure, P,		N/m^2	:	1.013×10^5
12.	Constants,	A'_i,	K	:	-7200.8
		B'_1		:	10.2261
		B'_2		:	11.3247
		B'_3		:	12.4233

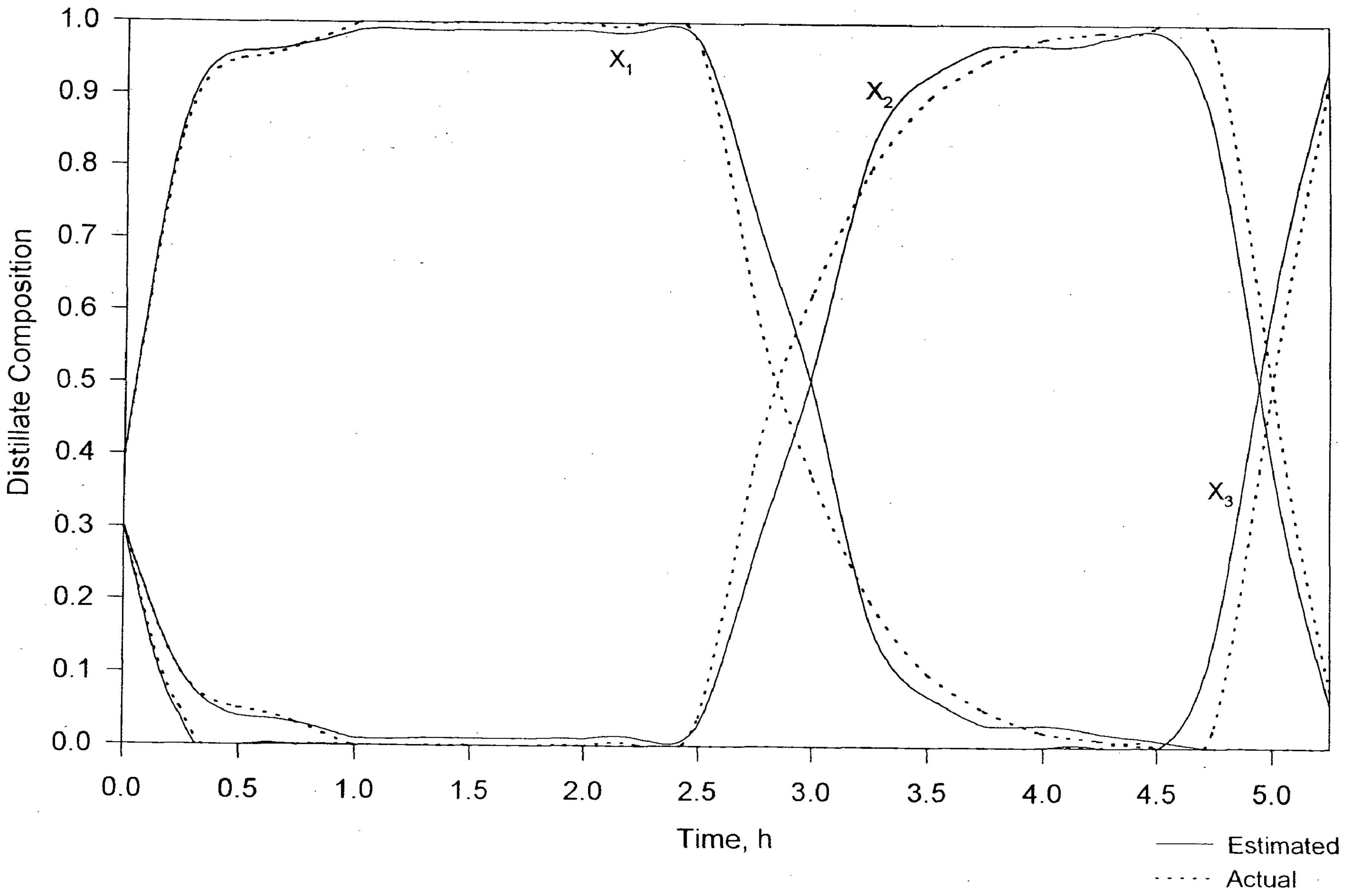


Fig.5.1 Distillate Composition for the system α =1/3/9; product purity=95%

Based on the summary of the compositions of distillate (shown in Table5.2), the total moles of the products (P_1, P_2, and P_3) and slop cuts (S_1 and S_2) were computed. Also the average compositions of the products and slop cuts were computed over the period of collection. These results are presented in Table 5.3, showing a comparison with their corresponding actual values.

The objective of the estimator was to obtain a correct estimate of top product composition. As shown in Fig. 5.1, we observe that estimated compositions are very close to the actual values as reported by *Quintero-Marmol and Luyben (1992)*. The comparison of the estimated compositions at the top tray with corresponding actual values at selected times may be given as follows.

At time t = 1 h.

$x_1 = 0.00$ $x_2 = 0.01$ $x_3 = 0.99$,

$x_{a1} = 0.00$ $x_{a2} = 0.00$ $x_{a3} = 1.00$.

At time t = 2.75 h,

$x_1 = 0.00$ $x_2 = 0.27$ $x_3 = 0.73$

$x_{a1} = 0.00$ $x_{a2} = 0.40$ $x_{a3} = 0.60$

At time t = 3.0 h,

$x_1 = 0.00$ $x_2 = 0.52$ $x_3 = 0.48$

$x_{a1} = 0.00$ $x_{a2} = 0.63$ $x_{a3} = 0.37$

At time t = 3.25 h,

$x_1 = 0.00$ $x_2 = 0.83$ $x_3 = 0.17$

$x_{a1} = 0.00$ $x_{a2} = 0.80$ $x_{a3} = 0.20$

At time t = 3.5 h,

$x_1 = 0.00$ $x_2 = 0.93$ $x_3 = 0.07$

$x_{a1} = 0.00$ $x_{a2} = 0.90$ $x_{a3} = 0.10$

Table 5.2

Summary of distillate composition obtained from estimator at different times for the system α=1/3/9, product purity = 95%

Time, h	Distillate Fractional Composition					
	Estimated			Actual		
	X_1	X_2	X_3	X_{a1}	X_{a2}	X_{a3}
0.00	0.30	0.30	0.40	0.30	0.30	0.40
0.25	0.04	0.10	0.86	0.05	0.10	0.85
0.50	0.00	0.04	0.96	0.00	0.05	0.95
0.75	0.00	0.03	0.97	0.00	0.03	0.97
1.00	0.00	0.01	0.99	0.00	0.00	1.00
1.25	0.00	0.01	0.99	0.00	0.00	1.00
1.50	0.00	0.01	0.99	0.00	0.00	1.00
1.75	0.00	0.01	0.99	0.00	0.00	1.00
2.00	0.00	0.01	0.99	0.00	0.00	1.00
2.25	0.00	0.01	0.99	0.00	0.00	1.00
2.50	0.00	0.03	0.97	0.00	0.04	0.96
2.75	0.00	0.27	0.73	0.00	0.40	0.60
3.00	0.00	0.52	0.48	0.00	0.63	0.37
3.25	0.00	0.83	0.17	0.00	0.80	0.20
3.50	0.00	0.93	0.07	0.00	0.90	0.10
3.75	0.00	0.97	0.03	0.00	0.95	0.05
4.00	0.00	0.97	0.03	0.00	0.98	0.02
4.25	0.00	0.98	0.02	0.00	0.99	0.01
4.50	0.00	0.99	0.01	0.00	1.00	0.00
4.75	0.15	0.85	0.00	0.03	0.97	0.00
5.00	0.61	0.39	0.00	0.50	0.50	0.00
5.25	0.94	0.06	0.00	0.92	0.08	0.00

Table 5.3

Comparison of results between actual and estimated values of products and slop cuts.

Initial feed F = 300 mols

System $\alpha = 9/3/1$ Purity = 95%	Actual	Estimated
P_1, mols	83.7450	84.1500
$x_{P_{11}}$	0.9450	0.9550
$x_{P_{12}}$	0.0544	0.0400
$x_{P_{13}}$	0.0006	0.0050
S_1, mols	45.900	44.1000
$x_{S_{11}}$	0.2242	0.2100
$x_{S_{12}}$	0.7758	0.7600
$x_{S_{13}}$	0.0000	0.0300
P_2, mols	48.0250	47.2500
$x_{P_{21}}$	0.0119	0.0080
$x_{P_{22}}$	0.9415	0.9800
$x_{P_{23}}$	0.0466	0.0120
S_2, mols	0.0000	0.0000
P_3, mols	122.3300	124.5000
$x_{P_{31}}$	0.0000	0.0000
$x_{P_{32}}$	0.0377	0.0550
$x_{P_{33}}$	0.9623	0.9450

We observe that except for the time interval t = 2.75 h to 3.25 h, there is a very close match between the estimated and actual values. The reason for mismatch between time interval t = 2.75 h to 3.25 h may be given as follows :

(i) Equimolal flow rate may not be achieved because heat of vaporization/condensation of the three components in the temperature range from tray no. 1 to tray no. 40 may be significantly different.

(ii) Assumption of constant relative volatility for all trays may be approximate.

The composition profiles developed at different times are shown in Fig. 5.2 to Fig.5.9 and values are tabulated in Appendix B (Table B-1 to Table B-8).

In Fig. 5.2 , initial compositions are assumed be same on all the trays at t=0 h, so it gives straight line.

Fig. 5.3 at t=0.66 h shows that in column above 30th stage (trays are numbered from top to bottom as shown in Fig. 3.1), separation is rapid. At the top, component 3 is almost totally separated from component 2 and 1. Below 30th stage, x_2 increases from stage 30 to 35, then decreases slightly from stage 35 to 40. This may be due to the fact that the amount of component 1 (heaviest component) carried up is smaller and reboiler holdup is very large as compared to the tray holdups. So still composition changes very slowly with the time.

In Fig.5.4 at time t=1.5 h, the front where component 3 builds up is moving upwards. At this time, it is around 25th stage. 35th stage onwards, separation of component 2 from the other components is continuously decreasing whereas x_1 is increasing 25th stage onwards.

In Fig.5.5 at time t=2.25 h, the front where component 3 builds up has further moved upwards. At this time, it is around 20th stage. 30th stage onwards, separation of component 2 from the other components is continuously decreasing whereas x_1 is increasing 10th stage onwards. So, it is similar to the profile obtained for time t = 1.5 h, but position of the front for component 3 has changed.

In Fig. 5.6 at time t=3.0 h, component 3 is missing as it was completely separated out. In the upper section component 2 is dominant and contributes to the second product (P_2).

In Fig. 5.7 at time t=3.75h, the front where component 2 builds up has started moving up which is around 35th stage. Above the front, x_2 is greater than x_1. So the product is rich in component 2.

In Fig. 5.8 at time t=4.5 h, the front has further moved up. It is now around 25th stage. Rest of the profile is similar to the profile at t = 3.75 h.

In Fig. 5.9 at time t=5.25 h component 2 has been totally separated and only component 1 is remaining in the column.

The results discussed above using the present model, considering the dynamic behaviour of the batch distillation column, were found in good agreement to the results obtained by *Quintero-Marmol and Luyben (1992)*, considering an approximate quasi-dynamic behaviour of the column.

In view of the foregoing discussion, it was observed that the estimator is good enough and will provide accurate estimation of the product compositions and compositions at other trays based on measured values of temperatures.

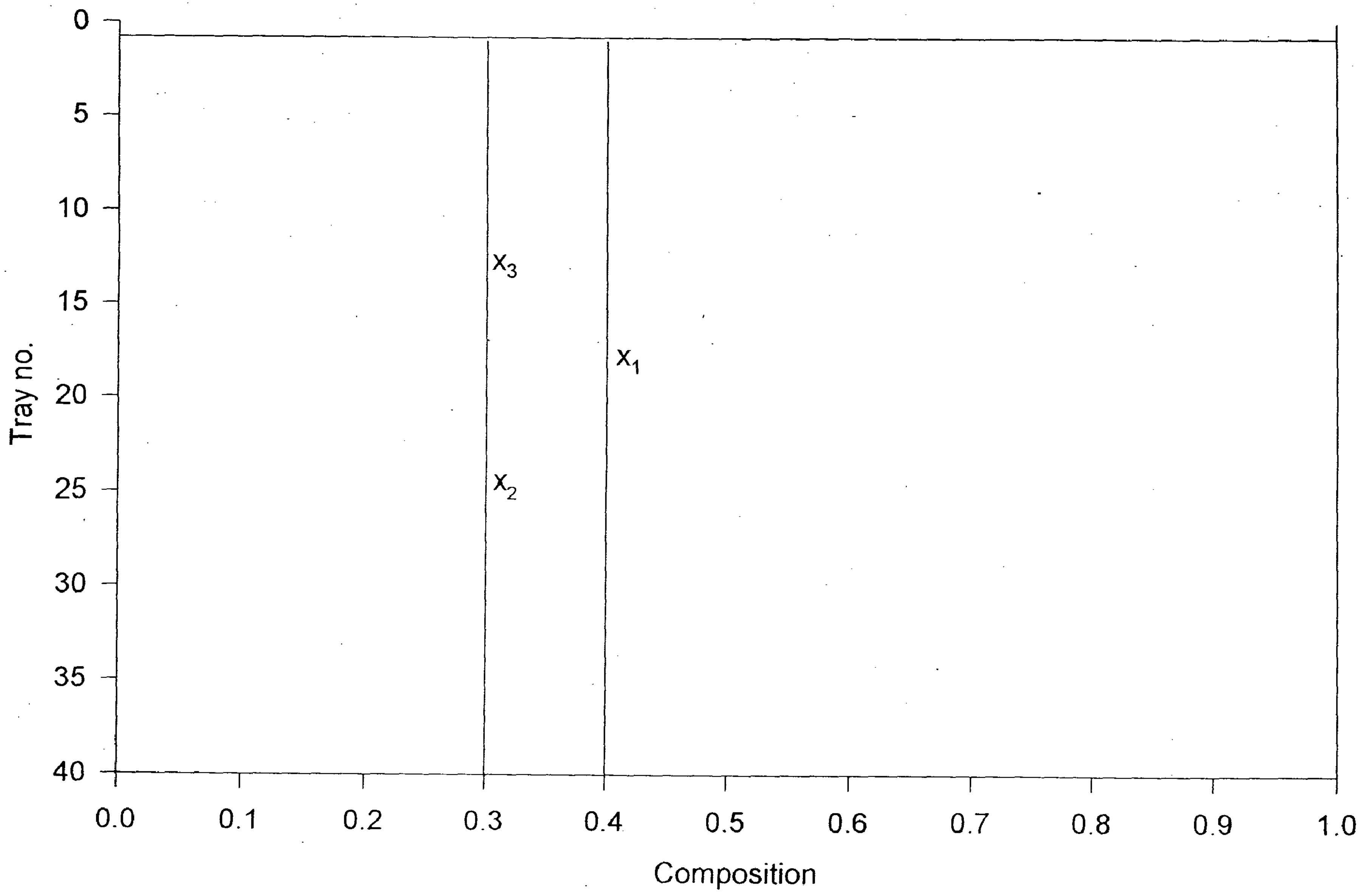


Fig. 5.2 Instantaneous column composition profile at time t=0.0 h

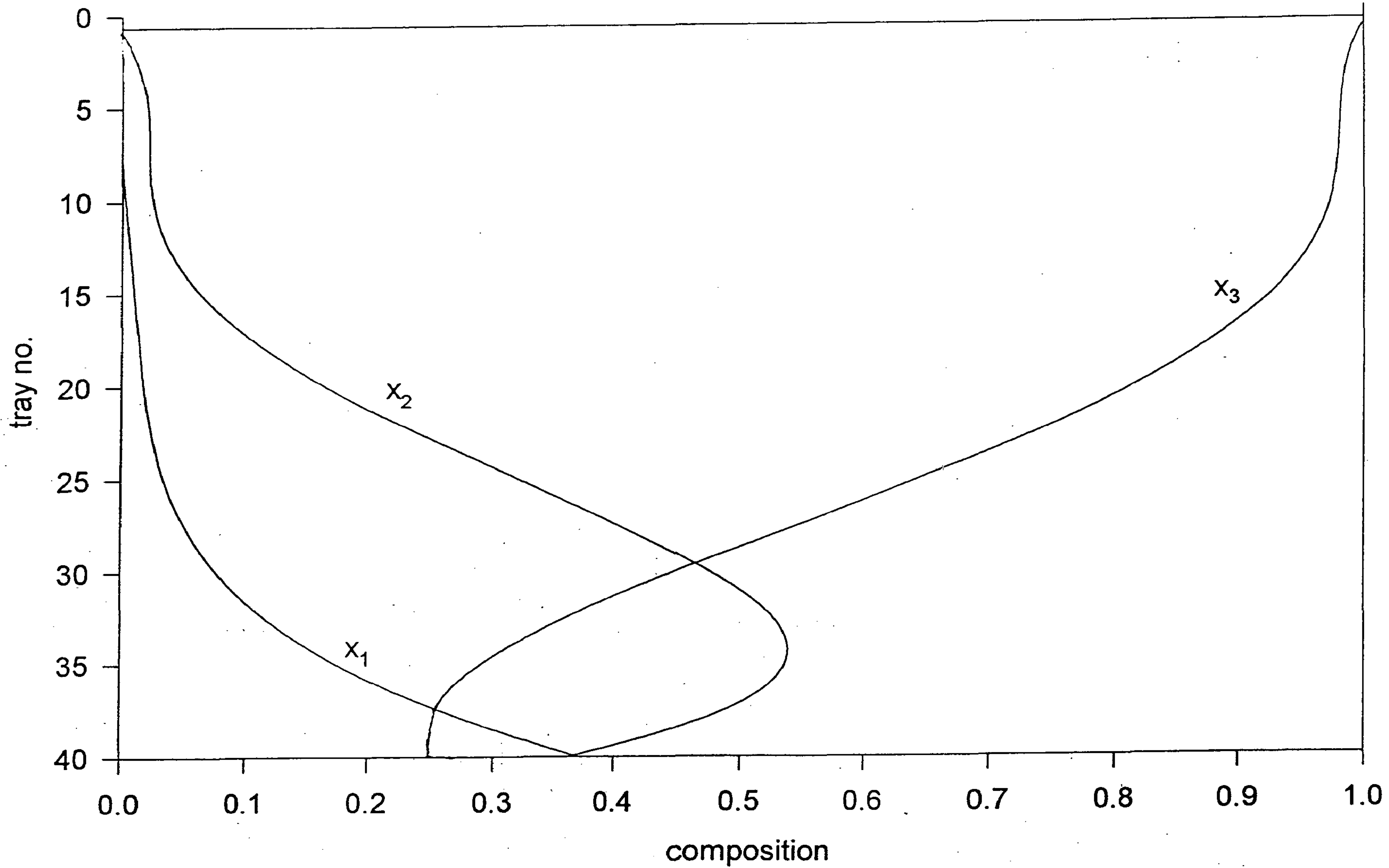


Fig. 5.3 Instantaneous column composition profile at time t=0.66 h

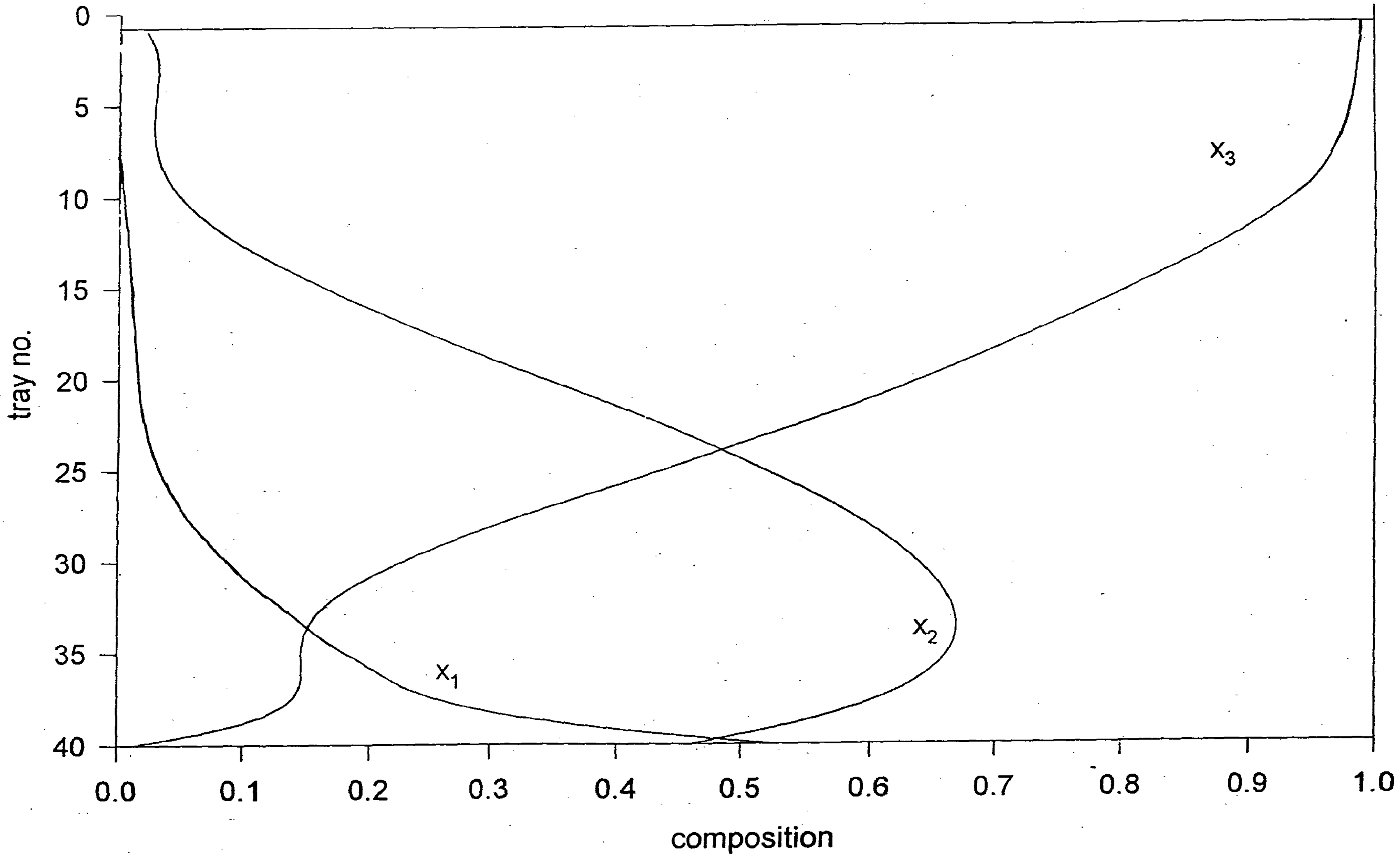


Fig. 5.4 Instantaneous column composition profile at time t=1.50 h

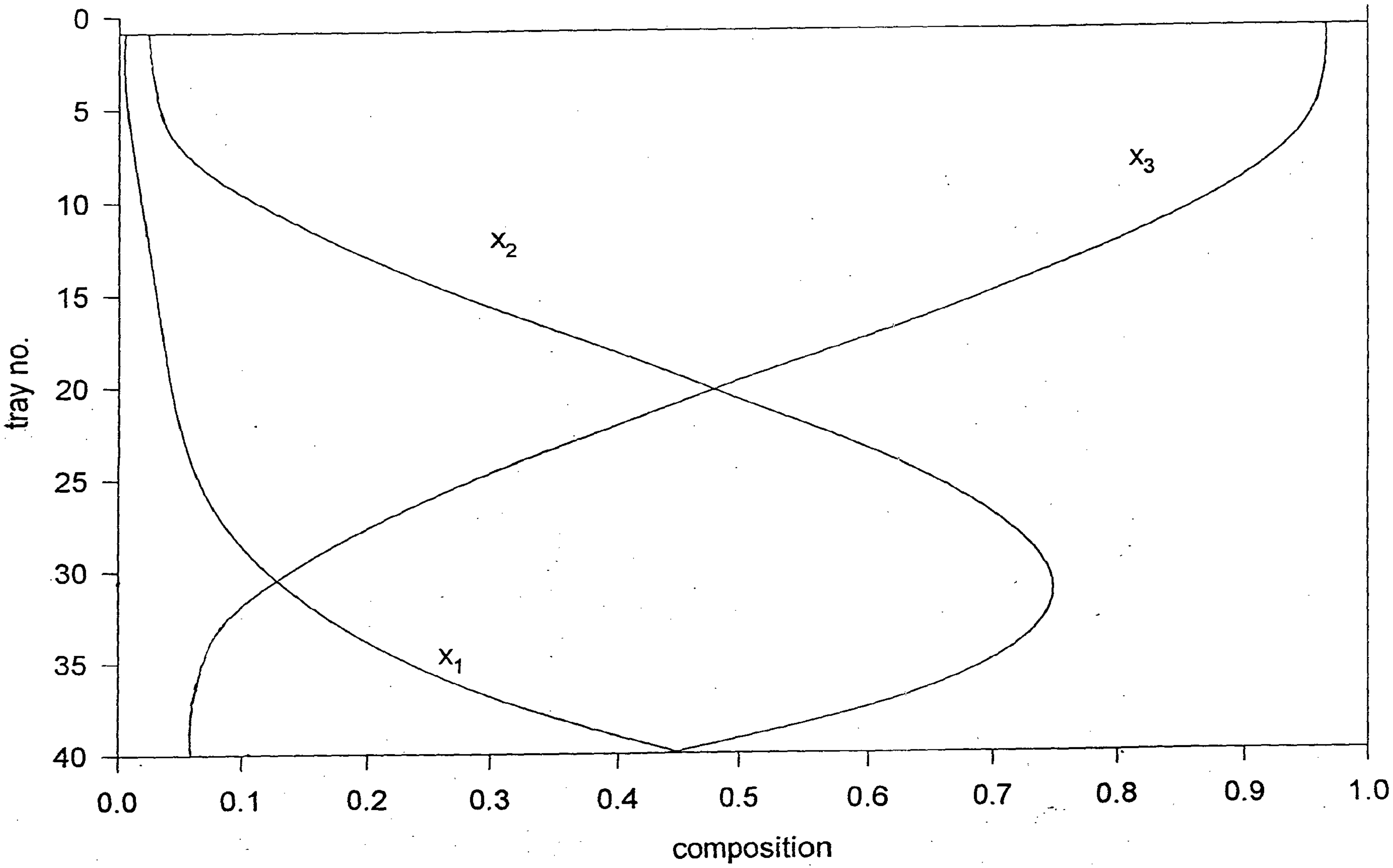


Fig. 5.5 Instantaneous column composition profile at time t=2.25 h

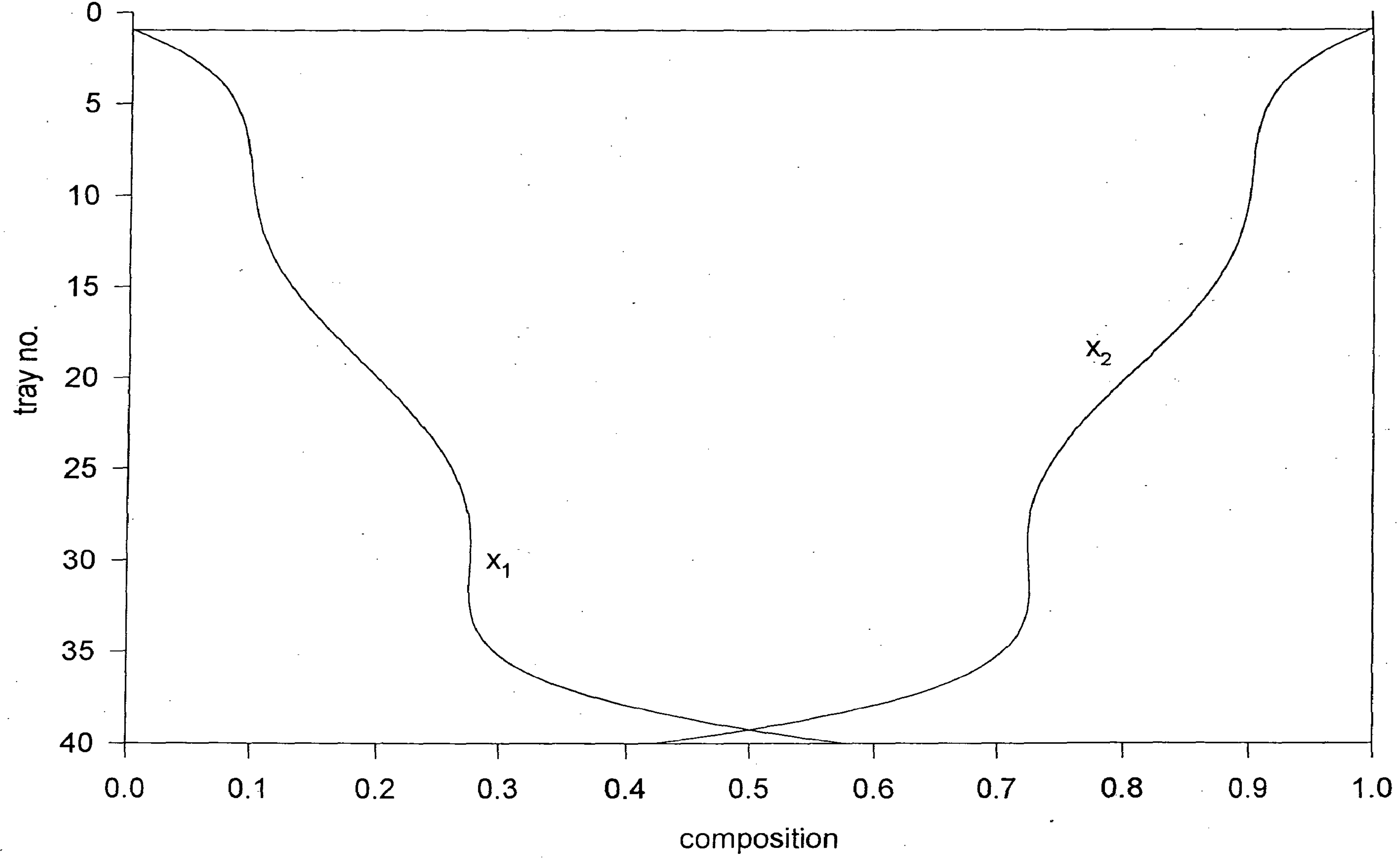


Fig. 5.6 Instantaneous column composition profile at time t=3.0 h

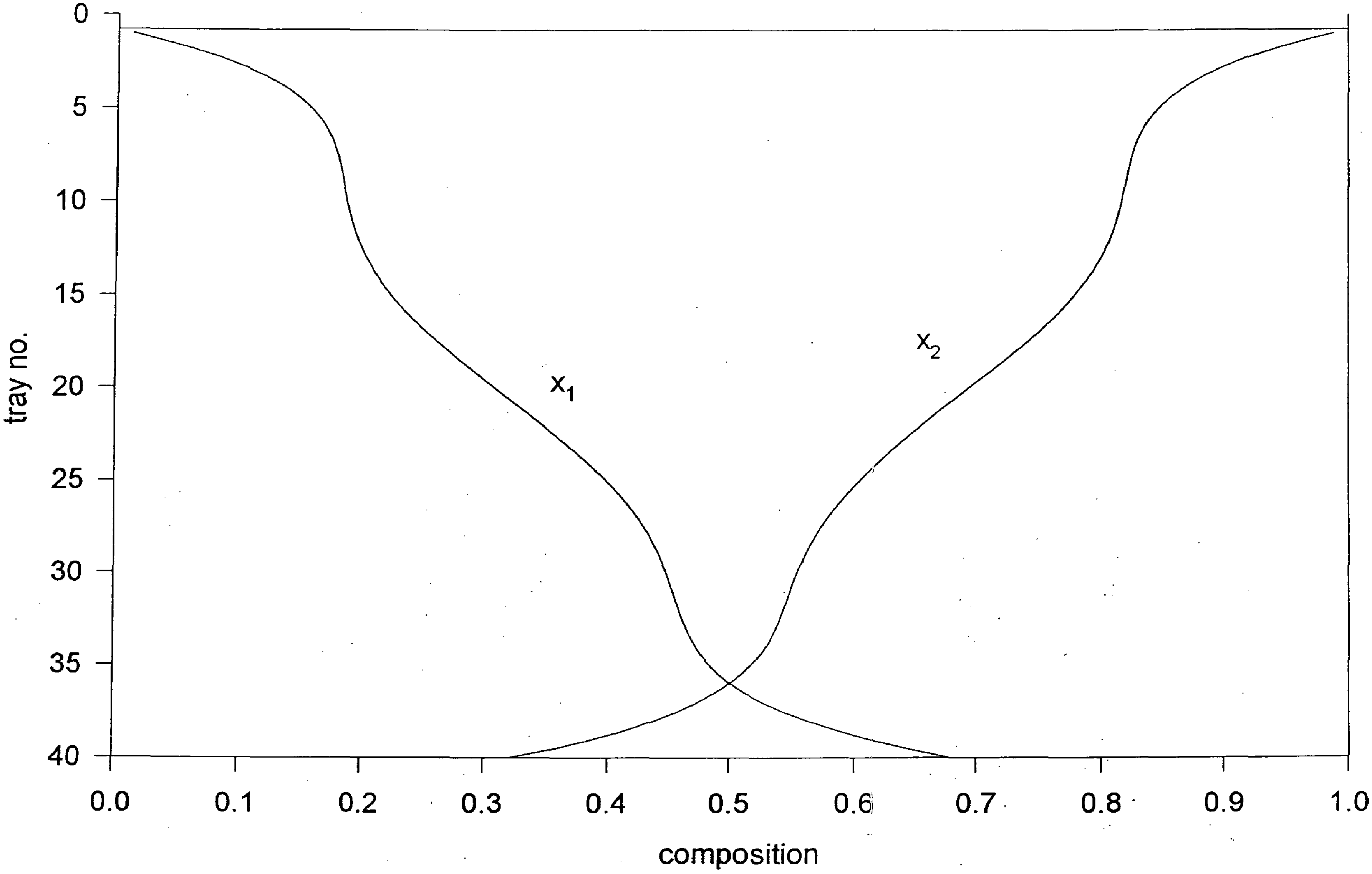


Fig. 5.7 Instantaneous column composition profile at time t=3.75 h

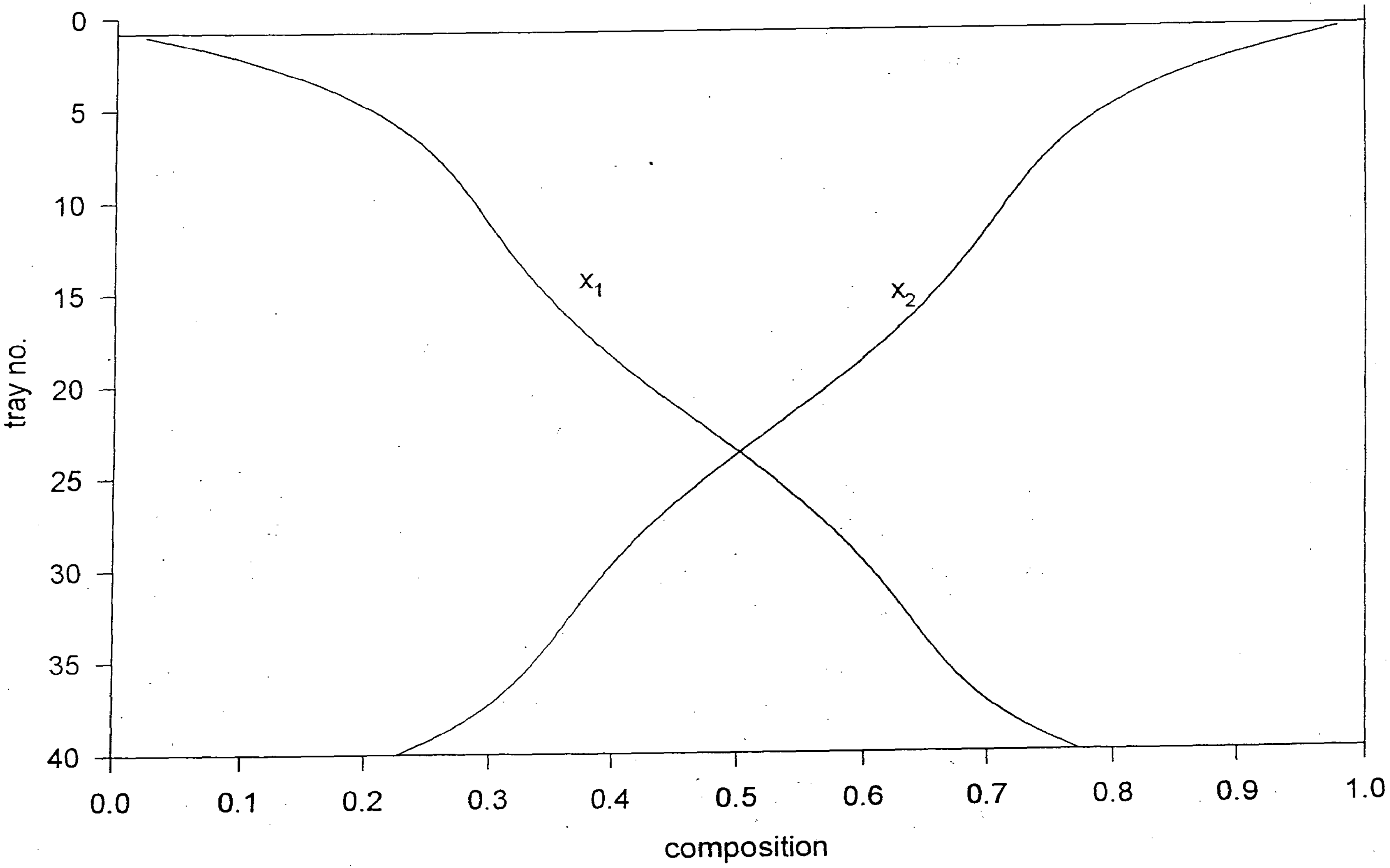


Fig. 5.8 Instantaneous column composition profile at time t=4.5 h

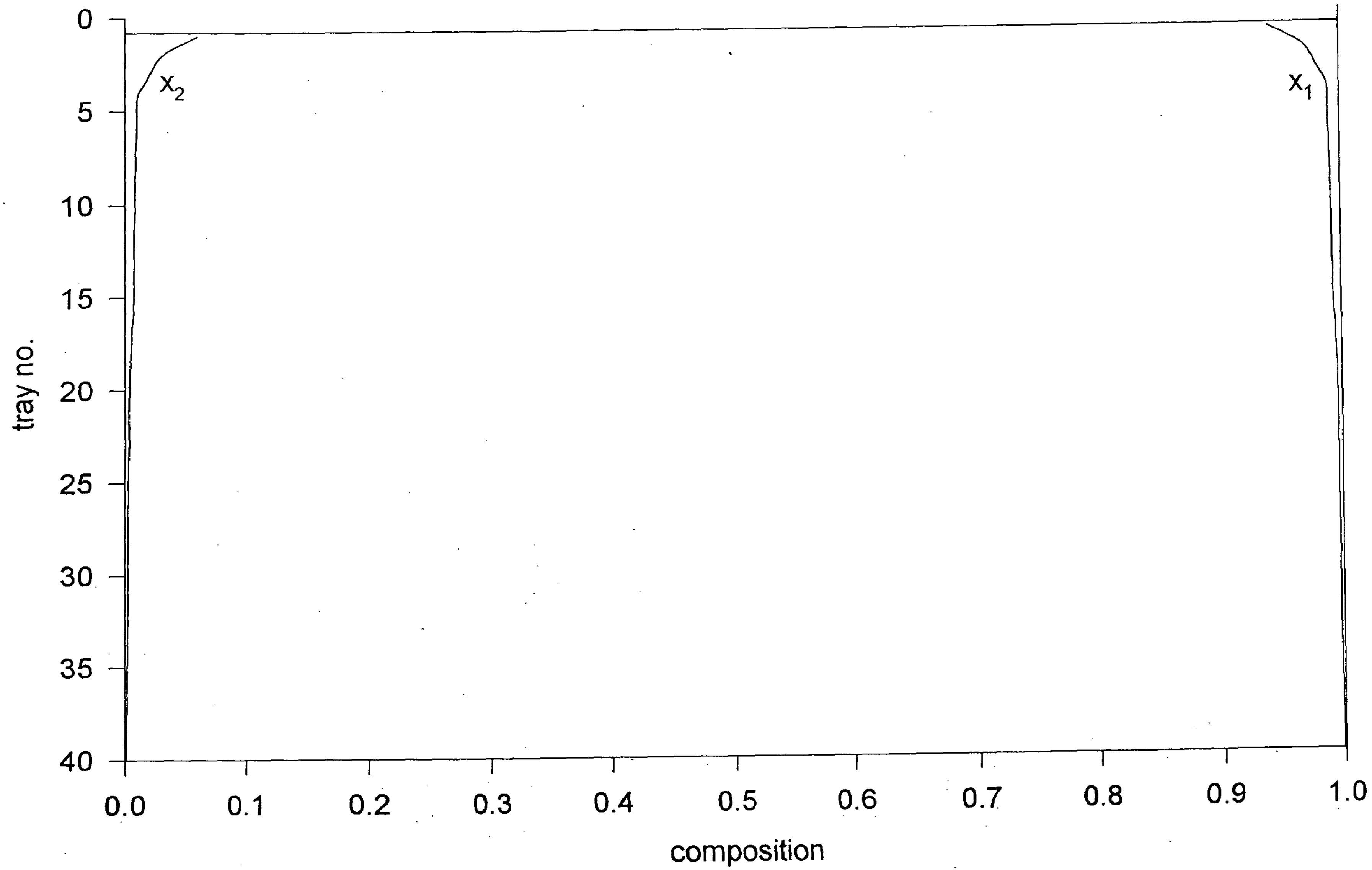


Fig. 5.9 Instantaneous column composition profile at time t=5.25 h

CONCLUSIONS AND RECOMMENDATIONS

CONCLUSIONS

1. A suitable and efficient estimator for a batch distillation column has been developed using a more realistic dynamic model of the column. The developed program can be used for estimating reasonable values of product compositions for all the three components at different times using measured values of tray temperatures.

2. The estimator being a critical component of the inferential control closed loop system of a batch distillation column, it may be further used for the design of the control system.

3. This estimator is general enough and may be used with some modifications for systems of more than three components.

RECOMMENDATIONS

1. Other elements of the closed loop control system of the batch distillation column such as process, measuring element, controller, control valve etc. may be modelled.

2. Using the models of the closed loop system, the response of inferential control may be studied.

3. Estimators, using enthalpy balance in the dynamic model may also be developed and studied to find its effects on the accuracy of the results.

4. A suitable adaptive control strategy may also be developed and studied.

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APPENDIX - A

/* Computer Program for Estimator for Start Up Period */

```
#include<iostream.h>
#include<iomanip.h>
#include<math.h>
#include<conio.h>

const int NP =40;
const int NC = 3;
void main()
{
int      j,i,j7,i6,k1,p1,q1;
double H[NP+2][NC+2],Kb[NP+2],K[NP+2][NC+2],TAU[NP+2],M[NP+2][NC+2];
double G[NP+2][NC+2],uc[NP+2][NC+2],v[NP+2][NC+2],l[NP+2][NC+2],SIG;
double Tt,Tb,h[NP+2],u[NP+2][NC+2],A[NP+2][NC+2],X[NP+2][NP+2],g[NP+2],SU;
float    ALPHA[NC+2],L[NP+2],V[NP+2],T[NP+2],y[NP+2][NC+2],U[NP+2],sum6 ;
float    BC[NC+2] , conv[NP+2], sum5[NP+2], ntheta[NP+2] ,nT[NP+2], Yc[NP+2];
float    x[NP+2][NC+2],d[NC+2],P[NP+2][NC],theta[NP+2],dc[NC+2],t1,sum9[NP+2];
float    ua[NP+2][NC+2],Uc[NP+2],la[NP+2][NC+2],Lc[NP+2], diff, sum8[NP+2];
float    va[NP+2][NC+2],Vc[NP+2],xa[NP+2][NC+2],Xc[NP+2],ya[NP+2][NC+2] ;
float    l1[NP+2][NP+2],gg[NP+2],u1[NP+2][NP+2],sum3[NC+2],s3[NC+2];
float    sum,sum1[NC+2],sum2[NP+2],s1[NC+2],s2[NC+2],sum7[NP+2];

/*       Input values   */

cout << "\nEnter the values of AC,F,D,t,DELTandPHI";
cout<<"AC = ";cin >> AC;
cout<<"F = ";cin >> F;
cout<<"D = ";cin >> D;
cout<<"t = ";cin >> t;
cout<<"DELT = ";cin >> DELT;
cout<<"PHI = ";cin >>PHI;
for(i=1;i<=NC;++i){
cout << "\nEnter the values of ALPHA[i]";
cout<<"ALPHA["<<i<<"] = ";
cin >> ALPHA[i];
cout << "\nEnter the values of BC[i]";
cout<<"BC["<<i<<"] = ";
cin >> BC[i];}
for(j=2;j<=NP-1;++j){
cout << "\nEnter the values of U[j]";
cout<<"\nU["<<j<<"] =";
cout<<U[j];}
for(j=2;j<=NP;++j){
cout << "\nEnter the values of V[j]";
cout<<"\nV["<<j<<"] =";
```

```
cout<<V[j];}
V[1]=D;
SIG=(1-PHI)/PHI;
for(j=1;j<=NP;++j) {
g[j]=0.002;
theta[j]=1;
conv[j]=0.2;}

/*      Initial estimation of temperatures  */

cout << "\nEnter the values of Tt and Tb";
cout<<"Tt =";
cin>>Tt;
cout<<"Tb =";
cin>>Tb;*/
T[1]=(((Tt-273.0)*9.0/5.0)+492.0);
T[NP] =(((Tb-273.0)*9.0/5.0)+492.0);
diff = (T[NP]-T[1])/(NP-1);
t1=T[1];
for( j=2;j<=NP;++j){
T[j]=t1+diff;
t1=T[j];}
for(j=1;j<=NP-1;++j)
SU +=U[j];
for(j=1;j<=NP-1;++j)
L[j]=V[j+1]-D;
U[NP]=F-SU-D*t;

for(int j=1;j<=NP;++j){
        while(conv[j] > 0.00001){

/*      Calculation of K's values for all components for all tray */
        for(j=1;j<=NP;++j){
                for(i=1;i<=NC;++i){
                K[j][i]=exp((AC/T[j])+BC[i]);
                y[j][i]=x[j][i]*K[j][i];}}

/*      Calculation of tridiagonal matrix form for vji's    */
        for(j=2;j<=NP;++j){
                for(i=1;i<=NC;++i)
                v[j][i]=y[j][i]*V[j];}
        for(i=1;i<=NC;++i)
        l[1][i]=v[2][i];
        for(i=1;i<=NC;++i)
        A[1][i]=1;
        for(j=2;j<=(NP-1);++j){
                for(i=1;i<=NC;++i)
                A[j][i]=L[j]/(K[j][i]*V[j]);}
```

```
for(i=1;i<=NC;++i)
u[1][i]=U[1]*v[2][i]/V[2];
for(j=2;j<=NP-1;++j){
        for(i=1;i<=NC;++i)
        u[j][i]=U[j]*A[j][i]*v[j][i]/L[j];}
for(i=1;i<=NC;++i){
u[NP][i]=U[NP]*y[NP][i]/K[NP][i];}
for(j=2;j<=NP-1;++j){
        for(i=1;i<=NC;++i){
        l[j][i]=A[j][i]*v[j][i];}}
for(j=1;j<=NP-1;++j){
        for(i=1;i<=NC;++i){
        TAU[j]=U[j]/(L[j]*PHI*DELT);}}
for(i=1;i<=NC;++i){
M[1][i]=-(1+TAU[1]);
M[NP][i]=-(1+U[NP]/(V[NP]*PHI*DELT*K[NP][i]));
P[1][i]=-(SIG*(v[2][i]-l[1][i])+u[1][i]/(PHI*DELT));
P[NP][i]=-(SIG*(l[NP-1][i]-v[NP][i])+u[NP][i]/(PHI*DELT));
H[1][i]=1/M[1][i];
G[1][i]=P[1][i]/M[1][i];}
for(j=2;j<=NP-1;++j){
        for(i=1;i<=NC;++i){
        M[j][i]=-(1+A[j][i]*(1+TAU[j]));
        P[j][i]=-(SIG*(v[j+1][i]+l[j-1][i]-v[j][i]-l[j][i])+u[j][i]/(PHI*DELT));
        H[j][i]=1/(M[j][i]-A[j-1][i]*H[j-1][i]);}}
for(j=2;j<=NP;++j){
        for(i=1;i<=NC;++i)
        G[j][i]=(P[j][i]-A[j-1][i]*G[j-1][i])/(M[j][i]-A[j-1][i]*H[j-1][i]);}
for(i=1;i<=NC;++i)
v[NP][i]=G[NP][i];
for(j=NP-1;j>=1;--j){
        for(i=1;i<=NC;++i){
        v[j][i]=G[j][i]-H[j][i]*v[j+1][i];}}
```

Calculation of θ_j's by Newton Raphson Method */

```
for(int j3=2;j3<=NP;++j3){
while(fabs(g[j3]) > 0.0001){
        for(int j3=2;j3<=NP;++j3)
        g[j3]=u[j3][1]+u[j3][2]+u[j3][3]-U[j3];
        for(i=1;i<=NC;++i){
                for(j=1;j<=NP;++j){
                sum3[i]+=u[j][i];}}
        for(j=2;j<=NP;++j){
                for(i=1;i<=NC;++i){
                sum9[j-2] + = (uc[j][i]*u[1][i]/uc[1][I])*
                                (1theta[j]*u[1][i]*uc[j][i])/(F*x[NP][i]*uc[1][i]));}
        X[j-2][j-2]=sum9[j-2];}
        for(int m2=2;m2<=NP;++m2){
```

```
                for(j=2;j<=NP;++j){
                if (m2!=j)
                X[m2-2][j-2] = -theta[m2]*(((uc[m2][1]*uc[j][1]*u[1][1]*u[1][1])
                            /(uc[1][1]*uc[1][1]*F*x[NP][1]))+((uc[m2][2]
                            *uc[j][2]*u[1][2]*u[1][2])/(uc[1][2]*uc[1][2]*F*
                            x[NP][2]))+((uc[m2][3]*uc[j][3]*u[1][3]*u[1][3])/
                            (uc[1][3]*uc[1][3]*F*x[NP][3])));
                            }
                    }

LU Decomposition Method */
        for(i6=0;i6<NP-1;++i6){
        l1[i6][0]=X[i6][0];}
        for(j7=0;j7<NP-1;++j7){
        u1[0][j7]=X[0][j7]/X[0][0];}
        for(j7=1;j7<NP-1;++j7){
                for(i6=j7;i6<=NP-1;++i6){
                sum=0.0;
                        for(k1=0;k1<j7;++k1){
                        sum=sum+l1[i6][k1]*u1[k1][j7];}
                l1[i6][j7]=X[i6][j7]-sum;}
        p1=j7;
        for(q1=0;q1<NP-1;++q1){
        sum=0.0;
                for(k1=0;k1<p1;++k1){
                sum=sum+l1[p1][k1]*u1[k1][q1];}
        u1[p1][q1]=(X[p1][q1]-sum)/l1[p1][p1];}}
        gg[0]=g[0]/l1[0][0];
        for(i6=1;i6<NP-1;++i6){
        sum=0.0;
                for(k1=0;k1<i6;++k1){
                sum=sum+l1[i6][k1]*gg[k1];}
        gg[i6]=(g[i6]-sum)/l1[i6][i6];}
        h[NP-2]=(gg[NP-2]);
        for(j7=NP-3;j7>=0;--j7){
        sum=0.0;
                for(k1=j7+1;k1<NP-1;++k1){
                sum=sum+u1[j7][k1]*h[k1];}
        h[j7]=(gg[j7]-sum);}
         for(j=2;j<=NP;++j){
        ntheta[j]=theta[j]+h[j-1];}
        for(j=2;j<=NP;++j){
                while ( ntheta[j]<0.0){
                h[j-1]=h[j-1]/2;
                ntheta[j]=theta[j]+h[j-1];}}
        for(j=2;j<=NP;++j){
        theta[j]=ntheta[j];}
        for(i=1;i<=NC;++i){
```

```
                        for(j=2;j<=NP;++j){
                        sum2[i]+=theta[j]*uc[j][i]/uc[1][i];}}
                for(i=1;i<=NC;++i){
                s2[i]=1+sum2[i];}
                for(i=1;i<=NC;++i){
                u[1][i]=F*x[NP][i]/s2[i];}}
        }

/*      Calculation of corrected xji's */

        for(j=2;j<=NP;++j){
                for(i=1;i<=NC;++i){
                u[j][i]=theta[j]*u[1][i]*uc[j][i]/uc[1][i];}}
        for(j=1;j<=NP;++j){
                for(i=1;i<=NC;++i){
                uc[j][i]=u[j][i];}}
        for(j=1;j<=NP;++j){
                for(i=1;i<=NC;++i){
                sum5[j] +=u[1][i]*uc[j][i]/uc[1][i];}}
        for(j=1;j<=NP;++j){
                for(i=1;i<=NC;++i){
                xa[j][i]=uc[j][i]*u[1][i]/(uc[1][i]*sum5[j]);}}
        for(j=1;j<=NP;++j){
                for(i=1;i<=NC;++i){
                Xc[j]+=xa[j][i];}}
        for(j=1;j<=NP;++j){
                for(i=1;i<=NC;++i){
                x[j][i]=xa[j][i]/Xc[j];}}

/*      Calculation of the corrected temperature profile (or Kb Method)

                for(j=1;j<=NP;++j){
        Kb[j]=1/(ALPHA[1]*x[j][1]+ALPHA[2]*x[j][2]+ALPHA[3]*x[j][3]);}
                for(j=1;j<=NP;++j){
                nT[j]=AC/(log(Kb[j]*ALPHA[1])-BC[1]);
                conv[j]=fabs(nT[j]-T[j])/T[j];
                T[j]=nT[j];}
        }
}
/*      Vapor composition for all components at every tray*/

for(j=1;j<=NP;++j){
        for(i=1;i<=NC;++i){
        ya[j][i]=ALPHA[i]*Kb[j]*x[j][i];}}
for(j=1;j<=NP;++j){
        for(i=1;i<=NC;++i){
        Yc[j]+=ya[j][i];}}
for(j=1;j<=NP;++j){
```

```
        for(i=1;i<=NC;++i){
        y[j][i]=ya[j][i]/Yc[j];}}

for(j=1;j<=NP;++j){
        for(i=1;i<=NC;++i){
        cout<< "y["<<j<<"]"<<"["<<i<<"]=";
        cout<< y[j][i];
        cout<<";";}
cout<<endl;}
cout<<endl;
for(j=1;j<=NP;++j){
        for(i=1;i<=NC;++i){
        cout<< "x["<<j<<"]"<<"["<<i<<"]=";
        cout<< x[j][i];
        cout<<";";}
cout<< "T["<<j<<"]=";
cout<< T[j]<<";";
cout<<endl;}
cout<<"\nU[NP] = "<<U[NP];
getche();
}
```

```
/* Computer Program for Estimator for Product Period */

#include<iostream.h>
#include<iomanip.h>
#include<math.h>
#include<conio.h>

const int NP =40;
const int NC = 3;
void main()
{
int     j,i,j7,i6,k1,p1,q1;
double BC[NC+2],H[NP+2][NC+2],Kb[NP+2],K[NP+2][NC+2],TAU[NP+2];
double G[NP+2][NC+2],uc[NP+2][NC+2],v[NP+2][NC+2],l[NP+2][NC+2],SIG;
double Tt,Tb,h[NP+2],u[NP+2][NC+2],A[NP+2][NC+2],X[NP+2][NP+2],g[NP+2],SU;
float   ALPHA[NC+2],L[NP+2],V[NP+2],T[NP+2],y[NP+2][NC+2],U[NP+2],sum6 ;
float   x[NP+2][NC+2],diff, conv[NP+2], M[NP+2][NC+2], ua[NP+2][NC+2], sum;
float   dc[NC+2],d[NC+2],P[NP+2][NC],theta[NP+2], sum5[NP+2],t1,sum9[NP+2];
float   Uc[NP+2],la[NP+2][NC+2],Lc[NP+2],nT[NP+2],ntheta[NP+2] ,sum8[NP+2];
float   va[NP+2][NC+2],Vc[NP+2],xa[NP+2][NC+2],Xc[NP+2],ya[NP+2][NC+2] ;
float   l1[NP+2][NP+2],gg[NP+2],u1[NP+2][NP+2],sum3[NC+2],s3[NC+2];
float   ;sum1[NC+2],sum2[NP+2],s1[NC+2],s2[NC+2],sum7[NP+2] ,Yc[NP+2];

/*      Input values   */

cout << "\nEnter the values of AC,F,D,t,DELTandPHI";
cout<<"AC = ";cin >> AC;
cout<<"F = ";cin >> F;
cout<<"D = ";cin >> D;
cout<<"t = ";cin >> t;
cout<<"DELT = ";cin >> DELT;
cout<<"PHI = ";cin >>PHI;
for(i=1;i<=NC;++i){
cout << "\nEnter the values of ALPHA[i]";
cout<<"ALPHA["<<i<<"] = ";
cin >> ALPHA[i];
cout << "\nEnter the values of BC[i]";
cout<<"BC["<<i<<"] = ";
cin >> BC[i];}
for(j=2;j<=NP-1;++j){
cout << "\nEnter the values of U[j]";
cout<<"\nU["<<j<<"] =";
cout<<U[j];}
for(j=2;j<=NP;++j){
cout << "\nEnter the values of V[j]";
cout<<"\nV["<<j<<"] =";
cout<<V[j];}
V[1]=D;
```

```
SIG=(1-PHI)/PHI;
for(j=1;j<=NP;++j) {
g[j]=0.002;
theta[j]=1;
conv[j]=0.2;}

/*      Initial estimation of temperatures  *

cout << "\nEnter the values of Tt and Tb";
cout<<"Tt =";
cin>>Tt;
cout<<"Tb =";
cin>>Tb;*/
T[1]=(((Tt-273.0)*9.0/5.0)+492.0);
T[NP] =(((Tb-273.0)*9.0/5.0)+492.0);
diff = (T[NP]-T[1])/(NP-1);
t1=T[1];
for( j=2;j<=NP;++j){
T[j]=t1+diff;
t1=T[j];}
for(j=1;j<=NP-1;++j)
SU +=U[j];
for(j=1;j<=NP-1;++j)
L[j]=V[j+1]-D;
U[NP]=F-SU-D*t;

for(int j=1;j<=NP;++j){
        while(conv[j] > 0.00001){

        Calculation of K's values for all components for all tray */
        for(j=1;j<=NP;++j){
                for(i=1;i<=NC;++i){
                K[j][i]=exp((AC/T[j])+BC[i]);
                y[j][i]=x[j][i]*K[j][i];}}

        Calculation of tridiagonal matrix form for di's and vji's  */
                for(i=1;i<=NC;++i){
                v[1][i]=D*y[1][i];
                d[i]=v[1][i];}
                for(j=2;j<=NP;++j){
                        for(i=1;i<=NC;++i)
                        v[j][i]=y[j][i]*V[j];}
                for(i=1;i<=NC;++i)
                A[1][i]=L[1]/K[1][i]*D;
                for(j=2;j<=(NP-1);++j){
                        for(i=1;i<=NC;++i)
                        A[j][i]=L[j]/(K[j][i]*V[j]);}
                for(j=1;j<=NP-1;++j){
```

```
        for(i=1;i<=NC;++i)
        u[j][i]=U[j]*A[j][i]*v[j][i]/L[j];}
    for(i=1;i<=NC;++i){
    u[NP][i]=U[NP]*y[NP][i]/K[NP][i];}
    for(j=1;j<=NP-1;++j){
        for(i=1;i<=NC;++i){
        l[j][i]=A[j][i]*v[j][i];
        TAU[j]=U[j]/(L[j]*PHI*DELT);}}
    for(j=1;j<=NP;++j){
        for(i=1;i<=NC;++i)
        uc[j][i]=u[j][i];}
    for(i=1;i<=NC;++i){
    M[1][i]=-(1+TAU[1]);
    M[NP][i]=-(1+U[NP]/(V[NP]*PHI*DELT*K[NP][i]));
    d[i]=v[1][i];
    P[1][i]=-(SIG*(v[2][i]-l[1][i]-d[i])+u[1][i]/(PHI*DELT));
    P[NP][i]=-(SIG*(l[NP-1][i]-v[NP][i])+u[NP][i]/(PHI*DELT));
    H[1][i]=1/M[1][i];
    G[1][i]=P[1][i]/M[1][i];}
    for(j=2;j<=NP-1;++j){
        for(i=1;i<=NC;++i){
        M[j][i]=-(1+A[j][i]*(1+TAU[j]));
        P[j][i]=-(SIG*(v[j+1][i]+l[j-1][i]-v[j][i]-l[j][i])+u[j][i]/
                (PHI*DELT));
        H[j][i]=1/(M[j][i]-A[j-1][i]*H[j-1][i]);}}
    for(j=2;j<=NP;++j){
        for(i=1;i<=NC;++i)
        G[j][i]=(P[j][i]-A[j-1][i]*G[j-1][i])/(M[j][i]-A[j-1][i]*H[j-1][i]);}
    for(i=1;i<=NC;++i)
    v[NP][i]=G[NP][i];
    for(j=NP-1;j>=1;--j){
        for(i=1;i<=NC;++i){
        v[j][i]=(G[j][i]-H[j][i]*v[j+1][i]);}}
    for(i=1;i<=NC;++i)
    dc[i]=v[1][i];
    for(i=1;i<=NC;++i)
    dc[i]=d[i]*D/(d[1]+d[2]+d[3]);
```

Calculation of θ_j's by Newton Raphson Method */

```
    for(int j3=0;j3<NP;++j3){
        while(fabs(g[j3]) > 0.0001){
        sum=0.0;
            for(int i3=1;i3<=NC;++i3)
            sum = sum+dc[i3];
            g[0]=sum-D;
            for(int j3=1;j3<NP;++j3)
            g[j3]=u[j3][1]+u[j3][2]+u[j3][3]-U[j3];
            for(i=1;i<=NC;++i){
```

```
          for(j=1;j<=NP;++j){
          sum3[i]+=u[j][i];}}
for(i=1;i<=NC;++i)
 s3[i]=(-SIG*dc[i]*PHI*DELT)+sum3[i];
for(i=1;i<=NC;++i){
sum6 += -(d[i]*d[i]*u[NP][i])/(s3[i]*dc[i]);}
X[0][0]=sum6;

for(j=1;j<NP;++j){
          for(i=1;i<=NC;++i){
          sum7[j] += -(d[i]*d[i]*u[j][i])/(s3[i]*dc[i]);}
 X[0][j]=sum7[j];}

for(int m1=1;m1<NP;++m1){
          for(i=1;i<=NC;++i){
          sum8[m1] + =(-theta[m1+1]*u[m1][i]*u[NP][i]*
                    d[i]*d[i])/(dc[i]*dc[i]*s3[i]);}
X[m1][0]=sum8[m1];}

for(j=1;j<NP;++j){
          for(i=1;i<=NC;++i){
          sum9[j] + = u[j][i]*d[i]*(1-(theta[j+1]*d[i]*u[j][i])/
                    (s3[i]*dc[i]))/dc[i];}
X[j][j]=sum9[j];}

for(int m2=1;m2<NP;++m2){
          for(j=1;j<NP;++j){
          if (m2!=j)
          X[m2][j]=-theta[m2+1]*(((u[m2][1]*u[j][1]*d[1]
                    *d[1])/(dc[1]*dc[1]*s3[1]))+
                  ((u[m2][2]*u[j][2]*d[2]*d[2])dc[2]*dc[2]*
                  s3[2]))+((u[m2][3]*u[j][3]*d[3]*d[3])/
                  (dc[3]*dc[3]*s3[3])));}}
```

LU Decomposition Method */

```
for(i6=0;i6<NP;++i6){
l1[i6][0]=X[i6][0];}
for(j7=0;j7<NP;++j7){
u1[0][j7]=X[0][j7]/X[0][0];}
for(j7=1;j7<NP;++j7){
          for(i6=j7;i6<=NP;++i6){
          sum=0.0;
                    for(k1=0;k1<j7;++k1){
                    sum=sum+l1[i6][k1]*u1[k1][j7]; }
          l1[i6][j7]=X[i6][j7]-sum;}
p1=j7;
for(q1=0;q1<NP;++q1){
```

```
            sum=0.0;
                for(k1=0;k1<p1;++k1){
                sum=sum+l1[p1][k1]*u1[k1][q1];}
            u1[p1][q1]=(X[p1][q1]-sum)/l1[p1][p1];}}
            gg[0]=g[0]/l1[0][0];
            for(i6=1;i6<NP;++i6){
            sum=0.0;
                for(k1=0;k1<i6;++k1){
                sum=sum+l1[i6][k1]*gg[k1];}
            gg[i6]=(g[i6]-sum)/l1[i6][i6];}
            h[NP-1]=(gg[NP-1]);

            for(j7=NP-2;j7>=0;--j7){
            sum=0.0;
                for(k1=j7+1;k1<NP;++k1){
                sum=sum+u1[j7][k1]*h[k1];}
                h[j7]=(gg[j7]-sum);}
            for(j=1;j<=NP;++j){
            ntheta[j]=theta[j]+h[j-1];}
            for(j=1;j<=NP;++j){
                while ( ntheta[j]<0.0){
                h[j-1]=h[j-1]/2;
                ntheta[j]=theta[j]+h[j-1];}}
            for(j=1;j<=NP;++j){
            theta[j]=ntheta[j];}

alculation of corrected di's and xji's */
            for(i=1;i<=NC;++i){
                for(j=1;j<=NP;++j){
                sum1[i]+=u[j][i];}
            s1[i]=-SIG*dc[i]+sum1[i]/(PHI*DELT);}
            for(i=1;i<=NC;++i){
                for(j=2;j<=NP;++j){
                sum2[i]+=theta[j]*u[j-1][i]/dc[i];}}
            for(i=1;i<=NC;++i){
            s2[i]=1+((theta[1]*u[NP][i]/dc[i])+sum2[i])/(PHI*DELT);}
            for(i=1;i<=NC;++i){
            d[i]=s1[i]/s2[i];}
        }
    }
    for(j=1;j<NP;++j){
        for(i=1;i<=NC;++i){
        u[j][i]=theta[j+1]*d[i]*uc[j][i]/dc[i];}}
    for(i=1;i<=NC;++i){
    u[NP][i]=d[i]*theta[1]*uc[NP][i]/dc[i];}
    for(j=1;j<=NP;++j){
        for(i=1;i<=NC;++i){
        uc[j][i]=u[j][i];}}
```

```
        for(j=1;j<=NP;++j){
            for(i=1;i<=NC;++i){
            sum5[j] +=dc[i]*u[j][i]/d[i];}}
        for(j=1;j<=NP;++j){
            for(i=1;i<=NC;++i){
            xa[j][i]=u[j][i]*d[i]/(dc[i]*sum5[j]);}}
        xa[NP][1]=(l[NP-1][1]+U[NP]*x[NP][1])/(L[NP-1]+U[NP]);
        for(j=1;j<=NP;++j){
            for(i=1;i<=NC;++i){
            Xc[j]+=xa[j][i];}}
        for(j=1;j<=NP;++j){
            for(i=1;i<=NC;++i){
            x[j][i]=xa[j][i]/Xc[j];}}
```

Calculation of the corrected temperature profile (or Kb Method)

```
        for(j=1;j<=NP;++j){

    Kb[j]=1/(ALPHA[1]*x[j][1]+ALPHA[2]*x[j][2]+ALPHA[3]*x[j][3]);}
        for(j=1;j<=NP;++j){
        nT[j]=AC/(log(Kb[j]*ALPHA[1])-BC[1]);
        conv[j]=fabs(nT[j]-T[j])/T[j];
        T[j]=nT[j];}
    }
```

Vapor composition for all components at every tray*/

```
    for(j=1;j<=NP;++j){
        for(i=1;i<=NC;++i){
        ya[j][i]=ALPHA[i]*Kb[j]*x[j][i];}
    for(j=1;j<=NP;++j){
        for(i=1;i<=NC;++i){
        Yc[j]+=ya[j][i];}}
    for(j=1;j<=NP;++j){
        for(i=1;i<=NC;++i){
        y[j][i]=ya[j][i]/Yc[j];}}
    for(i=1;i<=NC;++i){
    d[i]=y[1][i]*D;
    cout<<"d["<<i<<"]="<<d[i]<<", ";}
    cout<<endl;

for(j=1;j<=NP;++j){
    for(i=1;i<=NC;++i){
    cout<< "y["<<j<<"]"<<"["<<i<<"]=";
    cout<< y[j][i];
    cout<<";";}
    cout<<endl;}
cout<<endl;
```

```
 for(j=1;j<=NP;++j){
          for(i=1;i<=NC;++i){
          cout<< "x["<<j<<"]"<<"["<<i<<"]=";
          cout<< x[j][i];
          cout<<";";}
cout<< "T["<<j<<"]=";
cout<< T[j]<<";";
cout<<endl;}
cout<<"\nU[NP] = "<<U[NP];
getche();
}
```

APPENDIX - B

Table B-1

Response of the estimator to obtain column compositions for the system α=1/3/9 , product purity = 95%,at time t = 0.0 h

Tray No.	X_1	X_2	X_3
1	0.4000	0.3000	0.3000
2	0.4000	0.3000	0.3000
3	0.4000	0.3000	0.3000
4	0.4000	0.3000	0.3000
5	0.4000	0.3000	0.3000
6	0.4000	0.3000	0.3000
7	0.4000	0.3000	0.3000
8	0.4000	0.3000	0.3000
9	0.4000	0.3000	0.3000
10	0.4000	0.3000	0.3000
11	0.4000	0.3000	0.3000
12	0.4000	0.3000	0.3000
13	0.4000	0.3000	0.3000
14	0.4000	0.3000	0.3000
15	0.4000	0.3000	0.3000
16	0.4000	0.3000	0.3000
17	0.4000	0.3000	0.3000
18	0.4000	0.3000	0.3000
19	0.4000	0.3000	0.3000
20	0.4000	0.3000	0.3000
21	0.4000	0.3000	0.3000
22	0.4000	0.3000	0.3000
23	0.4000	0.3000	0.3000
24	0.4000	0.3000	0.3000
25	0.4000	0.3000	0.3000
26	0.4000	0.3000	0.3000
27	0.4000	0.3000	0.3000
28	0.4000	0.3000	0.3000
29	0.4000	0.3000	0.3000
30	0.4000	0.3000	0.3000
31	0.4000	0.3000	0.3000
32	0.4000	0.3000	0.3000
33	0.4000	0.3000	0.3000
34	0.4000	0.3000	0.3000
35	0.4000	0.3000	0.3000
36	0.4000	0.3000	0.3000
37	0.4000	0.3000	0.3000
38	0.4000	0.3000	0.3000
39	0.4000	0.3000	0.3000
40	0.4000	0.3000	0.3000

Table B-2

Response of the estimator to obtain column compositions for the system α=1/3/9,product purity = 95%,at time t = 0.66 h

Tray No.	X_1	X_2	X_3
1	0.0001	0.0100	0.9899
2	0.0002	0.0099	0.9899
3	0.0003	0.0098	0.9899
4	0.0010	0.0101	0.9889
5	0.0020	0.0151	0.9829
6	0.0030	0.0151	0.9818
7	0.0040	0.0151	0.9808
8	0.0040	0.0161	0.9798
9	0.0050	0.0172	0.9778
10	0.0050	0.0182	0.9768
11	0.0055	0.0202	0.9743
12	0.0050	0.0202	0.9748
13	0.0061	0.0303	0.9637
14	0.0071	0.0403	0.9526
15	0.0081	0.1008	0.8911
16	0.0091	0.1008	0.8901
17	0.0101	0.1511	0.8388
18	0.0111	0.1511	0.8378
19	0.0121	0.1511	0.8368
20	0.0131	0.1511	0.8358
21	0.0141	0.1612	0.8247
22	0.0151	0.1712	0.8136
23	0.0151	0.2014	0.7835
24	0.0201	0.3018	0.6780
25	0.0201	0.3520	0.6279
26	0.0302	0.3519	0.6179
27	0.0502	0.4020	0.5478
28	0.0703	0.4219	0.5078
29	0.0904	0.4519	0.4578
30	0.1004	0.4518	0.4478
31	0.1104	0.5017	0.3879
32	0.1204	0.5117	0.3679
33	0.1304	0.5216	0.3480
34	0.1504	0.5315	0.3181
35	0.1805	0.5314	0.2882
36	0.1905	0.5313	0.2782
37	0.2005	0.5213	0.2782
38	0.2406	0.5012	0.2583
39	0.2506	0.4911	0.2583
40	0.4736	0.2767	0.2497

Table B-3

Response of the estimator to obtain column compositions for the system α=1/3/9,product purity = 95%,at time t = 1.50 h

Tray No.	X_1	X_2	X_3
1	0.0003	0.0251	0.9747
2	0.0005	0.0248	0.9747
3	0.0008	0.0246	0.9747
4	0.0025	0.0253	0.9722
5	0.0050	0.0376	0.9574
6	0.0075	0.0375	0.9550
7	0.0100	0.0375	0.9525
8	0.0100	0.0399	0.9501
9	0.0125	0.0423	0.9453
10	0.0124	0.0447	0.9429
11	0.0136	0.0495	0.9369
12	0.0124	0.0495	0.9381
13	0.0146	0.0730	0.9123
14	0.0168	0.0958	0.8874
15	0.0176	0.2199	0.7625
16	0.0198	0.2196	0.7606
17	0.0206	0.3083	0.6711
18	0.0226	0.3079	0.6695
19	0.0247	0.3075	0.6678
20	0.0267	0.3071	0.6662
21	0.0284	0.3231	0.6485
22	0.0300	0.3387	0.6313
23	0.0289	0.3845	0.5866
24	0.0343	0.5133	0.4523
25	0.0326	0.5691	0.3983
26	0.0484	0.5635	0.3881
27	0.0755	0.6025	0.3220
28	0.1020	0.6101	0.2880
29	0.1255	0.6258	0.2487
30	0.1383	0.6205	0.2412
31	0.1448	0.6562	0.1990
32	0.1554	0.6588	0.1858
33	0.1658	0.6612	0.1730
34	0.1869	0.6585	0.1546
35	0.2193	0.6438	0.1369
36	0.2297	0.6390	0.1312
37	0.2418	0.6270	0.1312
38	0.2859	0.5940	0.1201
39	0.2978	0.5821	0.1201
40	0.5732	0.4268	0.0000

Table B-4

Response of the estimator to obtain column compositions for the system α=1/3/9,product purity = 95%,at time t = 2.25 h

Tray No.	X_1	X_2	X_3
1	0.0005	0.0474	0.9521
2	0.0010	0.0469	0.9521
3	0.0014	0.0464	0.9521
4	0.0048	0.0477	0.9475
5	0.0094	0.0699	0.9207
6	0.0140	0.0697	0.9163
7	0.0186	0.0694	0.9120
8	0.0185	0.0738	0.9077
9	0.0230	0.0778	0.8992
10	0.0229	0.0821	0.8950
11	0.0250	0.0904	0.8847
12	0.0228	0.0905	0.8867
13	0.0263	0.1306	0.8432
14	0.0295	0.1677	0.8028
15	0.0280	0.3481	0.6239
16	0.0314	0.3471	0.6215
17	0.0306	0.4561	0.5133
18	0.0335	0.4550	0.5114
19	0.0365	0.4539	0.5096
20	0.0395	0.4528	0.5077
21	0.0414	0.4705	0.4881
22	0.0432	0.4873	0.4694
23	0.0405	0.5365	0.4231
24	0.0440	0.6568	0.2992
25	0.0405	0.7047	0.2549
26	0.0598	0.6934	0.2468
27	0.0896	0.7133	0.1971
28	0.1187	0.7084	0.1729
29	0.1430	0.7110	0.1460
30	0.1569	0.7021	0.1411
31	0.1605	0.7257	0.1137
32	0.1711	0.7234	0.1055
33	0.1813	0.7212	0.0975
34	0.2024	0.7113	0.0863
35	0.2353	0.6890	0.0758
36	0.2458	0.6819	0.0724
37	0.2587	0.6690	0.0724
38	0.3041	0.6301	0.0658
39	0.3167	0.6174	0.0658
40	0.5775	0.3031	0.1194

Table B-5

Response of the estimator to obtain column compositions for the system α=1/3/9,product purity = 95%,at time t = 3.00 h

Tray No.	X_1	X_2	X_3
1	0.0144	0.9853	0.0003
2	0.0287	0.9710	0.0003
3	0.0429	0.9569	0.0003
4	0.0764	0.9236	0.0000
5	0.0880	0.9119	0.0000
6	0.0880	0.9120	0.0000
7	0.0960	0.9040	0.0000
8	0.0980	0.9020	0.0000
9	0.1038	0.8962	0.0000
10	0.1038	0.8962	0.0000
11	0.1104	0.8896	0.0000
12	0.1115	0.8885	0.0000
13	0.1125	0.8875	0.0000
14	0.1133	0.8867	0.0000
15	0.1533	0.8467	0.0000
16	0.1153	0.8847	0.0000
17	0.1265	0.8733	0.0002
18	0.1618	0.8380	0.0001
19	0.1944	0.8056	0.0000
20	0.2022	0.7978	0.0001
21	0.2246	0.7754	0.0001
22	0.2246	0.7754	0.0001
23	0.2246	0.7753	0.0001
24	0.2786	0.7213	0.0001
25	0.2658	0.7341	0.0001
26	0.2658	0.7341	0.0001
27	0.2868	0.7131	0.0001
28	0.2848	0.7151	0.0001
29	0.2987	0.7012	0.0001
30	0.2435	0.7565	0.0000
31	0.2416	0.7584	0.0000
32	0.2541	0.7459	0.0000
33	0.2658	0.7342	0.0000
34	0.2907	0.7093	0.0000
35	0.3297	0.6703	0.0000
36	0.3417	0.6583	0.0000
37	0.3577	0.6423	0.0000
38	0.4101	0.5899	0.0000
39	0.4249	0.5751	0.0000
40	0.6020	0.3980	0.0000

Table B-6

Response of the estimator to obtain column compositions for the system α=1/3/9,product purity = 95%,at time t = 3.75 h

Tray No.	X_1	X_2	X_3
1	0.0288	0.9712	0.0000
2	0.0565	0.9435	0.0000
3	0.0832	0.9168	0.0000
4	0.1436	0.8564	0.0000
5	0.1636	0.8364	0.0000
6	0.1636	0.8364	0.0000
7	0.1771	0.8229	0.0000
8	0.1804	0.8196	0.0000
9	0.1901	0.8099	0.0000
10	0.1901	0.8099	0.0000
11	0.2010	0.7990	0.0000
12	0.2028	0.7972	0.0000
13	0.2043	0.7957	0.0000
14	0.2057	0.7943	0.0000
15	0.2089	0.7911	0.0000
16	0.2089	0.7911	0.0000
17	0.2269	0.7731	0.0000
18	0.2684	0.7316	0.0000
19	0.2812	0.7188	0.0000
20	0.3285	0.6716	0.0000
21	0.3393	0.6607	0.0000
22	0.3698	0.6302	0.0000
23	0.3698	0.6302	0.0000
24	0.3947	0.6053	0.0000
25	0.3923	0.6077	0.0000
26	0.4085	0.5915	0.0000
27	0.4232	0.5768	0.0000
28	0.4232	0.5768	0.0000
29	0.4390	0.5610	0.0000
30	0.4466	0.5534	0.0000
31	0.4491	0.5509	0.0000
32	0.4491	0.5509	0.0000
33	0.4537	0.5463	0.0000
34	0.4537	0.5463	0.0000
35	0.4992	0.5008	0.0000
36	0.5127	0.4873	0.0000
37	0.5302	0.4698	0.0000
38	0.5848	0.4152	0.0000
39	0.5996	0.4004	0.0000
40	0.6137	0.3207	0.0656

Table B-7

Response of the estimator to obtain column compositions for the system $\alpha=1/3/9$,product purity = 95%,at time t = 4.50 h

Tray No.	X_1	X_2	X_3
1	0.0564	0.9436	0.0000
2	0.0770	0.9230	0.0000
3	0.1078	0.8922	0.0000
4	0.1548	0.8452	0.0000
5	0.1548	0.8452	0.0000
6	0.2528	0.7472	0.0000
7	0.2528	0.7472	0.0000
8	0.2830	0.7170	0.0000
9	0.2830	0.7170	0.0000
10	0.3027	0.6973	0.0000
11	0.3075	0.6925	0.0000
12	0.3214	0.6786	0.0000
13	0.3214	0.6786	0.0000
14	0.3366	0.6634	0.0000
15	0.3391	0.6609	0.0000
16	0.3412	0.6588	0.0000
17	0.3431	0.6569	0.0000
18	0.3476	0.6524	0.0000
19	0.3719	0.6281	0.0000
20	0.4253	0.5747	0.0000
21	0.4411	0.5589	0.0000
22	0.4967	0.5033	0.0000
23	0.5088	0.4912	0.0000
24	0.5421	0.4579	0.0000
25	0.5421	0.4579	0.0000
26	0.5421	0.4579	0.0000
27	0.5681	0.4319	0.0000
28	0.5657	0.4343	0.0000
29	0.5821	0.4179	0.0000
30	0.5968	0.4032	0.0000
31	0.6219	0.3781	0.0000
32	0.6122	0.3878	0.0000
33	0.6262	0.3738	0.0000
34	0.6352	0.3648	0.0000
35	0.6678	0.3322	0.0000
36	0.6797	0.3203	0.0000
37	0.6948	0.3052	0.0000
38	0.7397	0.2603	0.0000
39	0.7513	0.2487	0.0000
40	0.7541	0.2459	0.0000

Table B-8

Response of the estimator to obtain column compositions for the system α=1/3/9,product purity = 95%,at time t = 5.25 h

Tray No.	X_1	X_2	X_3
1	0.9412	0.0588	0.0000
2	0.9700	0.0300	0.0000
3	0.9800	0.0200	0.0000
4	0.9891	0.0109	0.0000
5	0.9906	0.0094	0.0000
6	0.9906	0.0094	0.0000
7	0.9915	0.0085	0.0000
8	0.9917	0.0083	0.0000
9	0.9922	0.0078	0.0000
10	0.9922	0.0078	0.0000
11	0.9927	0.0073	0.0000
12	0.9928	0.0072	0.0000
13	0.9928	0.0072	0.0000
14	0.9929	0.0071	0.0000
15	0.9930	0.0070	0.0000
16	0.9937	0.0063	0.0000
17	0.9950	0.0050	0.0000
18	0.9953	0.0047	0.0000
19	0.9962	0.0038	0.0000
20	0.9964	0.0036	0.0000
21	0.9969	0.0031	0.0000
22	0.9969	0.0031	0.0000
23	0.9969	0.0031	0.0000
24	0.9971	0.0029	0.0000
25	0.9972	0.0028	0.0000
26	0.9973	0.0027	0.0000
27	0.9975	0.0025	0.0000
28	0.9975	0.0025	0.0000
29	0.9975	0.0025	0.0000
30	0.9976	0.0024	0.0000
31	0.9977	0.0023	0.0000
32	0.9977	0.0023	0.0000
33	0.9978	0.0022	0.0000
34	0.9979	0.0021	0.0000
35	0.9981	0.0019	0.0000
36	0.9982	0.0018	0.0000
37	0.9984	0.0016	0.0000
38	0.9987	0.0013	0.0000
39	0.9988	0.0012	0.0000
40	0.9990	0.0010	0.0000

APPENDIX - C

Two – Point Implicit Method

The two-point implicit method (or simply the implicit method) contains an adjustable parameter which may be selected such that the method reduces either to the Euler predictor or to a corrector. The method may be applied to either an integral -difference equation or to a differential equation. Consider

$$\int_{t_n}^{t_n+\Delta t} f(t,y)dt = y_{n+1} - y_n$$

which may be reduced to the differential equation

$$\frac{dy}{dt} = f(t,y)$$

When applied to these equations, the implicit method consists of approximating the integral by use of a weighted value of the integrand based on its values $t_n+\Delta t$ and t_n as follows:

$$\left[\phi f(t_n + \Delta t, y_{n+1}) + (1-\phi) f(t_n, y_n)\right] h = y_{n+1} - y_n$$

where $0 \le \phi \le 1$, and the truncation error is given by

$$E_{n+1} = \frac{h^2}{2}(1-2\phi)\, y^{(2)}(t_n) + \frac{h^3}{6}(1-3\phi) y^{(3)}(t_n) + O(h^4)$$

APPENDIX - D

Solution of Tridiagonal System :

Consider the system of equations defined by

$$b_1 v_1 + c_1 v_2 = d_1$$

$$a_2 v_1 + b_2 v_2 + c_2 v_3 = d_2$$

$$a_3 v_2 + b_3 v_3 + c_3 v_4 = d_3$$

$$\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots$$

$$a_{N-1} v_{N-2} + b_{N-1} v_{N-1} + c_{N-1} v_N = d_{N-1}$$

$$a_N v_{N-1} + b_N v_N = d_N$$

For the equations such as these , which are seen to be of tridiagonal torm, the unknown v_j's may be found by use of the following recurrence formulas, sometimes called Thomas algorithm. The recurrence formulas are applied in the order stated

$$f_1 = c_1 / b_1 \; ; \qquad g_1 = d_1 / b_1 \; ;$$

$$f_k = \frac{c_k}{b_k - a_k f_{k-1}} \qquad (k = 2,3,\ldots\ldots,N-1)$$

$$g_k = \frac{d_k - a_k g_{k-1}}{b_k - a_k f_{k-1}} \qquad (k = 2,3,\ldots\ldots,N-1)$$

After the f's and g's have been computed , the values of $v_N, v_{N-1}, \ldots\ldots, v_2, v_1$, are computed as follows :

$$v_N = g_N \quad v_k = g_k - f_k v_{k+1} \qquad (k = N-1, N-2, \ldots\ldots, 2, 1)$$

This procedure has been found to be very efficient for use on a digital computer.