

A SIMPLIFIED MODEL FOR PREDICTING DISTILLATION COLUMN DYNAMICS

By

DAVID LEROY REYNOLDS

Bachelor of Science

Oklahoma State University

Stillwater, Oklahoma

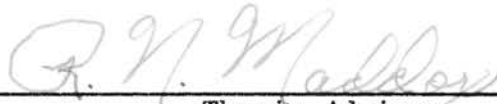
1962

Submitted to the faculty of the Graduate School of  
the Oklahoma State University  
in partial fulfillment of the requirements  
for the degree of  
Master of Science  
May, 1964

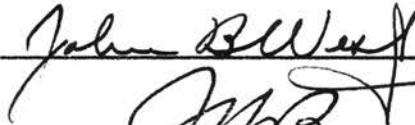
JAN 8 1965

A SIMPLIFIED MODEL FOR PREDICTING DISTILLATION COLUMN DYNAMICS

Thesis Approved:

  
\_\_\_\_\_

Thesis Adviser

  
\_\_\_\_\_

  
\_\_\_\_\_

Dean of the Graduate School

570332

## PREFACE

Two systems of simultaneous differential equations that simulate a distillation column are presented in this thesis. The derivation of equations and the difference between these systems and those of other authors are explained.

Comparison was made between the results of the derived equations and those obtained by digital computer solution of a plate-to-plate calculation, both at steady state.

I sincerely appreciate and would like to thank my adviser Dr. R. N. Maddox for all the advice, helpful criticism, time, and efforts that were necessary to make this thesis possible. I would like to thank the Oklahoma State University Graduate School for permission to make further study. I also appreciate the talks I had with Dr. J. B. West and Mr. Dale Bush on the mass-transfer concept; they were very beneficial. Also, I would like to thank Mr. Dale Bush for his instructions on the operation of the analog computer. Last, but by no means least I would like to thank my wife, Glenda, for the encouragement and self-sacrifices that were made so that I could obtain the degree, Master of Science.

## TABLE OF CONTENTS

Chapter	Page
I. INTRODUCTION.....	1
II. CHARACTERISTICS OF UNSTEADY-STATE DISTILLATION.....	2
III. LITERATURE SURVEY.....	4
IV. DERIVATION OF EQUATIONS.....	10
Simplified Method I.....	10
Simplified Method II.....	18
V. DISCUSSION OF DERIVATIONS AND RESULTS.....	22
VI. APPARATUS.....	43
VII. CONCLUSIONS.....	45
VIII. RECOMMENDATIONS.....	46
A SELECTED BIBLIOGRAPHY.....	47
APPENDIX A - PROGRAM FOR ANALOG COMPUTER OF SIMPLIFIED METHOD I.....	49
APPENDIX B - PROGRAM FOR ANALOG COMPUTER OF SIMPLIFIED METHOD II.....	52
APPENDIX C - PROGRAM FOR IBM 1620 FOR SPECIAL PROBLEM <sup>(5)</sup> ...	54
APPENDIX D - PROGRAM FOR IBM 1620 FOR SPECIAL PROBLEM <sup>(5)</sup> USING AVERAGE COMPOSITIONS.....	57
APPENDIX E - PROGRAM FOR IBM 1620 OF SIMPLIFIED METHOD I..	61
NOMENCLATURE.....	65

## LIST OF TABLES

Table	Page
I. Summary of Equations for Simplified Method I.....	19
II. Summary of Equations for Simplified Method II.....	21
III. Initial Conditions for Problems 1 and 2.....	25
IV. Distillate Rate Results from Problem 1 Using Simplified Method I.....	26
V. Distillate Rate Results from Problem 2 Using Simplified Method I.....	27
VI. Distillate Rate Results from Problem 1 Using Simplified Method II.....	32
VII. Distillate Rate Results from Problem 2 Using Simplified Method II.....	33
VIII. Summary of Equations for Special Problem (5).....	38
IX. Summary of Equations for Special Problem (5) Using Average Compositions.....	40

## LIST OF FIGURES

Figure	Page
1. Schematic Diagram of a Simple Fractionator.....	11
2. Typical Distillate-Time Curves for Step Changes in Feed Composition from Problem 1 Using Simplified Method I.....	28
3. Distillate Rate as Function of Feed Rate for Benzene from Problem 1 Using Simplified Method I.....	30
4. Typical Distillate-Time Curves for Step Changes in Feed Composition from Problem 1 Using Simplified Method II.....	34
5. Distillate Rate as Function of Feed Rate for Benzene from Problem 1 Using Simplified Method II.....	35
6. Mass Transfer Rate as Function of Feed for Benzene from Problem 1.....	36
7. Comparison of Mathematical Models and Experimental Data.....	42

## CHAPTER I

### INTRODUCTION

The study of controlling distillation columns has become more pronounced in the past few years. All previous investigators (with the exception of the ones who used a material balance for distillation column control) have used the idea of the individual plate which contained a certain amount of holdup for the basis of their equations. The individual plate models use excessive time on the digital computer and excessive equipment on the analog computer (16).

In 1962, Marr (16) presented a paper on distillation column dynamics where column parameters (weir height, weir length, plate spacing, tower diameter, etc.) were used to develop a mathematical model of a distillation column. Marr introduced the idea of not using an individual plate in a mathematical model. Marr, however used the plate concept in his model in that plate holdup was an assumption for his equations.

The purpose of this work was to devise a mathematical model of a distillation column which would not use the plate concept. The model would be such that it accurately represented the composition change of any component. Also, it would not be so complex that the equations couldn't be used as the basis for a control system of a continuous distillation column.

## CHAPTER II

### CHARACTERISTICS OF UNSTEADY-STATE DISTILLATION

The transient effects in composition of counter-current distillation are of interest in three separate cases: 1 - during a batch distillation run, 2 - during start-up of a continuous column, and 3 - a control system for maintaining product specifications during disturbances in the column.

For Case 1, a batch distillation system is such that the feed composition is continually changing with time, i.e., at any point in the system, the composition and temperature change continually. The distillate increases and the residue decreases in the more volatile component as the process starts operation. Often the column is operated at total reflux until the product has the right composition before the product is withdrawn. As the distillation proceeds, the distillate and residue become less concentrated with the more volatile component until the still has vaporized the liquid and the run is complete.

In Case 2, the continuous column operates at unsteady-state during start-up. The column is generally filled with a liquid feed or a vapor generated from a liquid feed and operated for some time until counter-current reflux and vapor produce the enrichment for which the column was designed.



For Case 3, a distillation column is initially at steady state prior to an upset. An upset can be caused by a feed disturbance (composition or quantity change), reflux fluctuation, or a vapor rate change caused by the reboiler.

The literature reports two types of feed upsets that have been represented by differential equations. These are step changes and sinusoidal changes. Although these types of disturbances are not usually found in industry, they give the investigator a look at the transient effects involved in unsteady-state distillation.

The response to a step-change in the feed was reported by Armstrong and Wilkinson (2) to become slower as the distance from the feed point increased. The sinusoidal disturbance produces results similar to those of a step change.

With the use of distillation control equipment in industry and the performance of the equipment being well understood in some instances, the design of control systems has been hampered by the insufficient understanding of the dynamic characteristics of a distillation column. The necessary data needed for control system design are the equations to represent the disturbance, the equipment to represent the equations, and the equipment to make the control action.

This thesis will present two sets of equations which can be used on an analog computer to represent the change in composition of the distillate because of a change in the feed composition.

## CHAPTER III

## LITERATURE SURVEY

Since the first works on unsteady-state distillation by Bardeen (6), Cohen (9), and Huffman and Urey (13), many investigators have attempted to simulate a distillation column and its approach to steady state. These include: Acrivos and Amundson (1), Berg and James (7), Davidson (10), Jackson and Pigford (14), Marr (16), Rose and Johnson (18), Rose, Williams, and Johnson (19), Rosenbrock (21)(22), and others.

Several investigators (Armstrong and Wilkinson (2), Rose and Williams (20), Rosenbrock (23), Wilkinson and Armstrong (25), and Williams and Harnett (26)) have studied transient effects in distillation because of a feed change.

A few investigators (Armstrong and Wood (3), Baber and Gerster (4) (5), and Weber, Martin, Pink, and Hargett (24)) have studied distillation equilibrium after a change in reflux or vapor rate. Baber and Gerster are the only investigators who have actually presented experimental data on unsteady-state distillation. This work was only to the degree of changing the reflux rate from a total to a stripping condition. Weber, Martin, Pink, and Hargett applied a material balance about the top of a distillation column for a control system to operate the column at maximum vapor capacity.

All previous investigators who studied unsteady-state distillation have used essentially the same basis to derive their dynamic relations. The basis is liquid holdup on a plate, a parameter which has an uncertain value since it is almost impossible to measure or estimate accurately within a distillation column.

The equations derived by most of the investigators mentioned above will be presented below. There are some supplementary equations that have variations between authors but the main equations are based on holdup. The variation of equations shown in the literature was generally in the equilibrium relationships.

The assumptions generally made by previous investigators were about all the same with few exceptions in each case.

For the case of start-up the assumptions usually made are like the ones made in the Davidson (10) paper. These are:

1. Liquid feed is supplied at a constant rate.
2. The mole fractions of the feed are fixed.
3. The column operates adiabatically.
4. The reboiler holdup has a fixed value.
5. The reboiler produces a constant heat supply.
6. There is a constant number of moles of liquid holdup on each plate that is perfectly mixed.
7. Each plate has the same efficiency.
8. At time  $t=0$  the liquid on each tray, and in the reboiler, has the same composition.
9. The mixture has molal latent heat that is independent of composition.
10. The relation between the liquid and vapor is in the form  $y = Bx$ , where  $(B)$  is a constant.

For the case of a feed change during steady-state operation the assumptions generally made are like the ones presented in the paper by Wilkinson and Armstrong (25). These are:

1. There is  $H$  moles of liquid holdup on each tray that is constant and perfectly mixed.
2. The vapor holdup is neglected.
3. The plate efficiency is independent of composition.

4. The column operates adiabatically.
5. The time to attain fluid dynamic equilibrium is small compared with that for mass transfer.
6. The mixture has constant molal latent heat.
7. The mixture has constant molal volume.
8. The equilibrium relation between the liquid and vapor can be approximated by two straight lines.

For the case of a reflux or vapor rate change during steady-state operation the following assumptions are generally made (3).

1. The column is at equilibrium when the change in the reflux rate is made at  $t = 0$ .
2. The plate efficiency is the same for all plates and reboiler, and is independent of composition and reflux rate.
3. The plate efficiency is constant during the non-equilibrium conditions.
4. The liquid holdup on the plate is perfectly mixed and independent of the liquid flow rate.
5. The column operates adiabatically.
6. The molar volumes and latent heats are independent of composition.
7. The pressure in the column is constant.
8. The system being distilled is a binary mixture and the vapor-liquid equilibrium data may be represented by straight lines.
9. The heat transfer along the column due to boiling point-concentration relationship is negligible.
10. The time to attain fluid dynamic equilibrium is small compared with the time for mass transfer.
11. The feed enters the column as saturated liquid.

From the above sets of assumptions, it is readily apparent that the assumptions of a feed change or vapor or reflux change are essentially the same. The assumptions presented by (10) which are different than the assumptions of feed change (25) are: 1, 2, and 8 of (10). The assumption presented by (3) that is different than the assumptions for start-up (10) is number one of (3).

The derivation proposed by previous investigators can be shown by writing a material balance around the condenser or any plate. Consider the  $n$ th plate and only one component. The plate contains  $H$  moles of liquid holdup and  $h$  moles of vapor holdup. A material balance for one component gives:

$$\frac{d(H_n x_n)}{dt} + \frac{d(h_n y_n)}{dt} = V_{n+1} y_{n+1} + L_{n-1} x_{n-1} - V_n y_n - L_n x_n$$

If the feed plate was considered then the above equation would include an  $(F x_F)$  term. For two components the form reduces to:

$$\frac{d(H_n + h_n)}{dt} = V_{n+1} + L_{n-1} - V_n - L_n$$

The assumptions that can be made to simplify the above equations are as follows:

With the assumption of negligible vapor holdup the equation reduces to:

$$\frac{d(H_n x_n)}{dt} = V_{n+1} y_{n+1} + L_{n-1} x_{n-1} - V_n y_n - L_n x_n$$

If  $H_n$  is a constant then the equation for the plate is:

$$H_n \frac{d(x_n)}{dt} = V_{n+1} y_{n+1} + L_{n-1} x_{n-1} - V_n y_n - L_n x_n$$

By assuming constant molar overflow the above equation reduces to:

$$H_n \frac{d(x_n)}{dt} = V(y_{n+1} - y_n) + L(x_{n-1} - x_n)$$

When at total reflux the total liquid rate and vapor rate are equal and the equation has the form:

$$H_n \frac{d(x_n)}{dt} = L(y_{n+1} + x_{n-1} - y_n - x_n)$$

To obtain a steady-state solution from a set of differential equations (one for each plate) after a disturbance, the initial condition for each equation is necessary. An equilibrium relationship between the vapor and liquid also has to be available.

The sequence of the calculations involved is stated below. For simplicity, take the rectifying section of a distillation column, a feed composition disturbance, and the assumptions given by Wilkinson and Armstrong (25).

1. Integrate the equation for plate (m), the feed plate. The result is the liquid composition ( $x_m$ ) on the feed plate.
2. The vapor composition ( $y_m$ ) is obtained from ( $x_m$ ) with the appropriate equilibrium relationship.
3. The new value of ( $y_m$ ) is then used in the equation for plate (n) to integrate a new value for the liquid composition ( $x_n$ ).
4. ( $x_n$ ) gives ( $y_n$ ) with the equilibrium relationship, ( $y_n$ ) gives ( $x_{n-1}$ ) from the integration, and the same procedure is followed until the results for the top of the column have been calculated to give the new steady-state values of the overhead.

The most recent development in distillation column dynamics was by Marr (16). Marr introduces the idea of omitting the discrete accounting of each plate.

The method proposed by Marr deals with column parameters, as stated previously. He uses a space variable which is distance up the column instead of plates. However, his equations use the same basis as in previous work, that of plate holdup.

An assumption required for his model was that column composition and temperature profiles are established as continuous functions of distance in the column, i.e., phases are in counter-

current flow. Marr also assumed phase physical properties are continuous functions of distance in the column.

The equations presented in the paper by Marr (16) are presented below.

By assuming that mass is being transferred from the vapor to the liquid, a material balance for the liquid in the section of height ( $d\beta$ ) is:

$$\frac{\partial(Hx_i)}{\partial t} = \frac{\partial(Lx_i)}{\partial \beta} + K_i (y_i - y_i^*)$$

For the vapor in the same section the material balance is:

$$\frac{\partial(hy_i)}{\partial t} = \frac{\partial(Vy_i)}{\partial \beta} - K_i (y_i - y_i^*)$$

Similar equations to the ones above will be derived and simplified in the following chapter of this thesis.

A recent paper on the simulation of a liquid-liquid extraction column by Biery and Boylan (8) presents several mathematical models. One model is also similar to the equations derived in the next chapter of this thesis. The difference between the two methods is the way the liquid and vapor holdup terms are expressed.

## CHAPTER IV

### DERIVATION OF EQUATIONS

The purpose of the following derivations is to present a mathematical model for a distillation column which will respond to a feed disturbance and show the product variation. These equations can then in turn be the basis for an economical, accurate control system for distillation.

The assumptions involved in these derivations are presented as follows:

1. Constant Molal Overflow.
2. Non-uniform Mixing in the Rectifying and Stripping Sections.
3. The rectifying and stripping sections are in unsteady-state.
4. The column is at steady-state when the change in feed composition is made.
5. The column operates adiabatically.
6. The column pressure is constant.
7. There is a constant heat supply from the reboiler.

#### Simplified Method I

The schematic of a simple fractionator presented in Figure 1 shows the flows that are represented in the derived equations.

The equations to be derived for the Simplified Method I are accumulation and depletion balances about the rectifying and stripping section of a distillation column.

The derivation of equations are thus presented with statements made for convenience and the assumptions involved. Take a volume



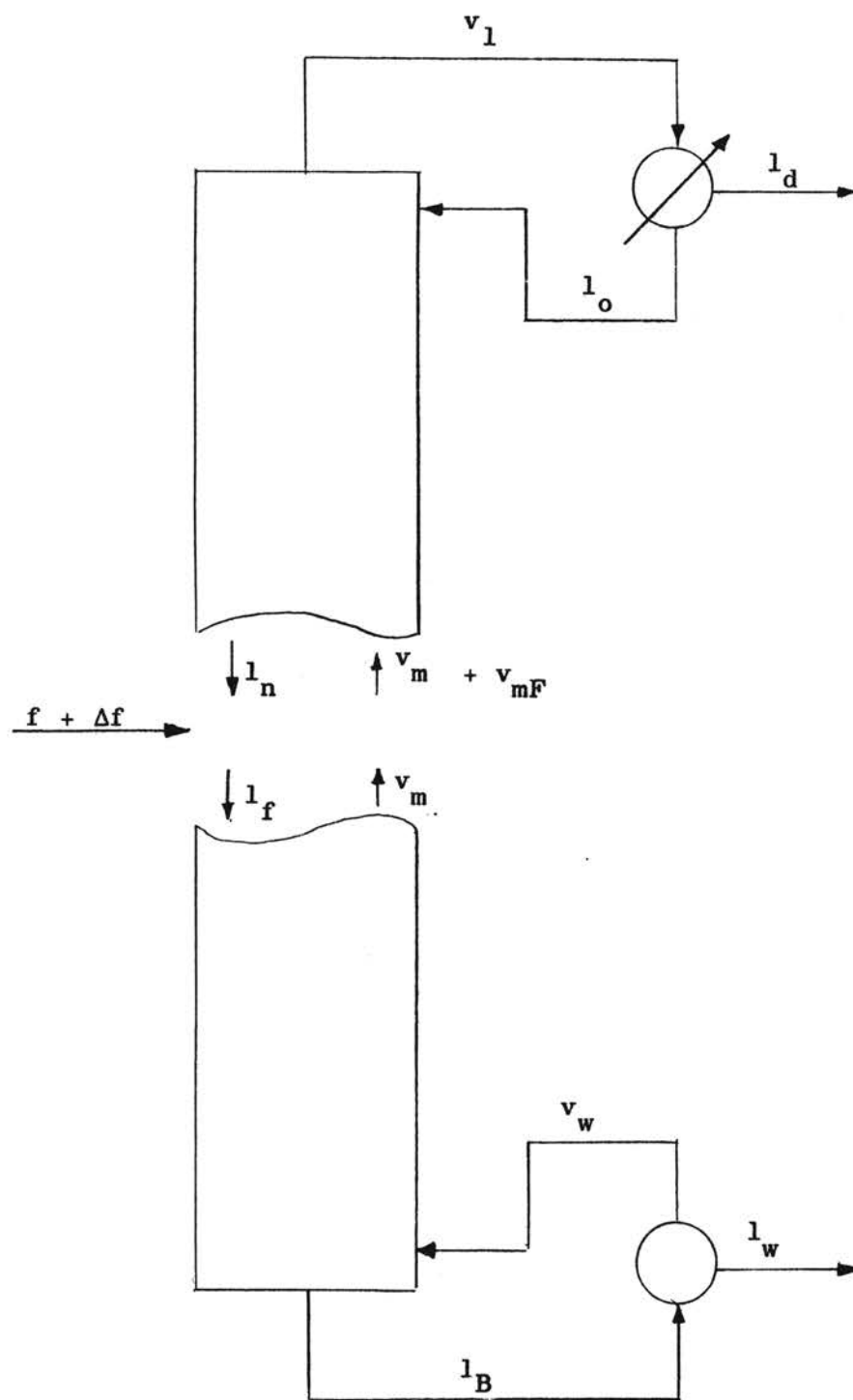
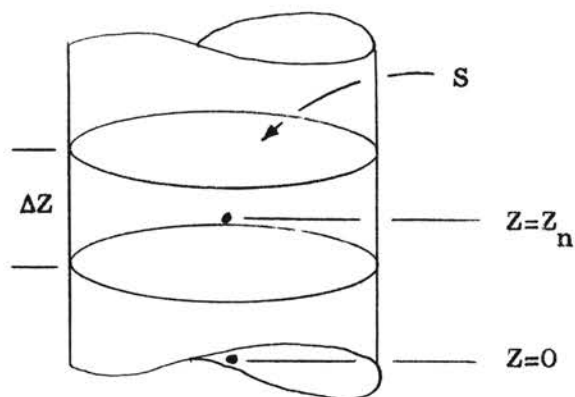


Figure 1 Schematic of a Simple Fractionator

section that has a cross sectional area (S) and consider an increment ( $\Delta Z$ ).



For convenience, take the origin for the following equations at the bottom of the section from which the height  $Z$  is zero at that point. There are two phases present in the section. Each phase has a certain volume fraction ( $\mu$ ) and average molar density ( $\rho_M$ ) in the section. The composition of the vapor in the increment is ( $y$ ) and the composition of the liquid in the increment is ( $x$ ).

The rate of accumulation with time at point  $Z_n$  for vapor is:

$$\frac{\partial (S)(\Delta Z)(\mu_V)(\rho_{MV})(y)}{\partial t} \quad (1)$$

The rate of change of material of one component in respect to  $Z_n$  as ( $\Delta Z$ ) goes to zero is:

$$\frac{\partial (V)(y)(\Delta Z)}{\partial Z} \quad (2)$$

where:

$V$  = total vapor flow rate in moles/unit time

The mass transferred from the liquid phase to the vapor phase (the direction is arbitrary) is:

$N$  = moles transferred per time

$$N = K_G a S (y^* - y) \Delta Z \quad (3)$$

where:

$K_G$  = mass transfer coefficient, moles/square foot per unit time

$a$  = interfacial area, square feet/cubic foot

An accumulation balance is presented in the following statements and equations. By definition, the rate of accumulation of vapor with time is equal to the vapor rate into the particular section minus the vapor rate leaving the particular section. In equation form the following presents the accumulation balance after dividing through by  $(\Delta Z)$

$$\frac{\partial (S \mu_V \rho_{MV} y)}{\partial t} = \frac{\partial (Vy)}{\partial Z} + K_G a S (y^* - y) \quad (4)$$

Since we chose the direction of mass transfer from liquid to vapor the sign on the mass transfer term is plus and the sign on  $\partial(Vy)/\partial Z$  is positive when we choose the origin at the bottom of the column.

By assuming constant molal overflow the above equation reduces to:

$$\frac{\partial (S \mu_V \rho_{MV} y)}{\partial t} = V \frac{\partial y}{\partial Z} + K_G a S (y^* - y) \quad (5)$$

Since we only want the change of  $(x)$  and  $(y)$  with time, the change in composition with height is replaced with forward finite differences. The vapor composition  $(y_n)$  represents the vapor leaving the element  $(n)$  and the vapor composition  $(y_{n-1})$  represents the vapor leaving the increment  $(n-1)$ . The following equation represents the above statements:

$$\frac{\partial (S \mu_{Vn} \rho_{Mn} y_n)}{\partial t} = V \frac{(y_n - y_{n-1})}{\Delta Z} + K_G a S (y_n^* - y_n) \quad (6)$$

However, since the term  $V(y_n - y_{n-1})/\Delta Z$  represents depletion instead of accumulation the sign of this term has to be changed.

Changing the sign on the term stated above, multiplying the equation through by  $(\Delta Z)$ , and assuming over the increment that  $(\mu_{Vn})$  and  $(\rho_{Mn})$  are constant, the above equation reduces to:

$$\Delta Z S \mu_{Vn} \rho_{Mn} \frac{\partial y_n}{\partial t} = V (y_{n-1} - y_n) + K_G a S (y_n^* - y_n) \Delta Z \quad (7)$$

The vapor holdup in the element is  $= \Delta Z S \mu_{Vn} \rho_{Mn} V = \delta_V$

By using the new term for vapor holdup the above equation is in the following form:

$$\delta_V \frac{\partial y_n}{\partial t} = V (y_{n-1} - y_n) + K_{VR} (y_n^* - y_n) \quad (8)$$

where:

$$K_{VR} = K_G a S \Delta Z$$

The above equation can be applied to the rectifying section of a distillation column in the following manner. By using distillation column nomenclature the equation above has the following form:

$$\delta_{RV} \frac{\partial y_1}{\partial t} = V y_m - V y_1 + K_{VR} (y_1^* - y_1) \quad (9)$$

By assuming that the rectifying section has non-uniform mixing, the driving force below the section was taken to approximate the average mass transfer concentration driving force within the section.

$$\delta_{RV} \frac{\partial y_1}{\partial t} = V y_m - V y_1 + K_{VR} (y_n^* - y_m) \quad (10)$$

The changing of Equation 8 to Equation 9 by exaggeration of the size of the element might not be a valid procedure. In other words, the vapor composition leaving the rectifying section might not be the actual composition ( $y_1$ ) as given by the equation. Therefore, an approximation such as the average composition of the section might be more accurate. The approximation would then be  $(y_1 + y_w)/2.0 = \bar{y}$ , the average vapor composition.

$$\delta_{RV} \frac{\partial \bar{y}}{\partial t} = V y_m - V y_1 + K_{VR} (y_1^* - y_1) \quad (11)$$

or

$$\delta_{RV} \frac{\partial \bar{y}}{\partial t} = V y_m - V y_1 + K_{VR} (y_n^* - y_m) \quad (12)$$

where:

$$\bar{y} = (y_1 + y_w)/2 \quad (13)$$

Using an analogous procedure the equation for the liquid in the element ( $\Delta Z$ ) can be converted to use in simulating the distillation column at unsteady-state. The equation is converted as follows with the numbers on the following equations corresponding to numbers on the equations stated above, i.e., 1 corresponds to 1A, 2 corresponds to 2A, etc.

$$\frac{\partial (S \mu_L \rho_{ML} x)(\Delta Z)}{\partial t} \quad (1A)$$

$$\frac{\partial (Lx)(\Delta Z)}{\partial Z} \quad (2A)$$

$$N_L = K_L a S \Delta Z (x - x^*) \quad (3A)$$

or

$$-N_L = N_V = K_G a S (y^* - y) \Delta Z$$

$$\frac{\partial (S \mu_L \rho_{ML} x)}{\partial t} = \frac{-\partial(Lx)}{\partial Z} - K_G a S (y^* - y) \quad (4A)$$

$$\frac{\partial (S \mu_L \rho_{ML} x)}{\partial t} = \frac{-L \partial x}{\partial Z} - K_G a S (y^* - y) \quad (5A)$$

$$\frac{\partial (S \mu_{nL} \rho_{MLn} x_n)}{\partial t} = \frac{-L (x_{n+1} - x_n)}{\Delta Z} - K_G a S (y_n^* - y_n) \quad (6A)$$

$$(\Delta Z)(S)(\mu_{Ln})(\rho_{MLn}) \partial x_n / \partial t = L x_{n+1} - L x_n - K_G a S \Delta Z (y_n^* - y_n) \quad (7A)$$

$$\delta_L \frac{\partial x_n}{\partial t} = L (x_{n+1} - x_n) - K_{VR} (y_n^* - y_n) \quad (8A)$$

$$\delta_{RL} \frac{\partial x_n}{\partial t} = L x_o - L x_n - K_{VR} (y_n^* - y_n) \quad (9A)$$

$$\delta_{RL} \frac{\partial x_n}{\partial t} = L x_o - L x_n - K_{VR} (y_n^* - y_m) \quad (10A)$$

$$\delta_{RL} \frac{\partial \bar{x}}{\partial t} = L x_o - L x_n - K_{VR} (y_n^* - y_n) \quad (11A)$$

$$\delta_{RL} \frac{\partial \bar{x}}{\partial t} = L x_o - L x_n - K_{VR} (y_n^* - y_m) \quad (12A)$$

$$\bar{x} = (x_B + x_o) / 2.0 \quad (13A)$$

Similarly the preceding equations (10, 10A, 12, 12A) can be applied to the stripping section of a distillation column.

The equation for the vapor leaving the stripping section

has the following form:

$$\delta_{SV} \frac{dy_m}{dt} = Vy_w - Vy_m + K_{VS}(y_B^* - y_w)$$

The equation for the liquid leaving the stripping section has the form:

$$\delta_{SL} \frac{dx_B}{dt} = L x_f - L x_B - K_{VS}(y_B^* - y_w)$$

The material balances and stream ratios presented below are used in the accumulation and depletion balances to calculate the vapor leaving the reboiler, the liquid entering the stripping section from the feed section, the reflux entering the column, and the distillate product.

$$v_w = \frac{v_{wI}}{l_{BI}} (l_B)$$

where  $v_{wI}/l_{BI}$  is assumed constant for all calculations and:

$v_{wI}$  = vapor flow rate of a component leaving the reboiler at time  $t=0$ , moles/unit time

$l_B$  = liquid flow rate of a component leaving the bottom of the column after time  $t=0$ , moles/unit time

$l_{BI}$  = liquid flow rate of a component leaving the bottom of the column at time  $t=0$ , moles/unit time

$$l_f = x_n L + f_L + \Delta f_L$$

$f_L$  = liquid flow rate of feed of one component, moles/unit time

$\Delta f_L$  = liquid feed for a component that causes the upset in the column, moles/unit time

Assuming a total condenser:

$$l_o = \frac{L_o}{V_1} (y_1 V)$$

$$l_d = \frac{D}{V_1} (y_1 V)$$

The application of the preceding equations to multicomponent distillation can be made by using the above equations in terms of mole fractions.

Table I presents the four differential equations as simplified above with the supplementary equations necessary for programming on the analog and digital computers.

#### Simplified Method II

The following equations will be based on all the assumptions made at the beginning of this chapter with the exception of Assumption 2.

Simplified Method II will use the preceding equations of Simplified Method I with some simplifying assumptions. The equations will be reduced so that an equilibrium relationship is no longer needed.

By making the assumption that the mass transfer at steady state equals the mass transfer at any time, the mass transfer term will then be a constant and will be represented by the letter (C).

Also, the assumption will be made that the constant for mass transfer (C) in each accumulation or depletion balance is equal to some function of the difference between the inlet and outlet flows (determined by the accumulation and depletion balances).



TABLE I

## SUMMARY OF EQUATIONS FOR SIMPLIFIED METHOD I

$$\delta_{RL} \frac{d(x_n)}{dt} = l_o - (K_{L1}/L)(l_o - l_1^*) - l_n$$

$$\delta_{RV} \frac{d(y_1)}{dt} = v_m + v_{mF} + (K_{Vn}/V)(v_n^* - v_m) - v_1$$

$$\delta_{SL} \frac{d(x_B)}{dt} = l_f - (K_{Lm}/L)(l_f - l_m^*) - l_B$$

$$\delta_{SV} \frac{d(y_m)}{dt} = v_w + (K_{VB}/V)(v_B^* - v_w) - v_m$$

$$v_w = (v_{wI}/l_{BI})(x_B L)$$

$$l_f = x_n L + f_L + \Delta f_L$$

$$l_o = L_o(y_1 V)/V_1$$

$$l_d = D(y_1 V)/V_1$$

Since the equations have to satisfy the condition at steady state of being zero, the constant (C) is the difference between the inlet and outlet flows at time  $t=0$ .

Simplifying the four differential equations that are presented in Table I, the resulting equations are presented:

$$\delta_{RV} \frac{dy_1}{dt} = v_m + v_{mF} + C_1 - v_1$$

$$C_1 = v_{1I} - v_{mI} - v_{mFI}$$

$$\delta_{RL} \frac{dx_n}{dt} = l_o - C_n - l_n$$

$$C_1 = l_{oI} - l_{nI}$$

$$\delta_{SV} \frac{dy_m}{dt} = v_w + C_m - v_m$$

$$C_m = v_{mI} - v_{wI}$$

$$\delta_{SL} \frac{dx_B}{dt} = l_f - C_B - l_B$$

$$C_B = l_{fI} - l_{BI}$$

The above equations and the required supplementary equations are presented in Table II.

TABLE II

## SUMMARY OF EQUATIONS FOR SIMPLIFIED METHOD II

$$\delta_{RV} \, dy_1/dt = v_m + v_{mF} - v_{1F} - v_{mI} - v_{mFI} - v_1$$

$$\delta_{RL} \, dx_n/dt = l_o - l_{oI} + l_{nI} - l_n$$

$$\delta_{SV} \, dy_m/dt = v_w + v_{mI} - v_{wI} - v_m$$

$$\delta_{SL} \, dx_B/dt = l_f - l_{fI} + l_{BI} - l_B$$

$$v_w = (v_{wI}/l_{BI})(x_B L)$$

$$l_f = x_n L + f_L + \Delta f_L$$

$$l_o = (L_o/V_1)(y_1 V)$$

$$l_d = (D/V_1)(y_1 V)$$

## CHAPTER V

### DISCUSSION OF DERIVATIONS AND RESULTS

The differential equations presented in Table I and Table II are under the restriction of reducing to zero when the column is at steady state. The reason the equations reduce to zero is that the concentration at a point does not change with time. The mass-transfer coefficients were arbitrarily established from the above restriction for all the differential equations.

There were two ways that the differential equations of Table I were used to represent a transient effect. One method is to not assume any of the stream quantities are constant and let each term change with time with the exception of the mass-transfer coefficient. The second method is to use the assumption that the mass-transfer term remains constant if the feed composition changes only slightly. The other terms are allowed to change as a function of time. Both of the above methods were tested.

The mass-transfer coefficients were established from solving the differential equations at a condition of being at steady state. The initial values, equilibrium concentrations, and/or material balances were used to "back out" the mass-transfer coefficient for each section.

The results that are produced based on the first method stated above will be under the title Simplified Method I. The results

that are produced based on the second method stated above will be under the title of Simplified Method II.

The equations presented in the preceding chapter were programmed for the analog computer. The analog program for Simplified Method I is presented in Appendix A and the program for Simplified Method II is presented in Appendix B.

To check the results obtained from the analog computer, the use of the IBM 650 Digital Computer was necessary. A program for the plate-to-plate calculation of a distillation column, written by J. H. Erbar and R. N. Maddox (11), (12) and (15) was used to make the calculations.

The plate-to-plate program for the IBM 650 will make complete plate-to-plate calculations on a simple fractionator. The program is based on a given number of stages, reflux ratio, distillate rate, feed plate location, and feed composition. The program has limitations of 20 components, 98 theoretical trays, single feed stream, and two products.

There were two problems run on the digital and analog computers. The problems were formed from a binary system (Benzene-Toluene), with the equilibrium data obtained from Perry (17). The assumptions of constant molal overflow, bubble point feed, and total condenser were made in both cases. Problem 1 does not have as close a split in the distillate products as Problem 2. The split for Problem 1 was about 90 percent while the split for Problem 2 was about 99 percent.

The digital computer used the plate-to-plate program to calculate the steady-state values of stream flows. The feed

composition was the only change in the different examples of each problem. The initial conditions of the problems are presented in Table III.

The analog was set up at an initial feed condition of 50 percent benzene and 50 percent toluene, then a step change in the feed composition was made. The analog generated the results of the differential equations to their steady-state values. The step changes from the initial feed condition of one component were:  $\pm 5\%$ ,  $\pm 10\%$ ,  $\pm 50\%$ .

The programming of the equations for Simplified Method I used a total of 19 amplifiers and two function generators.

Tables IV and V are for Problem 1 and 2, respectively, using Simplified Method I. These tables present the feed rates, distillate rates from plate-to-plate calculations, distillate rates from analog computations, and percent differences between the two distillate rates based on the plate-to-plate results.

Figure 2 presents typical distillate-time curves of Problem 1 for the changes that were made in the feed composition. The feed change of 10 percent increase is the curve that has the largest distillate rate at steady state. The 50 percent decrease in feed composition is the curve with the lowest distillate rate at steady state. The curves in between are of the percentages stated above.

The results of Simplified Method I and Problem 1 had less than 3 percent difference for changes of feed composition ranging  $\pm 10$  percent when compared to distillate values of the light key from the plate-to-plate program.

The step change result for a 50 percent increase in feed

TABLE III

## INITIAL CONDITIONS FOR PROBLEM 1 AND 2

Problem 1		Problem 2	
	moles/hour		moles/hour
V	8.25	V	10.91
$v_1$	7.47	$v_1$	10.89
$v_m$	5.77	$v_m$	8.92
$v_w$	1.56	$v_w$	2.83
L	5.14	L	8.28
$l_d$	2.82	$l_d$	2.63
$l_o$	4.66	$l_o$	8.26
$l_n$	2.95	$l_n$	6.29
$l_f$	6.03	$l_f$	9.39
$l_B$	1.84	$l_B$	3.30

TABLE IV

Problem 1  
Simplified Method I

Feed Rate Benzene moles/hour	Distillate Rate Benzene Plate-to-Plate moles/hour	Distillate Rate Benzene Analog Computer moles/hour	Percent Difference Based on Plate-to- Plate
1.55	1.52	1.46	3.9
2.79	2.63	2.62	0.38
2.95	2.74	2.74	nil
3.1 (#)	2.82	2.82	----
3.26	2.88	2.96	2.8
3.41	2.92	3.03	3.8
4.00	3.00	3.23	7.7
4.65	3.03	----	----

(#) represents the feed from which the initial conditions were taken.



TABLE V

Problem 2  
Simplified Method I

Feed Rate Benzene moles/hour	Distillate Rate Benzene Plate-to-Plate moles/hour	Distillate Rate Benzene Analog Computer moles/hour	Percent Difference Based on Plate-to- Plate
1.55	1.55	1.34	13.5
2.79	2.6387	2.39	9.5
2.95	2.6337	2.53	3.8
3.1 (#)	2.6313	2.63	-----
3.26	2.6304	2.76	4.9
3.41	2.6308	2.87	9.1
4.65	2.6507	3.81	44.0

(#) represents the feed rate from which the initial conditions were taken

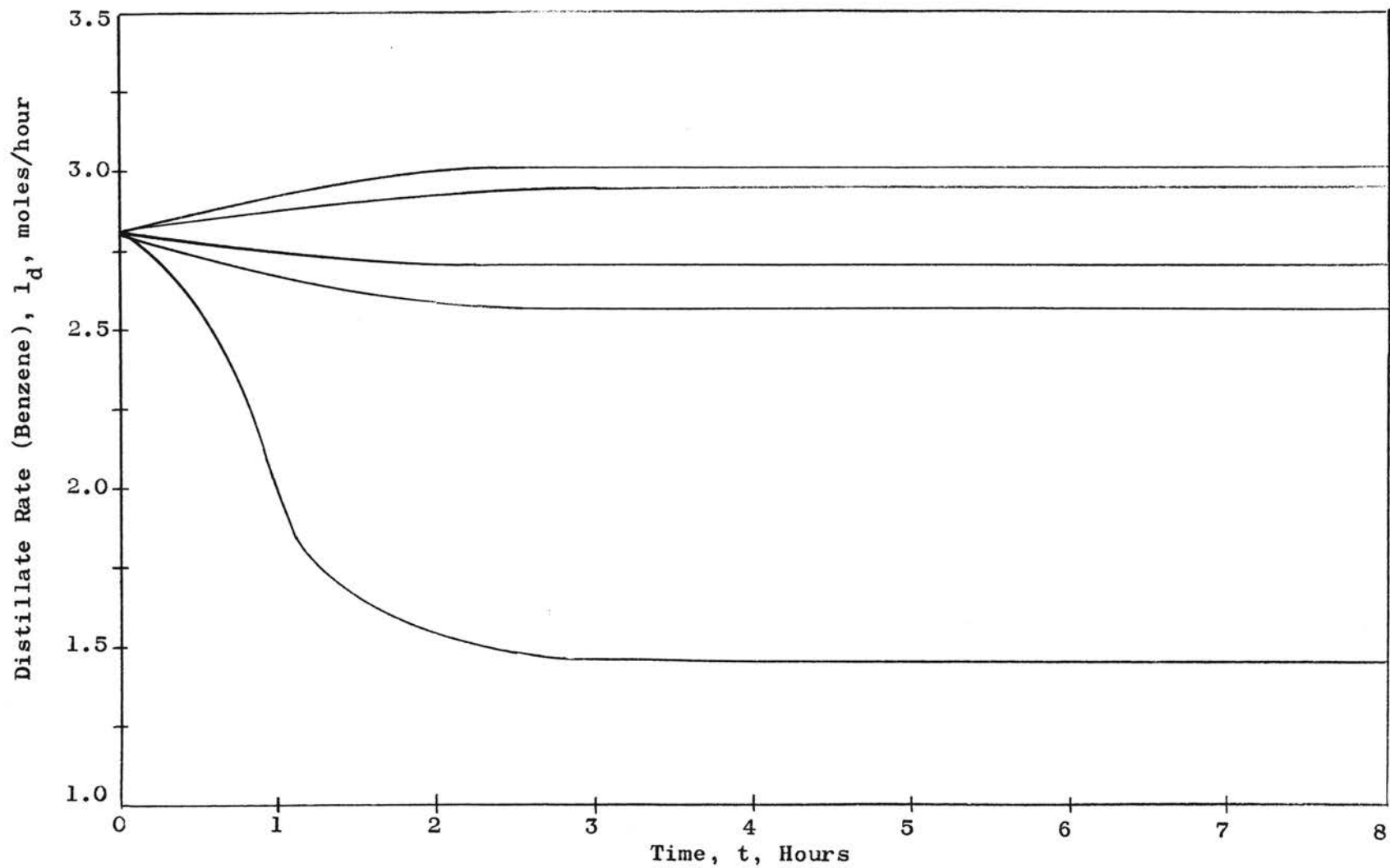


Figure 2 Typical Distillate Composition Curves for Step Changes in Feed Composition  
Simplified Method I - Problem 1

composition was not obtained with the equations presented in Table I. The reason for the limitation was because of the mass-transfer term in the equations for the rectifying section. The cause was in the driving force terms. The driving force would change sign after a disturbance of +30 percent was made with the conditions of Problem 1. When the disturbance was greater than +30 percent the equations would increase without limit until the amplifiers on the analog computer would overload.

The reason that this same effect did not happen when a large negative disturbance (-50%) in feed composition was made was because the mass-transfer driving force increased its difference as the feed composition was decreased.

The results from Table IV are plotted in Figure 3 and show the difference of the two sets of steady-state distillate values for the light key as a function of the feed rate.

The results for Problem 2 with Simplified Method I are presented in Table V. The analog solution shows a percent difference in distillate rates for the light key from the digital solutions over a range of 4 to 40 percent for all changes in feed composition. Problem 2 did not present a change in sign of the driving force for a +50 percent increase in feed composition as Problem 1. In other words, the difference in the terms of the driving force did not go to zero when the large change in feed composition was made.

The programming of the equations for Simplified Method II used a total of 9 amplifiers.

The steady-state analog solutions based on Simplified Method II

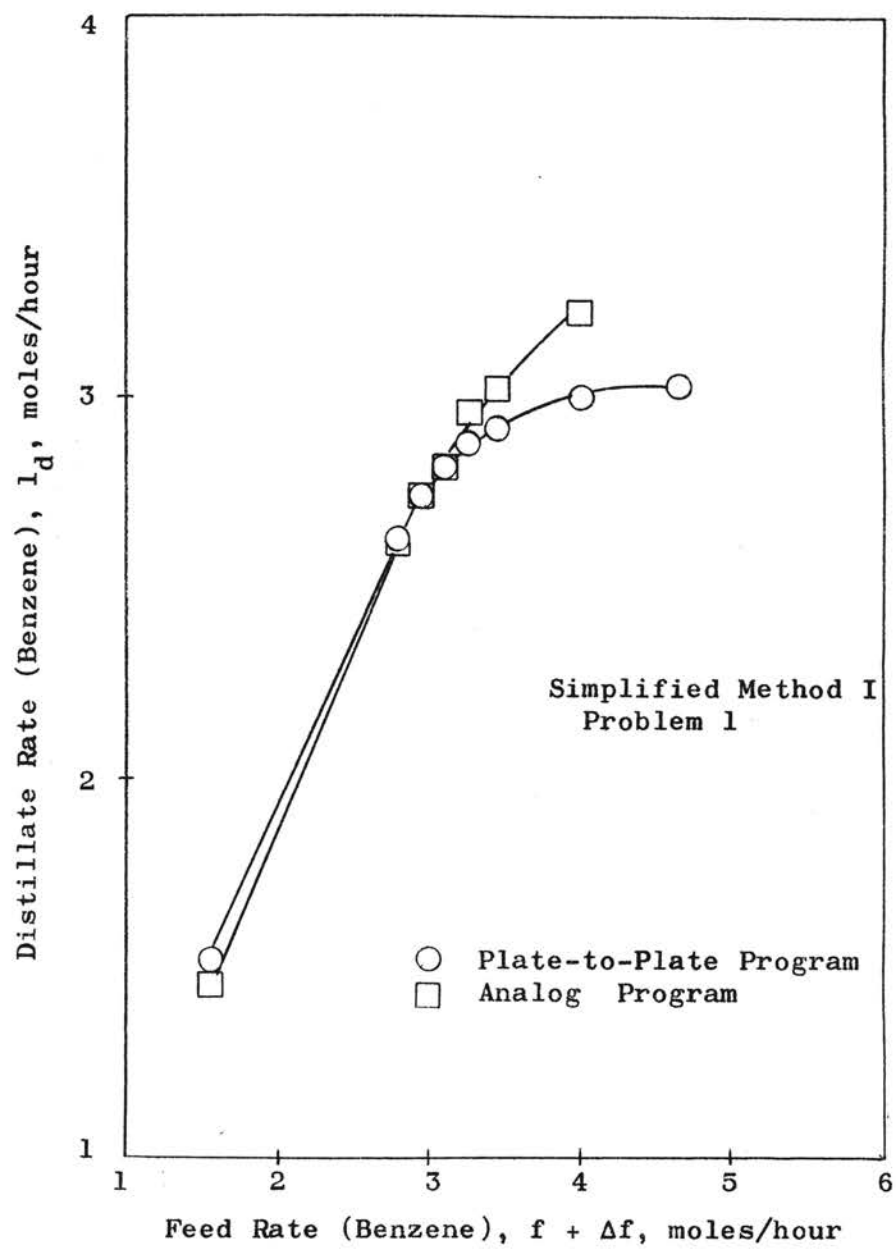


Figure 3 Distillate Rate as Function of Feed Rate (Light Key)

are presented in Table VI and VII. Table VI contains the results of Problem 1 in the same form as Table IV and V. Table VII contains the results of Problem 2 also in the same form as Table IV and V.

Figure 4 presents typical distillate-time curves of Problem 1 for the step change in feed composition from plus to minus 50 percent. The curve with the lowest distillate rate of the light key is for the 50 percent decrease in feed composition, while the curve with the highest distillate rate is for the increase in feed composition 50 percent.

Comparison of the distillate rates of the analog solutions with the plate-to-plate solutions shows that in Problem 1 the analog solution had a range of differences from 0.4 to 31 percent. Problem 2 had differences which were in the range of 1.9 to 35 percent. Figure 5 is for Problem 1 and presents a plot of distillate rates from the analog and digital computers as a function of the feed rate.

A reason for the large percent differences at large feed composition changes is because of the variation of the mass-transfer term with feed rate. These results are shown in Figure 6.

The results from the analog based on Simplified Method II show that the assumption of a constant mass-transfer term is not valid at large feed composition changes. The fact is that the equations were no longer in material balance, i.e., the distillate rate from the analog solution was greater than the entering feed rate for the case of 50 percent decrease in feed

TABLE VI

Problem 1  
Simplified Method II

Feed Rate Benzene moles/hour	Distillate Rate Benzene Plate-to-Plate moles/hour	Distillate Rate Benzene Analog Program moles/hour	Percent Difference Based on Plate-to- Plate
1.55	1.52	1.72	13.20
2.79	2.63	2.62	0.38
2.95	2.74	2.75	0.37
3.1 (#)	2.82	2.82	-----
3.26	2.88	3.00	4.20
3.41	2.92	3.08	5.50
4.65	3.03	3.98	31.40

(#) represents the feed rate from which the initial values used in analog program were obtained.

TABLE VII

Problem 2  
Simplified Method II

Feed Rate Benzene Moles/hour	Distillate Rate Benzene Plate-to-Plate moles/hour	Distillate Rate Benzene Analog Program moles/hour	Percent Difference Based on Plate-to- Plate
1.55	1.5484	1.64	5.80
2.79	2.6387	2.41	8.70
2.95	2.6337	2.52	4.20
3.1 (#)	2.6313	2.63	----
3.26	2.6304	2.68	1.90
3.41	2.6308	2.80	6.46
4.65	2.6507	3.57	34.70

(#) represents the feed rate from which the initial values used in the analog program were obtained.

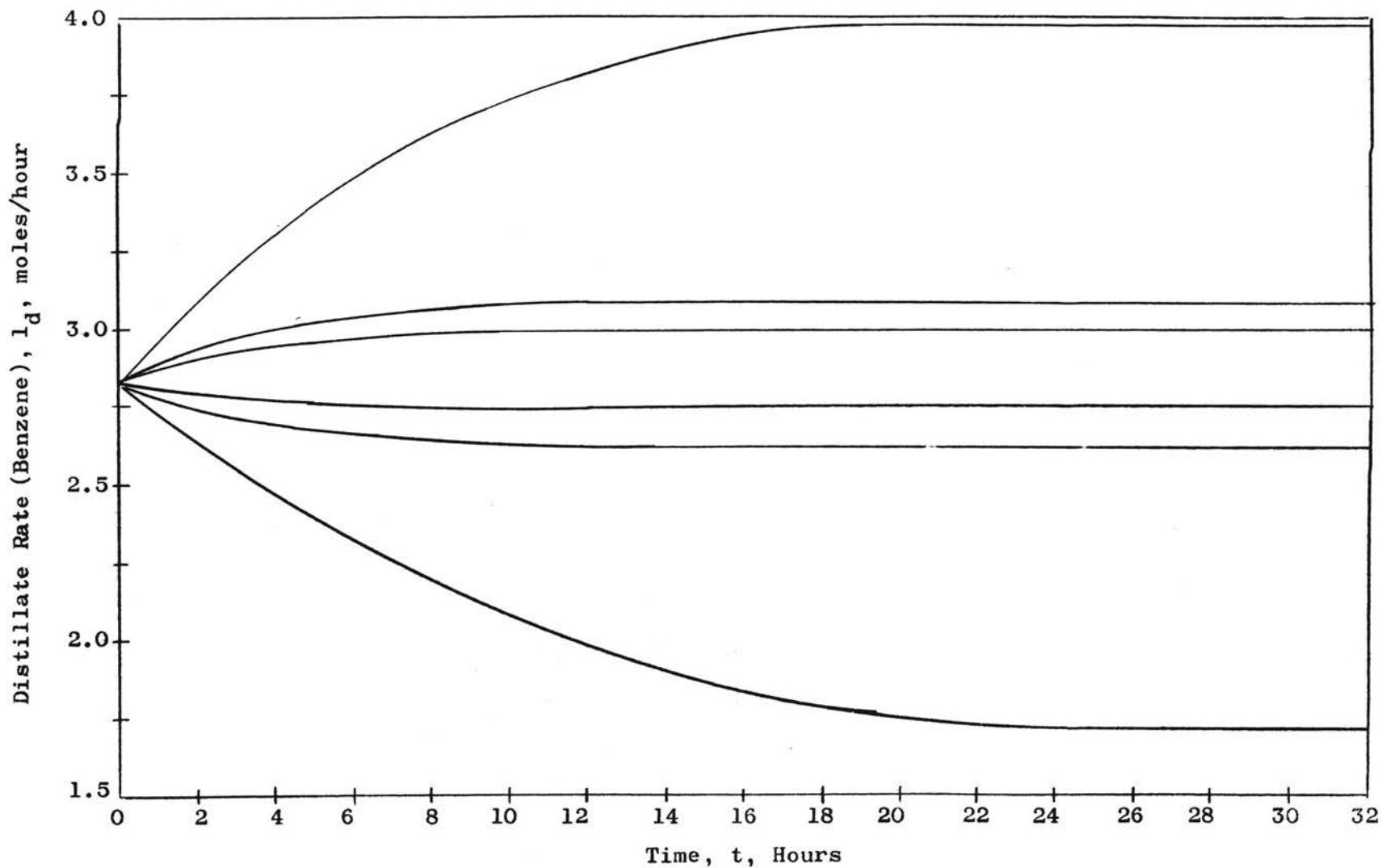


Figure 4 Typical Distillate - Time Curves for Step Changes in Feed Composition  
Simplified Method II - Problem 1



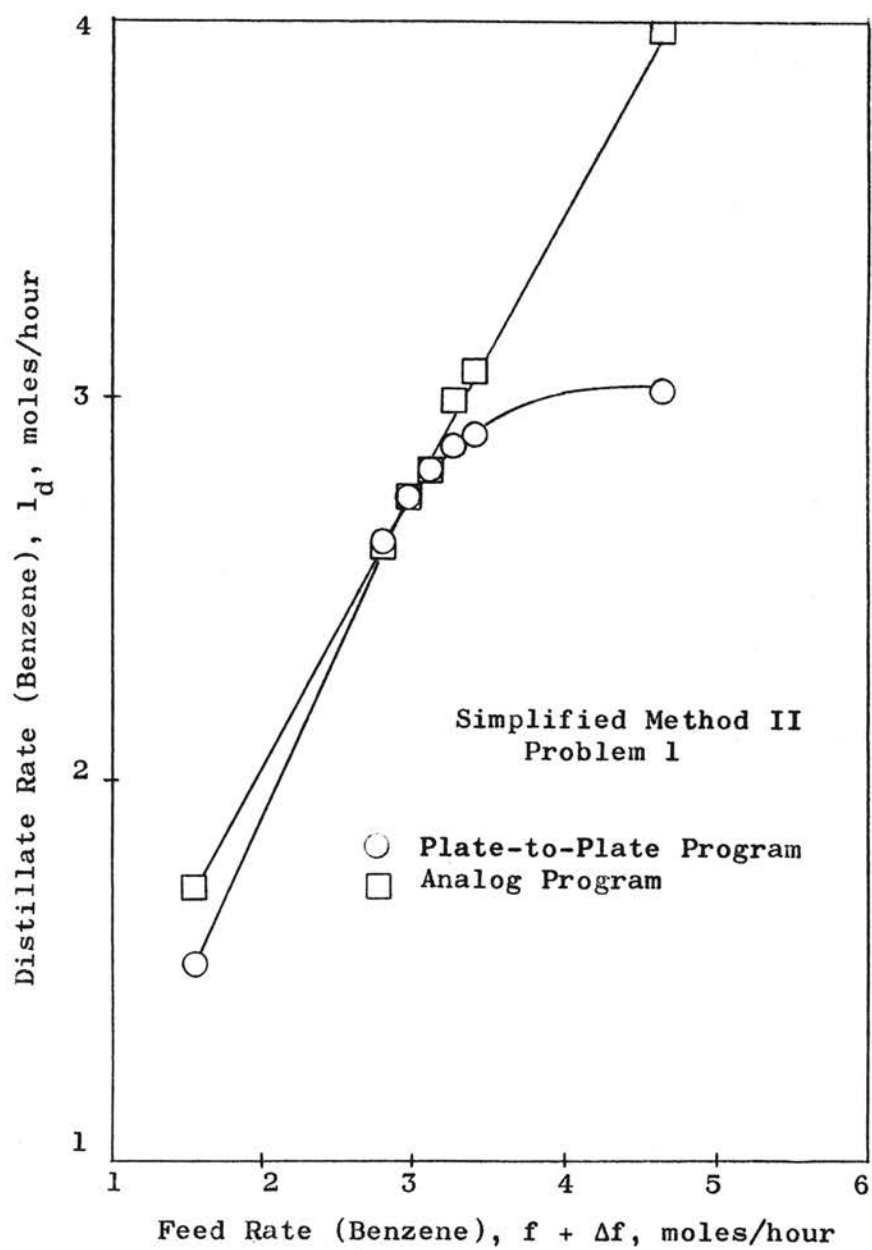


Figure 5 Distillate Rate as Function of Feed Rate (Light Key)

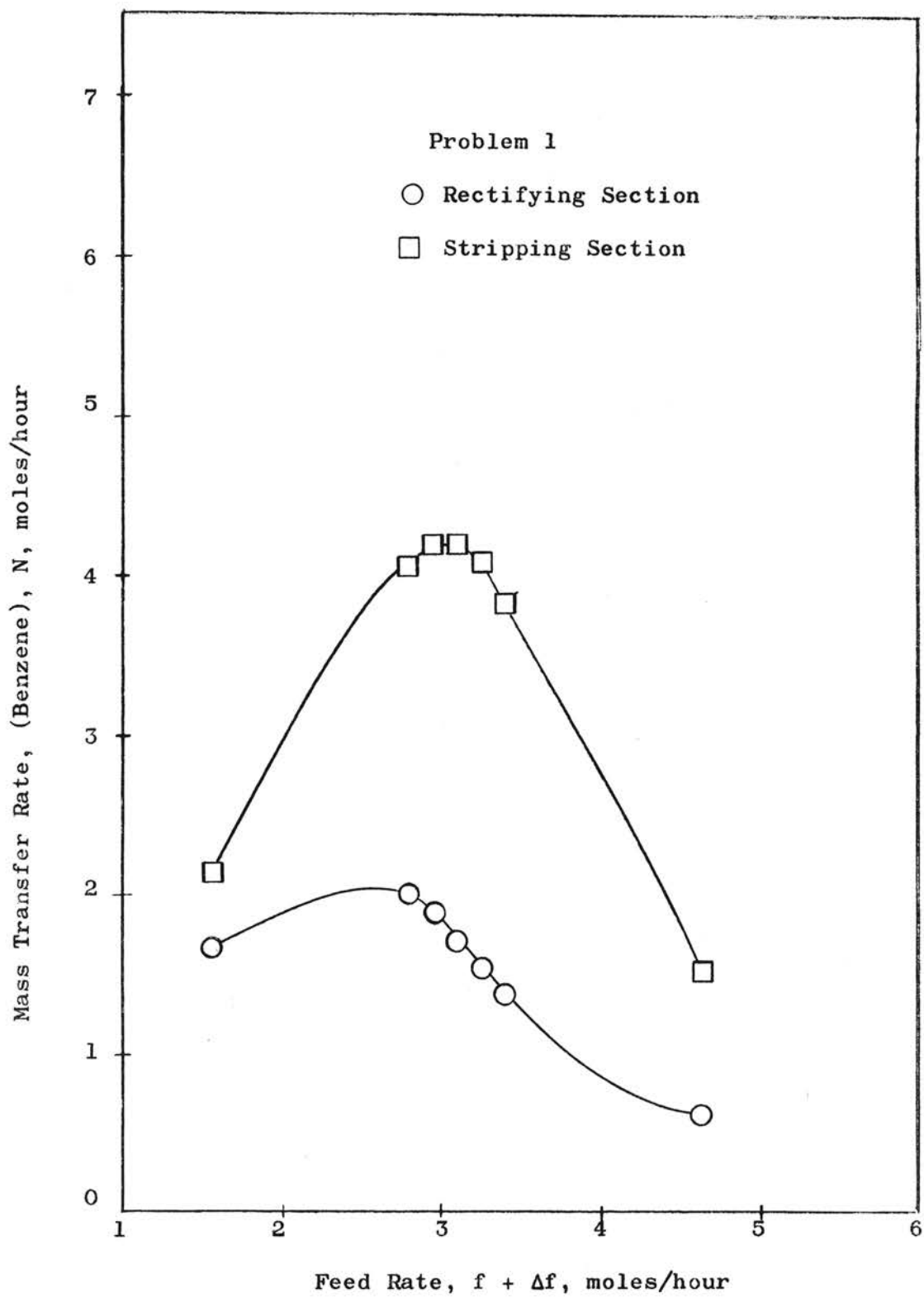


Figure 6 Mass Transfer Rate as Function of Feed (light Key)

composition. Therefore, by assuming that the mass-transfer term is constant a large number of amplifiers are saved but accuracy is lost.

The transient data presented by Barber and Gerster, et al., (5) were used with similar equations to the ones in Table I to see if the equations represent a reasonable model for distillation column simulation. The IBM 1620 Digital Computer was used since the equations were relatively easy to program. For the Case D-8 in (5) time-concentration data were presented and used in the equations derived for the situation presented in the paper. The equations derived for this particular case are presented in Table VIII.

The pseudo-equilibrium data for a Benzene-Acetone System (5) were curve fitted for the equilibrium concentration term in the driving force of the equations that were used.

To solve the two differential equations for the column on the digital computer, finite differences were used. The computer program is presented in Appendix C. An estimate of the liquid and vapor holdup was made in order that the time scale would be correct.

The liquid and vapor holdup were estimated by using the volume of the column, molar density, and fraction of section liquid or vapor. Since the values for the molar density and fraction liquid and vapor were not available, estimates were made and used in the computer program. An estimate of 150°F for the average column temperature, and 16 per cent liquid in the column were first used. The per cent liquid in the column was changed to 12 per cent and

TABLE VIII

SUMMARY OF EQUATIONS FOR SPECIAL PROBLEM<sup>(5)</sup>

$$\delta_L dx_B/dt = x_o L - K (y_B^* - y_w) - x_B L$$

$$\delta_V dy_1/dt = y_w V + K (y_B^* - y_w) - y_1 V$$

$$y_w = (v_{wI}/1_{BI})(L/V)x_B$$

$$y_B^* = 0.01368 + 1.9221(x_B) - 1.3639 (x_B^{2.0})$$

then to 20 percent to see the effect of liquid holdup. There was little effect on the time scale and none on the steady state composition.

The results based on the derivation presented in Table VIII are summarized in the following statements.

The experimental data presented the initial conditions for the equations that were derived for a one section distillation column. The results obtained after the use of finite differences in the derivation did not correspond to the results as presented by Gerster. The steady state overhead vapor composition obtained by using the derived equations was 1.8 per cent different from Gerster's experimental data value of the steady-state overhead vapor composition based on the steady-state value Gerster obtained. However, the time scale value at steady state based on the derived equations was over 7 times smaller than the time Baber and Gerster's data reached steady state (10 minutes).

The equations that were derived by assuming that the vapor and liquid compositions in the derivative were average values of composition are presented in Table IX and produced results as follows. The program of this method is presented in Appendix D. The steady state overhead vapor composition was the same as obtained without the previous made assumption but the time at which steady state was reached was over 14 times smaller than Gerster's data. Therefore, this method offers no improvement over the method formed initially.

The next step in finding a reason why the time scale did not give the correct results was to assume that a distillation

TABLE IX

SUMMARY EQUATION FOR SPECIAL PROBLEM<sup>(5)</sup>

$$\delta_L \frac{d\bar{x}}{dt} = x_o L - K (y_B^* - y_w) - x_B L$$

$$\delta_V \frac{d\bar{y}}{dt} = y_w V + K (y_B^* - y_w) - y_1 V$$

$$y_w = (v_{wI}/l_{BI})(L/V) x_B$$

$$y_B^* = 0.01368 + 1.9221 (x_B) - 1.3639 (x_B^{2.0})$$

$$\bar{x} = (x_o + x_B) / 2$$

$$\bar{y} = (y_1 + y_w) / 2$$

column would have a "lag time" because of a disturbance in an input flow. In other words, the response to a reflux composition change in the bottoms would be delayed until the composition profiles were changed throughout the column. Since the equations are in a closed loop and only one section is considered, they react instantaneously to the initial disturbance and therefore do not allow a correct time to be obtained.

Based on the above assumption and trial and error, the liquid and vapor holdup were each multiplied by the constant 10 and used in the equations to calculate the new value of time. The overhead steady-state composition was as previously calculated but the time to reach steady state was now approximately 10 minutes. A plot of the results obtained based on the derived equations is presented in Figure 7. Figure 7 also presents the experimental time-overhead composition data of Gerster. The maximum per cent difference between the two overhead vapor compositions based on the experimental data was 3.6 per cent at about 0.5 minute.

The equations using the derivative of the average compositions presented the same results when a multiple of 20 times the liquid and vapor holdup was used.

The equations of Table I were used as the basis for a program that was used on the IBM 1620. This program was written in order that the results computed by the analog computer might be checked and compared. This program is presented in Appendix E. The overall conclusion was that the digital computer verified the steady-state results as computed on the analog computer.

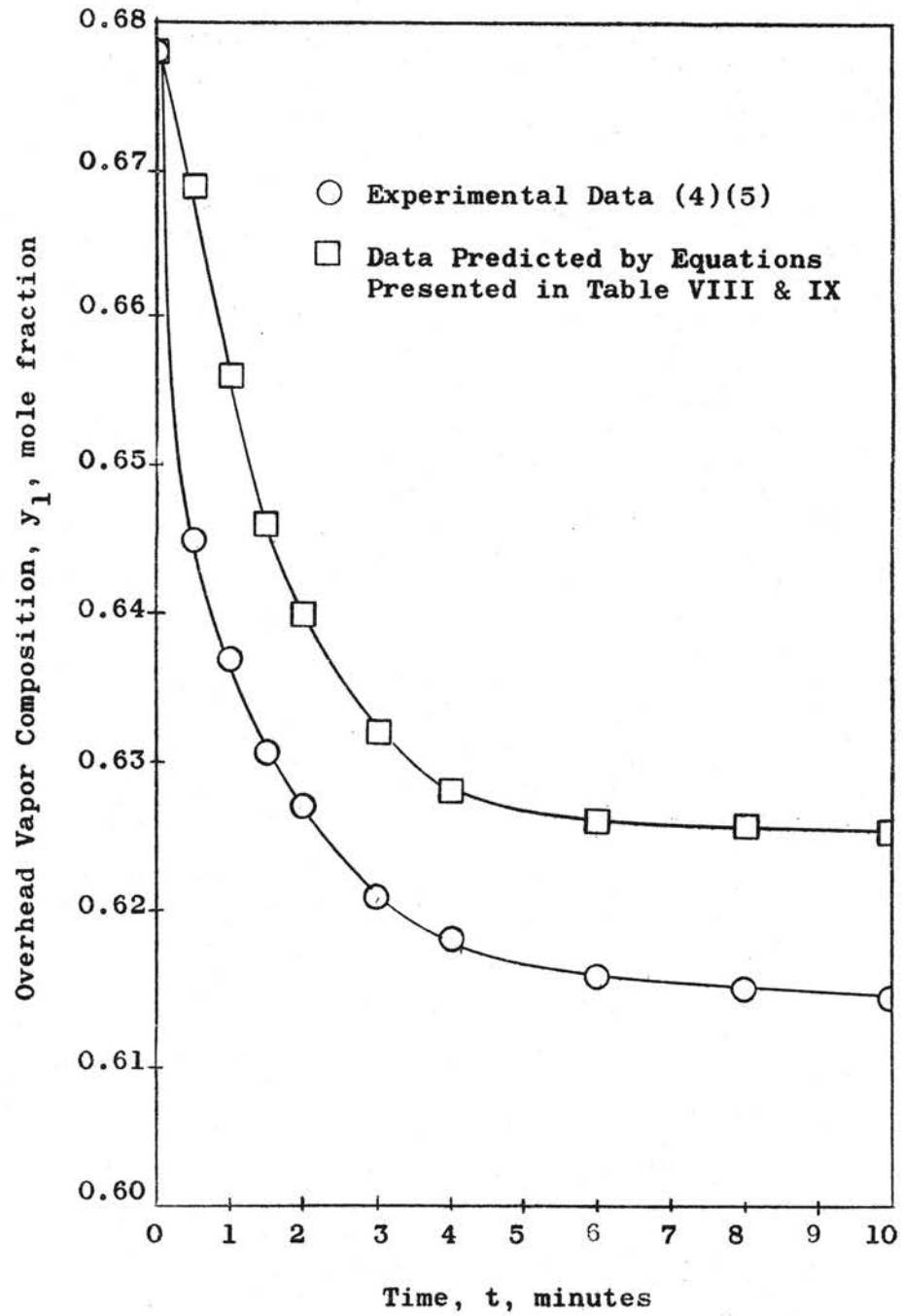


Figure 7 Comparison of Mathematical Models and Experimental Data.



## CHAPTER VI

### APPARATUS

The derived equations were programmed for the Donner Analog Computer. There were two analog computers which consisted of the following Donner Models: Model 3400, Model 3750, Model 3430, Model 3071, and Model 3073. An Electronics Associates Incorporated Variplotter (1100-E) was also available.

The Model 3400 contains ten d-c amplifiers and also is the control panel for the other accessories. The control panel includes power switch, initial condition settings, amplifier overload lights, voltmeter, and other instruments necessary for the analog operation.

The Model 3750 is a function generator which can simulate a continuous function of a variable. The curve can be approximated by 24 straight line segments. This unit was used to hold the equilibrium data.

The Model 3430 is a problem board which has terminals for the following:

- 10 operational amplifiers
- 5 initial condition supplies
- 2 electronic multiplier channels
- 1 function generator
- 10 ground points
- 2 fixed bias multipliers (105V and -105V)

The Model 3071 and Model 3073 are one-turn and ten-turn potentiometer strips, respectively. The Model 3073 is more

accurate than the Model 3071. These strips are used to obtain coefficients which are used to proportion voltages.

The variplotter (1100-E) is a table-top analog data recorder. The data can be plotted as a continuous inked line or as points along the contour of a curve. The variplotter plots one variable d-c voltage as a function of a second variable d-c voltage.

Resistors and capacitors are used across amplifiers for the purpose of obtaining a summer or integrator, respectively. Resistors are used to obtain the proper gain for summers and integrators. The accuracy of the resistors depends upon the magnitude of the resistance. The 5.0 and 10.0 meg-ohm resistors all have an accuracy of one percent. The 2.0, 1.0, 0.5, 0.2 and 0.1 meg-ohm resistors all have 0.1 percent accuracy. The 1.0, 0.1 and 0.01 micro-farad capacitors all have 0.1 percent accuracy.

## CHAPTER VII

### CONCLUSIONS

1. The equations of Simplified Method I will simulate a distillation column when large decreases in feed composition arise and for small increases in feed composition.
2. The equations of Simplified Method II will simulate a distillation column when only small changes in feed composition are made.
3. The results obtained, based on the derived equations which did not completely agree with experimental data, lead one to believe that exaggerating the element size is not a completely valid assumption.

## CHAPTER VIII

### RECOMMENDATIONS

- I. The literature survey has revealed that experimental unsteady-state data in distillation are insufficient. Therefore, I propose that experimental work be undertaken in a:
  - A. Batch Column
    1. Run other binary systems that are not presented in the paper by (4) under similar disturbances.
    2. Run ternary systems and then multicomponent systems under the disturbance conditions stated previously.
  - B. Continuous Column
    1. Build a continuous distillation column and operate using the following systems at unsteady-state:
      - a. binary systems
      - b. ternary systems
      - c. multicomponent systems.
- II. The use of unsteady-state data obtained in the manner stated in (I) above to verify the results produced from the derived equations would then show that the assumption of exaggerating the element size was valid or invalid.

#### A SELECTED BIBLIOGRAPHY

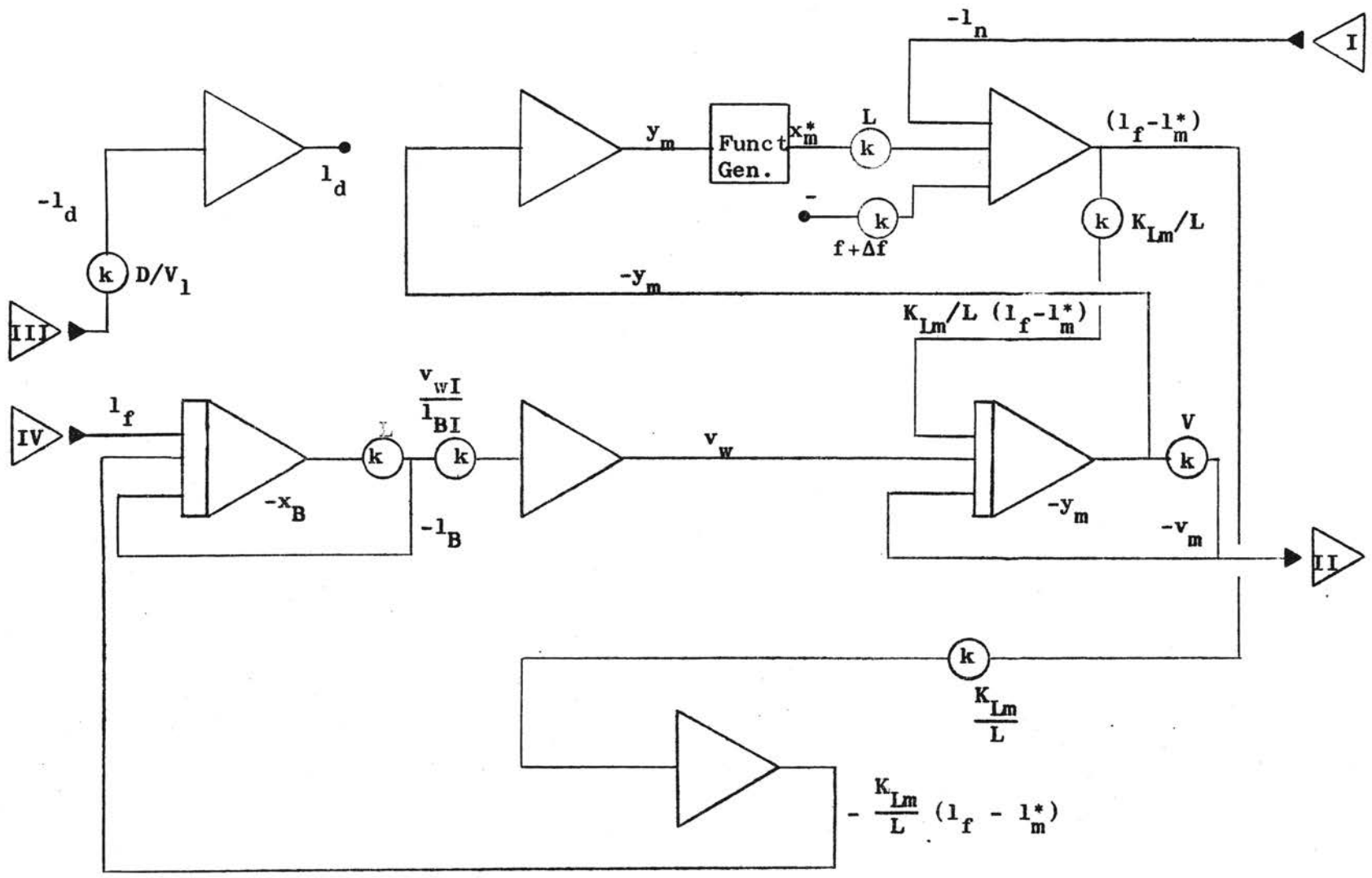
1. Acrivos, A. and Amundson, N. R., Ind. Eng. Chem., 45, 467, (1953).
2. Armstrong, W. D. and Wilkinson, W. L., Inst. Chem. Eng. Trans., 35, no. 5, 352-367, Oct., (1957).
3. Armstrong, W. D. and Wood, R. M., Inst. Chem. Eng. Trans., 39, no. 2, 65-79, (1961).
4. Baber, M. F. and Gerster, J. A., AICHE Jour., 8, no. 3, 407-415, July, (1962).
5. Baber, M. F., Edwards, L. L., Harper, W. T., Witte, M.D. & Gerster, J. A., CEP Sym., 57, no. 36, p. 141, (1961).
6. Barden, J., Phys. Rev., 57, 35, (1940).
7. Berg, C. and James, I. J., Chem. Eng. Prog., 44, 307, (1948).
8. Biery, J. C. and Boylan, D. R., Ind. Eng. Chem. Fund., 2, no. 1, Feb., (1963).
9. Cohen, K., Jour. Chem. Phys., 8, 588, (1940).
10. Davidson, J. F., AICHE Trans., 34, no. 1, 44-52, (1956).
11. Erbar, J. H., and Maddox R. N., Oil & Gas Journ., 57, no. 18, 116, (1959).
12. Erbar, J. H., and Maddox, R. N., Refining Engr., 31, no. 10, C-35, (1959).
13. Huffman, J. R. and Urey, H. C., Ind. Eng. Chem., 29, 521, (1937).
14. Jackson, R. F. and Pigford, R. L., Ind. Eng. Chem., 48, 1020-1026, June, (1956).
15. Maddox, R. N., and Erbar, J. H., "Plate-to-Plate Calculation on the IBM 650 Computer", Unpublished memorandum, School of Chemical Engineering, Oklahoma State University, Stillwater, Oklahoma, (1958).
16. Marr, G. R., National Meeting of AICHE, May, (1962).

17. Perry, J. H., "Chemical Engineers' Handbook", 3rd ed., (1950).
18. Rose, A. and Johnson, R. C., Chem. Eng. Prog., 49, 15, (1953).
19. Rose, A., Johnson, C. L. and Williams, T. J., Ind. Eng. Chem., 48, 2284, (1955).
20. Rose, A. and Williams, T. J., Ind. Eng. Chem., 47, 2284, (1955).
21. Rosenbrock, H. H., Inst. Chem. Eng. Trans., 35, no. 5, 347-352, Oct., (1957).
22. Rosenbrock, H. H., British Chem. Eng., 3, no. 7, 364-367, July, (1958).
23. Rosenbrock, H. H., Inst. Chem. Eng. Trans., 38, no. 6, 279-287, (1960).
24. Webster, W. D., Martin, R. L., Pink, J. F., and Hargett, J. T., Proc. Am. Petrol. Inst., 39, Sec. III, 114-119, (1959).
25. Wilkinson, W. L. and Armstrong, W. D., Chem. Eng. Sci., 7, No. 1-2, 1-7, (1957).
26. Williams, T. J. and Marnett, R. T., Chem. Eng. Prog., 53, no. 5, May, (1957).

**APPENDIX A**

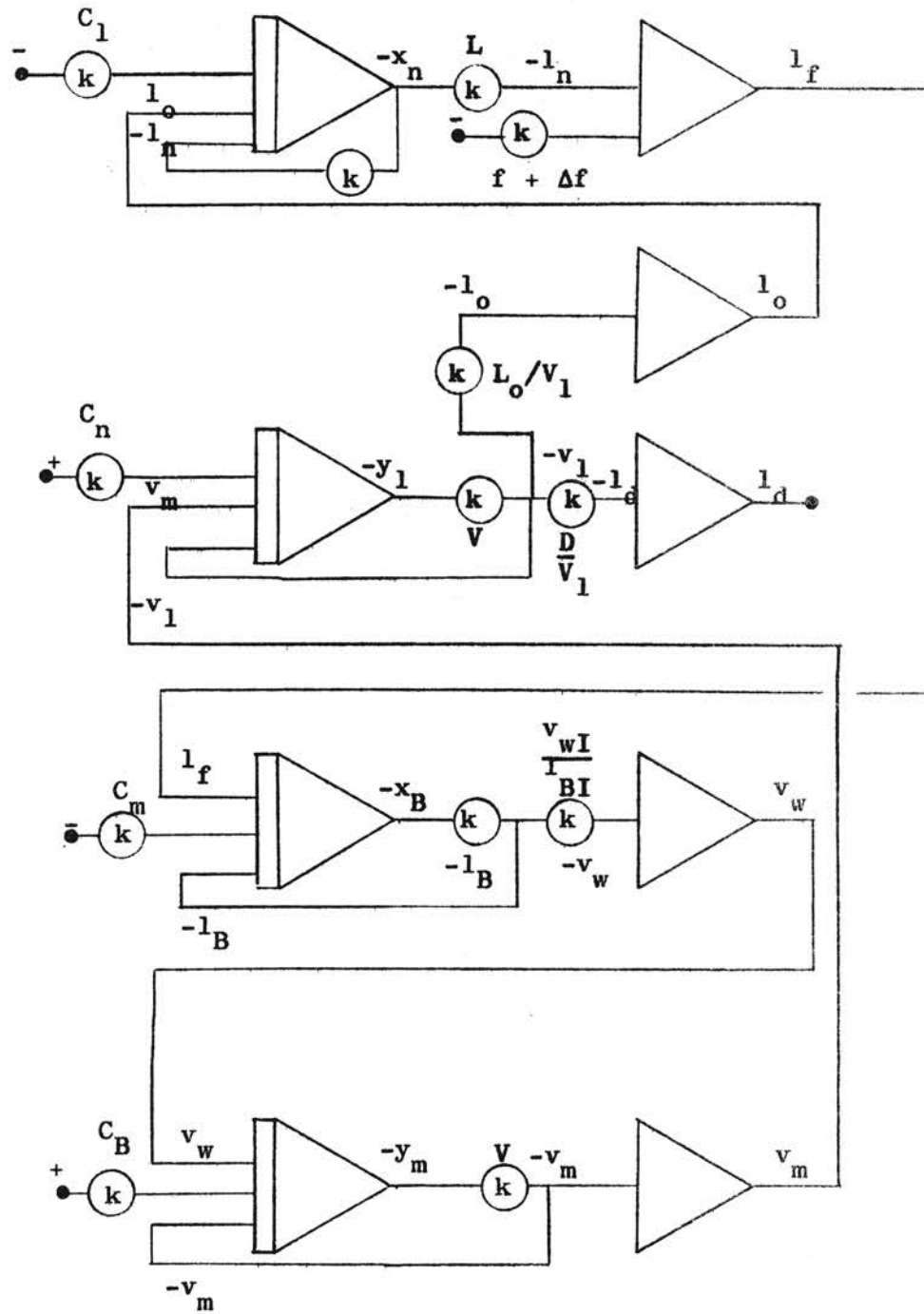






**APPENDIX B**

## Analog Program - Simplified Method II



**APPENDIX C**

FORTRAN STATEMENTS  
FOR SPECIAL PROBLEM (5)

```

160 READ 100,T,DELTA,HV,HA,L
    READ 110,YO,XB,COER,XO,A,V
100 FORMAT(F10.5,F10.5,F10.5,F10.5,I3)
110 FORMAT(F10.5,F10.5,F10.5,F10.5,F10.5,F10.5)
    K=0
    N=T/DELTA
    TIME =0.0
    PRINT 170
170 FORMAT (7X2HY05X4HD1Y09X2HXB5X4HD1XB7X4HTIME//)
180 DO 140 I=1,N
    TIME=TIME+DELTA
    K=K+1
    VER=0.013678+1.9221*XB-1.3639*(XB**2.0)
    YW=XB*(0.424)
    TRAR=COER*(VER-YW)
    YOT=YO+DELTA*(YW*V+TRAR-YO*V)/HV
    XBT=XB+DELTA*(XO*A-TRAR-XB*A)/HA
    DIYO=(YO-YOT)*100.0/YO
    DIXB=(XB-XBT)*100.0/XB
    YO=YOT
    XB=XBT
    IF (SENSE SWITCH 1) 150,160
150 IF (K-L)140,130,130
130 PRINT 99,YO,DIYO,XB,DIXB,TIME
    K=0
    99 FORMAT(F10.3,F10.5,F10.3,F10.5,F10.3)
140 CONTINUE
    GO TO 180
END

```

## FORTRAN SYMBOLS

- T = total time for machine to run.
- DELT = interval of time between each iteration.
- HV = vapor holdup, moles.
- HA = liquid holdup, moles.
- L = number of iterations before printout.
- YO = overhead vapor composition, mole fraction.
- XB = liquid composition leaving bottom of column, mole fraction.
- COER = mass transfer coefficient, moles/time (mass fraction).
- A = total liquid rate, moles/unit time.
- V = total vapor rate, moles/unit time.
- K = dummy variable which is used to print out after a certain number of iterations.
- N = number of iterations in time, T.
- TIME = initial time plus increment of time (DELT).
- VER = vapor equilibrium mole fraction obtained from curve-fit.
- YW = vapor composition leaving the reboiler, mole fraction.
- TRAR = mass transfer rate for vapor phase, moles/unit time.
- XBT = liquid composition leaving the bottom of the column at the new time (TIME + DELT), mole fraction.
- YOT = vapor composition leaving the top of the column at the new time (TIME + DELT), mole fraction.
- DIYO = percent difference between the previously calculated vapor composition (YO) and the one just calculated.
- DIXB = percent difference between the previously calculated liquid composition (XB) and the one just calculated.

**APPENDIX D**

FORTRAN STATEMENTS  
SPECIAL PROBLEM<sup>(5)</sup> USING AVERAGE COMPOSITIONS

```

160 READ 100,T,DELT,HV,HA,L
    READ 110,YO,XB,COER,XO,A,V
100 FORMAT(F10.5,F10.5,F10.5,F10.5,13)
110 FORMAT(F10.5,F10.5,F10.5,F10.5,F10.5,F10.5)
    K=0
    N=T/DELT
    TIME =0.0
    PRINT 170
170 FORMAT (7X2HY05X4HDIY09X2HXB5X4HDI XB7X4HTIME//)
180 DO 140 I=1,N
    TIME=TIME+DELT
    K=K+1
    VER=0.013678+1.9221*XB-1.3639*(XB**2.0)
    YW=XB*(0.424)
    TRAR=COER*(VER-YW)
    YOX=(YO+YW)/2.0
    XBX=(XB+XO)/2.0
    XBT=XBX+DELT*(XO*A-TRAR-XB*A)/HA
    XBT=2.0*XBT-XO
    YOT=YOX+DELT*(YW*V+TRAR-YO*V)/HV
    YOT=2.0*YOT-(0.424)*(XBT)
    DIYO=(YO-YOT)*100.0/YO
    DIXB=(XB-XBT)*100.0/XB
    YO=YOT
    XB=XBT
    IF (SENSE SWITCH 1) 150,160
150 IF (K-L)140,130,130
130 PRINT 99,YO,DIYO,XB,DIXB,TIME
    K=0
    99 FORMAT(F10.3,F10.5,F10.3,F10.5,F10.3)
140 CONTINUE
    GO TO 180
    END

```



## FORTRAN SYMBOLS

- T = total time for machine to run.
- DELT = interval of time between each iteration.
- HV = vapor holdup, moles.
- HA = liquid holdup, moles.
- L = number of iterations before printout.
- YO = overhead vapor composition, mole fraction.
- XB = liquid composition leaving bottom of column, mole fraction.
- COER = mass transfer coefficient, moles/time (mass fraction).
- A = total liquid rate, moles/unit time.
- V = total vapor rate, moles/unit time.
- K = dummy variable which is used to print out after a certain number of iterations.
- N = number of iterations in time, T.
- TIME = initial time plus increment of time (DELT).
- VER = vapor equilibrium mole fraction obtained from curve-fit.
- YW = vapor composition leaving the reboiler, mole fraction.
- TRAR = mass transfer rate for vapor phase, moles/unit time.
- YOX = average vapor composition in column.
- XBX = average liquid composition of the column as predicted by the derived equations.
- XBT = average liquid composition at time zero plus delta time (TIME + DELT).
- YOT = average vapor composition of the column as predicted by the derived equations at time zero plus delta time (TIME + DELT)

XBT = liquid composition leaving the bottom of the column at the new time (TIME + DELT), mole fraction.

YOT = vapor composition leaving the top of the column at the new time (TIME + DELT), mole fraction.

DIYO = percent difference between the previously calculated vapor composition (YO) and the one just calculated.

DIXB = percent difference between the previously calculated liquid composition (XB) and the one just calculated.

**APPENDIX E**



## FORTRAN SYMBOLS

- F = initial feed rate plus change of feed rate of one component, moles/hour.
- T = maximum time for machine to run.
- DELTA = interval of time between each iteration.
- L = number of iterations before printout.
- TVO = total vapor overhead rate, moles/hour.
- D = total distillate rate, moles/hour.
- V = total vapor rate in the column, moles/hour.
- A = total liquid rate in the column, moles/hour.
- TAO = total reflux rate into column, moles/hour.
- AB = liquid rate leaving the bottom of column, moles/hour.
- AF = liquid rate entering the feed section, moles/hour.
- VO = vapor rate of a component overhead, moles/hour.
- VF = vapor rate of a component leaving the feed section.
- VW = vapor rate of a component leaving the reboiler.
- COER = vapor mass transfer coefficient for the rectifying section, moles/ hour (mass fraction).
- COES = vapor mass transfer coefficient for the stripping section, moles/hour (mass fraction).
- K = dummy variable.
- COER = redefined as the rectifying section mass transfer coefficient over the total vapor rate, dimensionless.
- COES = redefined as the stripping section mass transfer coefficient over the total vapor flow rate, dimensionless.
- C = ratio of initial flow rates for the calculation of the vapor flow rate leaving the reboiler, dimensionless.

- CC = ratio of total flow rates for the calculation of the distillate flow rate of one component, dimensionless.
- CCC = ratio of total flow rates for the calculation of the reflux rate of one component, dimensionless.
- N = number of iterations in time, T.
- TIME = initial time plus increments as calculation proceeds, hours.
- VER = vapor equilibrium concentration rate in the rectifying section, moles/hour.
- TRAR = mass transfer rate of one component leaving the liquid phase in the rectifying section, moles/hour.
- AO = reflux rate of a component, moles/hour.
- AFT = liquid flow rate of a component entering the feed section after an increment of time, moles/hour.
- VOT = vapor flow rate of a component overhead after an increment of time, moles/hour.
- AD = distillate flow rate of one component, moles/hour.
- VES = vapor equilibrium concentration rate in the stripping section, moles/hour.
- TRAS = mass transfer rate of one component leaving the liquid phase in the stripping section.
- AFB = liquid flow rate of one component entering the stripping section.
- VFT = vapor flow rate of a component leaving the feed section after an increment of time.
- ABT = liquid flow rate of a component leaving the stripping section after an increment of time.

## NOMENCLATURE

- $a$  = interfacial area,  $\text{ft}^2/\text{ft}^3$ .
- $C$  = mass transfer rate for equations of Simplified Method II.
- $D$  = total value of the distillate rate, moles/unit time.
- $H$  = liquid holdup on a plate, moles.
- $h$  = vapor holdup on a plate, moles.
- $L$  = total liquid flow rate, moles/unit time.
- $l$  = liquid flow rate of a component, moles/unit time.
- $k$  = a potentiometer.
- $K$  = mass transfer coefficient, moles/unit time (mass fraction).
- $K_i$  = mass transfer coefficient, moles/unit time (mass fraction)  
volume.
- $N$  = moles transferred from one phase to another, moles/unit time.
- $n$  = number of components.
- $S$  = cross sectional area, square feet.
- $t$  = time, hours.
- $V$  = total vapor flow rate, moles/unit time.
- $v$  = vapor flow rate of a component, moles/unit time.
- $x$  = liquid mole fraction, dimensionless.
- $\bar{x}$  = average liquid mole fraction, dimensionless.
- $y$  = vapor mole fraction, dimensionless.
- $\bar{y}$  = average vapor mole fraction, dimensionless.
- $Z$  = height in a section

## GREEK LETTERS

$\beta$  = distance up the column.

$\delta_L$  = liquid holdup in a section, moles.

$\delta_V$  = vapor holdup in a section, moles.

$\mu_L$  = fraction of section liquid.

$\mu_V$  = fraction of section vapor.

$\rho_M$  = molar density, moles/unit volume.

## SUBSCRIPTS

B = bottom of the column.

d = distillate.

f = entering liquid to stripping section.

i = individual component.

I = initial value.

o = entering liquid to rectifying section.

l = top of distillation column.

L = liquid phase.

m = feed plate.

n = plate (n), bottom plate rectifying section.

R = rectifying section.

S = stripping section.

V = vapor phase.

w = reboiler output.

## SUPERSCRIPTS

\* = equilibrium concentration of liquid or vapor.



VITA

David LeRoy Reynolds

Candidate for the Degree of

Master of Science

Thesis: A SIMPLIFIED MODEL FOR PREDICTING DISTILLATION COLUMN  
DYNAMICS

Major Field: Chemical Engineering

Biographical:

Personal Data: Born in Enid, Oklahoma, May 7, 1939, the  
son of Clyde D. and Emily A. Reynolds. Married to  
Glenda L. Reed, Pond Creek, Oklahoma, in May, 1957.

Education: Attended elementary school in Pond Creek,  
Oklahoma; graduated from Pond Creek High School in  
1957; received the Bachelor of Science degree in  
Chemical Engineering from Oklahoma State University  
in 1962, completed requirements for the Master of  
Science degree May, 1964.

Professional Experience: Employed as a chemical engineer in  
Pilot Plant Laboratory with Continental Oil Company  
in the summer of 1962.