To the Graduate Council:

I am submitting herewith a thesis written by Qamar Haris Manzoor entitled "Computer Aided Distillation Design." I have examined the final copy of this thesis for form and content and recommend that it be accepted in partial fulfillment of the requirements for the degree of Master of Science, with a major in Chemical Engineering.

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COMPUTER AIDED DISTILLATION DESIGN

A Thesis

Presented for the

Master of Science

Degree

The University of Tennessee, Knoxville

Qamar Haris Manzoor

March 1984

ACKNOWLEDGEMENTS

The author would like to extend his sincere appreciation to Dr. G.C. Frazier for his guidance, advice, help and support throughout the duration of his stay at The University of Tennessee, Knoxville. He must also thank Dr. Fred Weber for assisting him in using the computer routine. He would also like to thank Dr. J.M. Holmes for the interest and cooperation extended by him during this work. Appreciation is also expressed to Mrs. Phyllis Davis, who assisted in the typing of this thesis.

Finally, his mother, who allowed him to be absent from responsibilities and kept him free from all worries, deserves to be mentioned. He is grateful to her.

ABSTRACT

A computer assisted distillation design code has been developed for optimizing distillation columns with respect to minimizing total annual cost for certain binary and certain multicomponent systems. Two classes of binary systems are considered. The first class contains systems whose vapor-liquid equilibrium data can be characterized by a single, constant value of relative volatility. This approximation holds reasonably well for ideal mixtures. An example of a system considered which is approximately ideal is the Benzene-Toulene system. The second class of binary systems considered is that whose members exhibit an inflexion point when their vapor-liquid equilibrium data are plotted as composition in liquid and vapor phase. This behavior is somewhat representative of relatively highly non-ideal systems. An example of this kind of system is the aqueous solution of ethanol. The computer code in both cases is based on the McCabe-Thiele method of determining the number of theoretical plates required to produce a specified distillate/bottom split for a specified reflux ratio. The code for the system is developed to optimize the design based upon minimizing the total annual cost using cost data and the cost as a function of tower size curves provided by Peters and Timmerhaus. The optimization is done by establishing the optimum reflux ratio which yields the minimum total annual cost.

In the multicomponent case, the systems which are reasonably ideal, such as mixture of certain light hydrocarbons, are considered. The code is based upon the short cut method as presented by Treybal, and the published computer code of Chang. The task common to all the programs is the development of analytical equations which provide a reasonable fit to the property data, especially to the vapor-liquid equilibrium data of the systems. This task is accomplished by a published regression analysis routine.

TABLE OF CONTENTS

CHAPTER	PAGE
1. INTRODUCTION	1
1.1 The Problem	1
1.2 Objectives of the Work	5
1.3 Methodology and Approach	5
2. LITERATURE BACKGROUND	7
2.1 Binary Distillation	7
2.2 Multicomponent Distillation	20
2.3 Curve Fitting Techniques for Property Data	26
2.4 Cost Estimation Methods for Distillation Columns	29
3. COMPUTER CODE FOR BINARY DISTILLATION	31
3.1 Models for the Equilibrium Curve and Data Fitting	33
3.2 Code for Column Design	40
3.3 Optimizing the Design	67
4. COMPUTER CODE FOR MULTICOMPONENT DISTILLATION	80
5. SUMMARY AND CONCLUSIONS	92
6. RECOMMENDATIONS FOR FUTURE WORK	96
LIST OF REFERENCES	99
APPENDICES	102
APPENDIX A. CODE FOR BINARY DISTILLATION	103
APPENDIX B. CODE FOR MULTICOMPONENT SYSTEM	112
VITA	118

LIST OF TABLES

TABLE		PAGE
1.1.	Specific Energy of Distillation for Petroleum Refining and Natural Gas Liquids Columns	2
2.1.	Equilibrium Concentration Data for Benzene-Toulene System	12
2.2.	Equilibrium Concentration Data for Ethanol-Water System	15
2.3.	Papers on Computer Assisted Binary Distillation	21
2.4.	Papers on Multicomponent Distillation	27
3.1.	Summary of Binary Equilibrium Data as fit by Six Models by Regression Analysis	43
3.2.	Code for Estimation of Number of Theoretical Plates	50
3.3.	Comparison of Results of a Benzene-Toulene Separation Example Problem for Q = 1.0	57
3.4.	Comparison of Results for a Benzene-Toulene Separation Example Problem for Q = 1.37	58
3.5.	Comparison of Results for an Ethanol-Water Separation Example Problem for Q = 1.37	63
3.6.	Code for Calculating Tower Diameter	68
3.7.	Cost Data for Condenser--Tube and Shell Heat Exchanger	73
3.8.	Cost Data for Reboiler--Tube and Shell Heat Exchanger	74

TABLE PAGE

3.9. Code for Calculating Total Annual Cost 77

3.10. Comparison of Results for an Example to Determine Total Annual Cost at Optimum Reflux Ratio 79

4.1. Summary of VLE Relationship for Selected Light Hydrocarbons at 150 psia as Fitted by a Model by Regression Analysis 83

4.2. Comparison of the Results for a Multicomponent Separation Example Problem 91

LIST OF FIGURES

FIGURE		PAGE
2.1.	Fractionater	9
2.2.	McCabe-Thiele Method for Benzene-Toulene System . . .	11
2.3.	McCabe-Thiele Method for Ethanol-Water System	13
2.4.	Ponchon-Savarit Method for Acetone-Water System . . .	17
3.1.	Equilibrium Data for Benzene-Toulene System at One Atmosphere	34
3.2.	Equilibrium Data for Benzene-Ethylenedichloride System at One Atmosphere	35
3.3.	Equilibrium Data for Ethanol-Water System at One Atmosphere, Models C and D	37
3.4.	Equilibrium Data for Ethanol-Water System at One Atmosphere, Model F	38
3.5.	Equilibrium Data for Ethanol-Water System at One Atmosphere, Model G and H	39
3.6.	Equilibrium Data for Methanol-Water System at One Atmosphere, Models C, D and E	41
3.7.	Equilibrium Data for Acetone-Water System at One Atmosphere, Model C	42
3.8.	Flow Chart for Estimating Number of Theoretical Plates for Ideal Systems	46
3.9.	Estimating Number of Theoretical Plates for Benzene-Toulene System	56

FIGURE PAGE

3.10. Calculating Minimum Reflux by Tangent for Ethanol-Water System 59

3.11. Calculating Minimum Reflux by Intersection of Q-Line and Equilibrium Curve for Ethanol-Water System 61

3.12. Flow Chart for Estimating Tower Diameter 65

3.13. Tray Spacing as a Function of Tower Diameter 66

3.14. Cost of Towers Including Installation and Auxiliaries 69

3.15. Optimum Reflux Ratio in Distillation Operation 75

3.16. Flow Chart for Calculating Total Annual Cost 76

4.1. VLE Relationships for Selected Light Hydrocarbons . . 82

4.2. Flow Chart for Short Cut Method for Multicomponent System 89

LIST OF SYMBOLS

A	Tower cross sectional area, ft^2
D	Quantity of distillate taken off
G'	Superficial gas mass velocity, lb/ft^2hr
L	Quantity of liquid passing down
L'	Superficial liquid mass velocity, lb/ft^2hr
N	Number of stages
N_m	Minimum number of stages
Q	Thermal condition feed stream
R	Reflux ratio
R_m	Minimum reflux ratio
TD	Tower diameter, ft
V	Quantity of vapor passing up
x	Liquid mole fraction
x_D	Mole fraction in distillate
x_W	Mole fraction in bottom
y	Vapor mole fraction
Z_F	Mole fraction in feed

Greek

α	Relative volatility (alpha)
ϕ	Parameter in Underwood's equation
Σ	Summation
σ	Surface tension, dyn/cm x 10^{-3}

Subscripts

i,J	Individual component identifier
LK	Light key component
HK	Heavy key component

CHAPTER 1

INTRODUCTION

1.1 The Problem

Distillation is a common and important operation in the chemical process industries. It is the most widely practiced technique for separating mixtures of chemical species (U.S. Department of Energy, 1980). Its application ranges from the separation of heavy petroleum fractions to the separation of liquefied air. Our society depends upon distillation to provide the abundant energy and synthetic materials so essential to our modern life-style.

Distillation is an energy intensive separation process. It is the key process in petroleum refining, refining of liquids derived from coal and organic chemical processing. The bulk of distillation energy is consumed in the petroleum, chemical and natural gas processing industries. A study based on these industries estimated the annual national distillation energy consumption to be about 3% of the total U.S. energy consumption, or the equivalent of 315 million barrels of fuel oil per year (U.S. Department of Energy, 1980). The values of the specific energy consumption of some typical distillation operations in chemical and petroleum industries are shown in Table 1.1. (U.S. Department of Energy, 1980). These energy consumptions depend upon nature of feed, the operating conditions and the most important being the reflux ratio.

Table 1.1. Specific Energy of Distillation for Petroleum Refining and Natural Gas Liquids Columns.

Column description	Specific distillation energy consumption, Btu/lb charged	Key components	Number of trays	Reboiler temperature, °F	Condenser temperature, °F
Petroleum operations					
Crude distillation	193	Light naphtha/heavy naphtha, light distillate/heavy distillate, atmospheric gas oil/reduced crude	20-65	650-750	100-350
Vacuum distillation	132	Light vacuum gas oil/heavy vacuum gas oil/residue	9-14	700-800	150-250
Alkylation					
H_2SO_4					
Deisobutanizer	510	Isobutane/n-butane/isopentane	50	330	165
Deisopropanizer	510	Propane/isobutane	27	200	120
HF					
Deisobutanizer	436	Isobutane/n-butane/isopentane	50	300-350	160
Depropanizer	382	n-Propane/isobutane	60	200	130
Propylene by-product	206	Propylene/propane	20	155	145
Rerun column	22	n-Butane/polymer	5	400	200
Catalytic hydrotreating and hydrorefining	101	Hydrogen sulfide, C_1-C_4/naphtha/furnace oil	20-40	300-600	150-330
Catalytic cracking fractionator	112	C_1-C_4/gasoline/light gas oil/heavy gas oil/slurry decant oil	30	675	150-300
Naphtha fractionator					
Catalytic cracking	132	n-Butane/isopentane	35	350-500	150-200
Crude atmospheric	132	n-Butane/isopentane	35	350-500	150-200
Thermal operations	132	n-Butane/isopentane	35	350-500	150-200
Catalytic hydrocracking	632	C_1-C_4/naphtha/diesel/bottoms	10-40	400-900	100-350
Catalytic reforming	132	C_1-C_4/gasoline	35	350-500	150-200
Sour-water strippers	240	Hydrogen sulfide/ammonia/water	40	260	240

Table 1.1. (Continued)

Column description	Specific distillation energy consumption, Btu/lb charged	Key components	Number of trays	Reboiler temperature, °F	Condenser temperature, °F
Light-ends processing					
Depropanizer	365	Propane/isobutane	30-50	220-260	120-140
De-ethanizer	137	Ethane/propane	20-40	190	50
Iso/n-butane splitter	153	Isobutane/n-butane	60-80	130-120	100-180
Debutanizer	44	n-Butane/isopentane	30-50	300-450	150-200
Isomerization					
C_4 feed deisobutanizer	1107	Isobutane/n-butane	60-80	130-210	100-180
C_5 feed deisopentanizer	664	Isopentane/n-pentane	60-80	135-215	120-200
C_5+C_6 feed deisopentanizer	664	Isopentane/n-pentane	60-80	150-250	120-200
Natural gas processing					
De-ethanizer	265	Ethane/propane	30-50	120-150	0-20
Depropanizer	235	Propane/isobutane	30-50	220-240	120-140
Iso/n-butane splitter	204	Isobutane/n-butane	60-80	130-210	100-180
Debutanizer	105	n-Butane/isopentane	30-50	260-280	150-200
Iso/n-pentane splitter	12	Isopentane/n-pentane	60-80	145-225	115-195
Depentanizer	6	n-Pentane/hexane	30-50	300-350	250

Data Source: Energy Conservation in Distillation, U.S. Department of Energy, 1980.

As reflux ratio is increased the number of theoretical stages required for given separation decreases. An increase in reflux ratio therefore may result in lower fixed charges for the distillation column and greater cost for the reboiler heat and condenser coolant. Proper distillation design is a compromise between energy consumption and the capital cost.

Established design procedures, e.g., McCabe and Thiele, Ponchon and Savarit, for binary systems are tedious and time consuming. In order to optimize a given separation with respect to minimizing total annual cost, these similar design procedures may have to be considered in which operating variables such as reflux ratio are varied over a wide range in order to find the optimum. Therefore, optimizing a process stream which includes distillation operation by hand calculations is especially very tedious and time consuming, more over, it involves quite complex calculations which are subject to error. Computers lend themselves readily to methods which involve repeated calculations. The calculation procedure which involves numbers of iterations are best done by computers to save a lot of time and money. Wide spread availability of computers ranging in size from small personal models to large main frame machines provides the opportunities in computer assisted distillation design.

In multicomponent distillation the procedure involves a lot of trial and error calculations which are far more tedious and subject to error. Using the computer could save a lot of time for

the calculation for the design procedure which itself is a very tedious process.

1.2 Objectives of the Work

The objective of this research is to develop a computer code to design a tray type distillation column for separation of certain binary systems and multicomponent mixtures. The code will calculate the minimum reflux, the feed plate and the total number of plates for a given reflux ratio. Another objective is to optimize the total annual operating cost for the distillation of binary systems using the cost data as provided by Peters and Timmerhous (1980).

1.3 Methodology and Approach

In developing the program two types of systems are to be considered:

(a) Binary systems and

(b) Multicomponent systems.

(a) For binary systems two types of cases are considered, case when alpha (relative volatility) can be represented reasonably well by a single, constant value, e.g., Benzene-Toulene System, and case when alpha is variable e.g., Ethanol-Water System. The program also takes into account the different thermal feed conditions e.g., sub-cooled feed, saturated feed and partially vaporized feed. The established design procedure of McCabe and Theile (Treybal, 1979; McCabe and Smith, 1976; Perry, 1973) is used to develop the program. The binary system of Ethanol-Water is

considered as an example of the variable alpha case. A number of curve fitting techniques are applied to find an equation for equilibrium curve, and the one giving the best fit to the experimental data is used. The program is developed for optimizing the total annual operating cost by determining the optimum reflux and using the cost data and method discussed by Peters and Timmerhaus (1980).

(b) A computer code is developed for multicomponent systems using the short cut distillation technique which calculates the minimum reflux and the number of theoretical plates. The short cut method is an established technique for preliminary designing the distillation operations for multicomponent mixtures, these have been discussed in a number of books (Treybal, 1979; McCabe and Smith, 1976; AIChE Modular Instruction, 1981). The method developed by Huan Chang (1980) is adopted as a basis for developing the program.

CHAPTER 2

LITERATURE BACKGROUND

2.1 Binary Distillation

The separation of binary mixtures by continuous distillation can be calculated by two methods. These methods are used to develop the relationship between the number of trays, liquid/vapor ratios and product composition. The first method is of McCabe and Thiele (Treybal, 1979) which is less rigorous and requires vapor-liquid equilibrium data for its application. This method also takes into account the relative volatility α defined as the separating factor. The relative volatility is defined as the ratio of the concentration ratio of components A and B in one phase to that in the other (Treybal, 1979), and is a measure of the separability. Mathematically

$$\alpha = \frac{y(1-x)}{x(1-y)} \quad . \tag{2.1}$$

The value of α ordinarily changes as x varies from 0 to 1.0. If $y = x$ (except at $x = 0$ or 1.0), $\alpha = 1.0$ and no separation is possible. The larger the value of α above unity, the greater is the degree of separability. The second method is the method of Ponchon and Savarit (Treybal, 1979) which requires detailed enthalpy data for its application.

2.1.1 McCabe and Thiele method. This method is based on the assumptions of constant molar overflow, steady state and no heat losses. This method is a representation of the material balance equations as straight lines upon the x-y diagram. This method is found adequate except where heat losses are unusually large. In plotting the equilibrium curve it is assumed that the pressure is constant throughout the tower. Hence, within any section of the column where no material or energy is added or withdrawn the liquid L mole/hr falling from each tray and the vapor V mole/hr rising from each tray are constant.

Total material balance for the enriching section for the fractionator shown in Figure 2.1 is

$$V = L+D = D(R+1) \quad . \tag{2.2}$$

For component A

$$Vy_{n+1} = Lx_n+Dx_D \quad . \tag{2.3}$$

The operating line for enriching section is

$$y_{n+1} = \frac{L}{V} x_n + \frac{D}{V} x_D \tag{2.4}$$

and

$$y_{n+1} = \frac{R}{R+1} X_n + \frac{x_D}{R+1} \quad . \tag{2.5}$$

This is the equation of straight line on x-y diagram of slope L/V and intercept of $x_D/(R+1)$. Substituting $x_n = x_D$ in the equation (2.5) shows $y_{n+1} = x_D$ so the line passes through the point

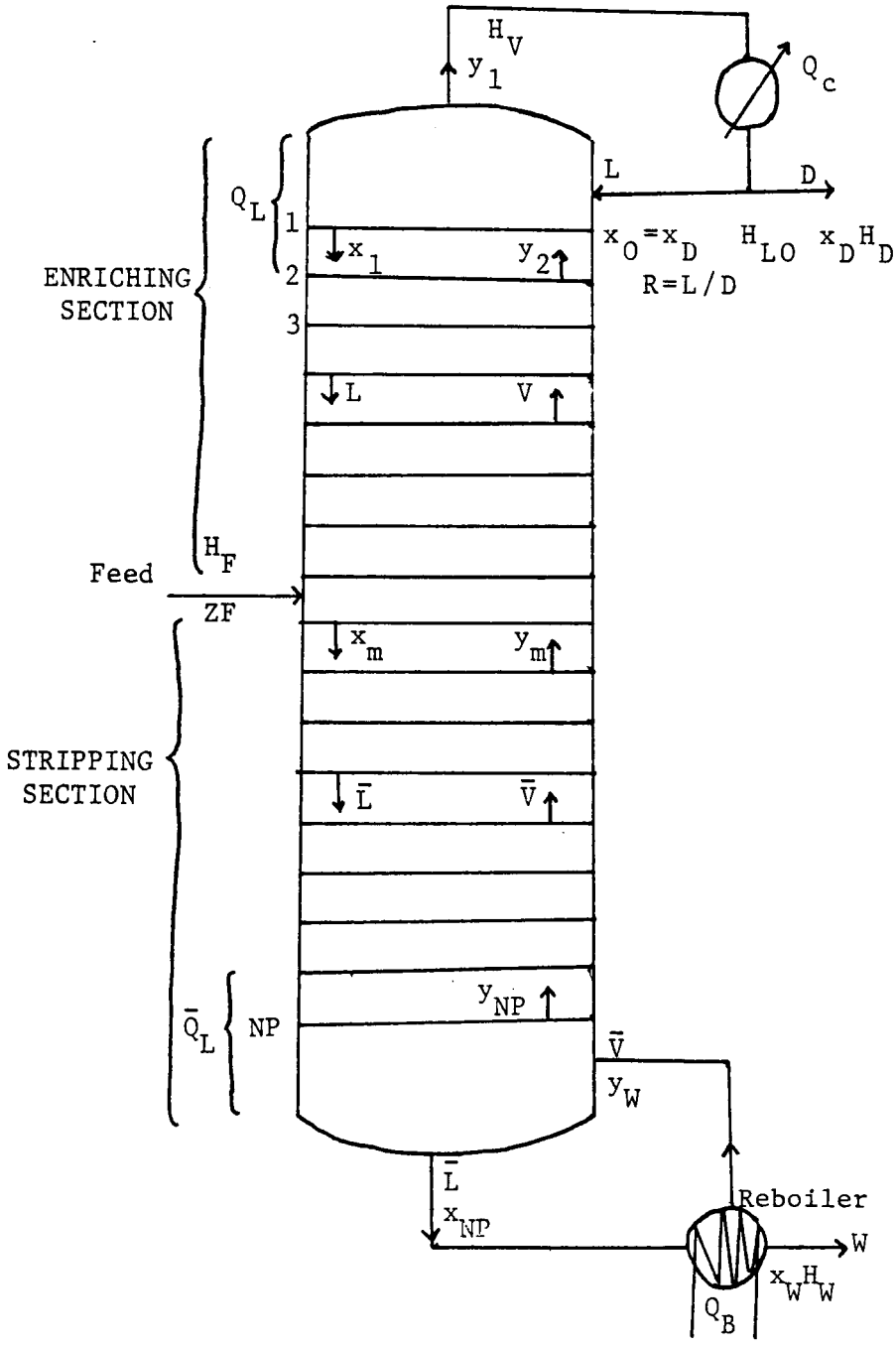


Figure 2.1. Fractionater.

$y = x = x_D$ on 45° diagonal. The staircase construction between operating line and equilibrium curve provides the theoretical plates. The construction cannot be carried further than the feed point.

A total material balance for stripping section for the fractionator (Figure 2.1) is

$$\bar{L} = \bar{V}+W \quad . \tag{2.6}$$

For component A

$$\bar{L}x_m = \bar{V}y_{m+1}+Wx_W \quad . \tag{2.7}$$

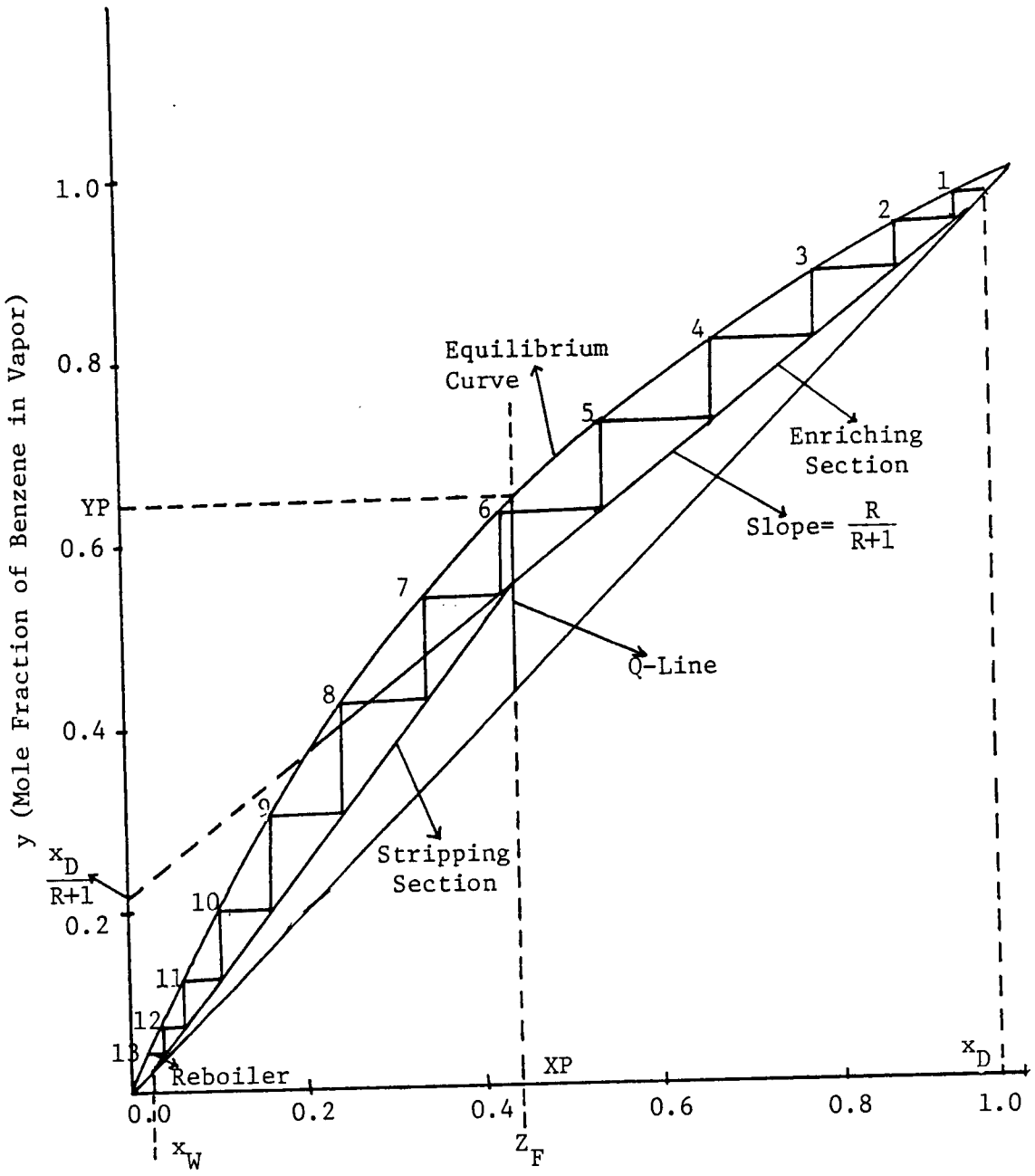
The equation of the stripping section operating line is

$$y_{m+1} = \frac{\bar{L}}{\bar{V}} x_m - \frac{W}{\bar{V}} x_W \tag{2.8}$$

and

$$y_{m+1} = \frac{\bar{L}}{\bar{L}-\bar{W}} x_m - \frac{W}{\bar{L}-\bar{W}} x_w \quad . \tag{2.9}$$

This is a straight line of slope $\bar{L}/\bar{V}$ and since when $x_m = x_W$, $y_{m+1} = x_W$ and the line passes through the point $x = y = x_W$ on the 45° diagonal. The number of trays are obtained by stepping down from equilibrium curve to the stripping section operating line. The Benzene-Toulene system is shown in Figure 2.2 and the equilibrium data is given in Table 2.1 as an example. The Ethanol-Water system is shown as an example of non constant alpha case in Figure 2.3 and the equilibrium data is given in



x (Mole Fraction of Benzene in Liquid)

Figure 2.2. McCabe-Thiele Method for Benzene-Toulene System.

Table 2.1. Equilibrium Concentration Data for Benzene-Toulene System.

Mol. Fraction of Benzene in Liquid,x	Mol. Fraction of Benzene in Vapor,y	Relative Volatility,
0.1	0.2063	2.339
0.2	0.3691	2.340
0.3	0.5007	2.340
0.4	0.6094	2.340
0.5	0.7006	2.340
0.6	0.7783	2.340
0.7	0.8452	2.340
0.8	0.9035	2.341
0.9	0.9547	2.342
1.0	1.0	-

Data Source: Unit Operations of Chemical Engineering, McCabe and Smith, 1976.

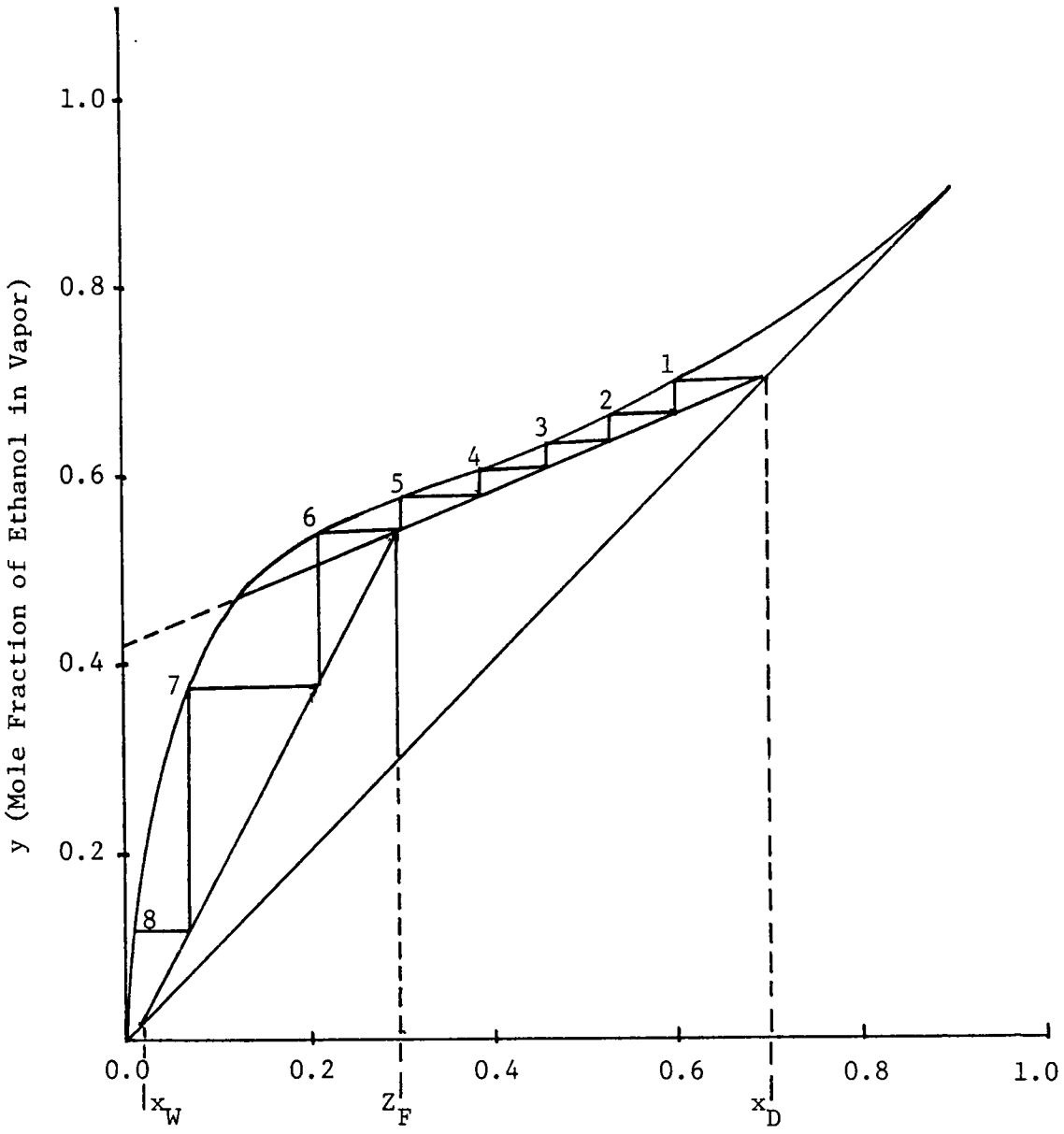


Figure 2.3. McCabe Thiele Method for Ethanol-Water System.

Table 2.2. The minimum reflux is obtained by the intersection points of equilibrium curve and Q-line and is calculated by the formula

$$R_m = (x_D - YP)/(YP - XP) \quad . \tag{2.10}$$

The method of McCabe and Thiele is used as the design procedure for the binary system distillation.

2.1.2 Ponchon and Savarit method. This method is more rigorous and does not require the same assumptions as described by previous method, but it requires detailed enthalpy data. The material balance on the fractionator gives

$$F = D+W \tag{2.11}$$

and

$$FZ_F = Dx_D + Wx_W \quad . \tag{2.12}$$

The complete enthalpy balance around the column is given as

$$Q_B = DH_D + WH_W + Q_C + Q_L - FH_F \quad . \tag{2.13}$$

In the absence of heat losses $Q_L = 0$ and we have

$$FH_F = DQ' + WQ'' \quad . \tag{2.14}$$

Eliminating F we get

$$\frac{D}{W} = \frac{Z_F - X_W}{X_D - Z_F} = \frac{H_F - Q''}{Q' - H_F} \quad . \tag{2.15}$$

Table 2.2. Equilibrium Concentration Data for Ethanol-Water System.

Mol. Fraction of Benzene in Liquid,x	Mol. Fraction of Benzene in Vapor,y	Relative Volatility,
0.0	0.0	
0.019	0.17	10.58
0.0721	0.3891	8.197
0.0966	0.4375	7.274
0.1238	0.4704	6.286
0.1661	0.5089	5.202
0.2337	0.5445	3.920
0.2608	0.5580	3.578
0.3273	0.5826	2.869
0.3965	0.6122	2.403
0.5079	0.6564	1.851
0.5198	0.6599	1.792
0.5732	0.6841	1.612
0.6763	0.7385	1.352
0.7472	0.7815	1.210
0.8943	0.8943	1.0

Data Source: Chemical Engineers Handbook, John H. Perry, IV Edition, 1963.

Equation (2.15) is the equation of straight line on the enthalpy diagram through (Q',x_D) at Δ_D, (H_F,Z_F) at F and (Q'',x_W) at Δ_W. In other words

$$F = \Delta_D + \Delta_W \quad . \tag{2.16}$$

After locating F and the concentration abscissas x_D and x_W corresponding to the product on the Hxy diagram, Δ_D is located vertically on line $x = x_D$ by computing Q. The line $\Delta_D F$ is extended to locate Δ_W. The operating curves intersect at M related to line $\Delta_D F \Delta_W$. Steps are drawn on the x-y diagram between operating curve and equilibrium curve beginning at x_D. The change is made from enriching to stripping curve at the feed tray. The Acetone-Water system is shown in Figure 2.4 as an example of the application of this method.

2.1.3 Computer assisted binary distillation. Wide spread availability of computing machinery provides the opportunity to use these tools in assisting the design work. The McCabe-Thiele and Ponchon-Savarit methods discussed are time consuming and tedious especially when the parameters such as reflux ratio are varied to optimize the process, hence using a computer saves a lot of time and effort and is less subject to error. A lot of codes have been developed for distillation--some of them are discussed below.

Walter H. Prahl (1979) has suggested a method for translating the McCabe-Thiele method into digital mode. The

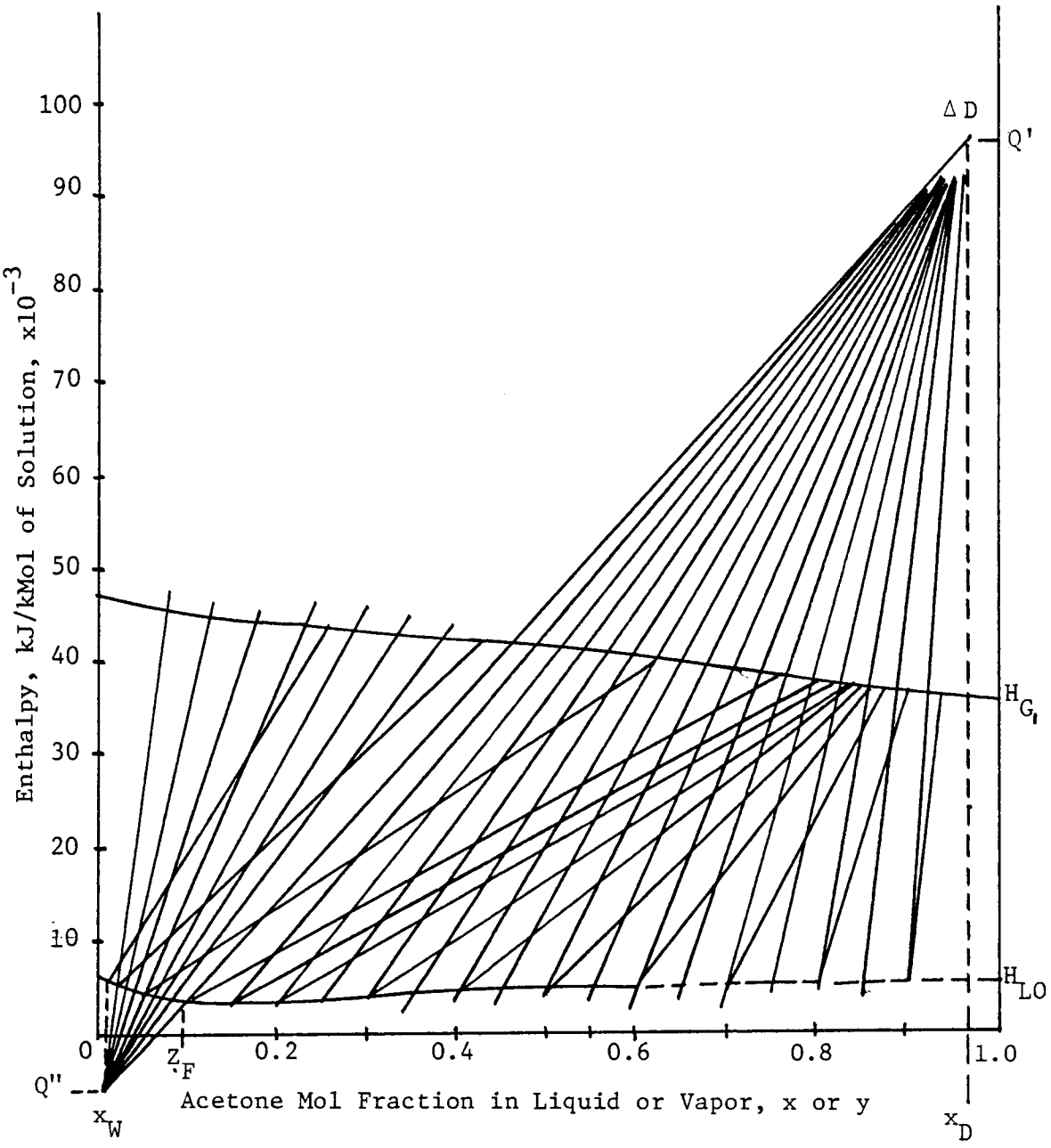


Figure 2.4. Ponchon-Savarit Method for Acetone-Water System.

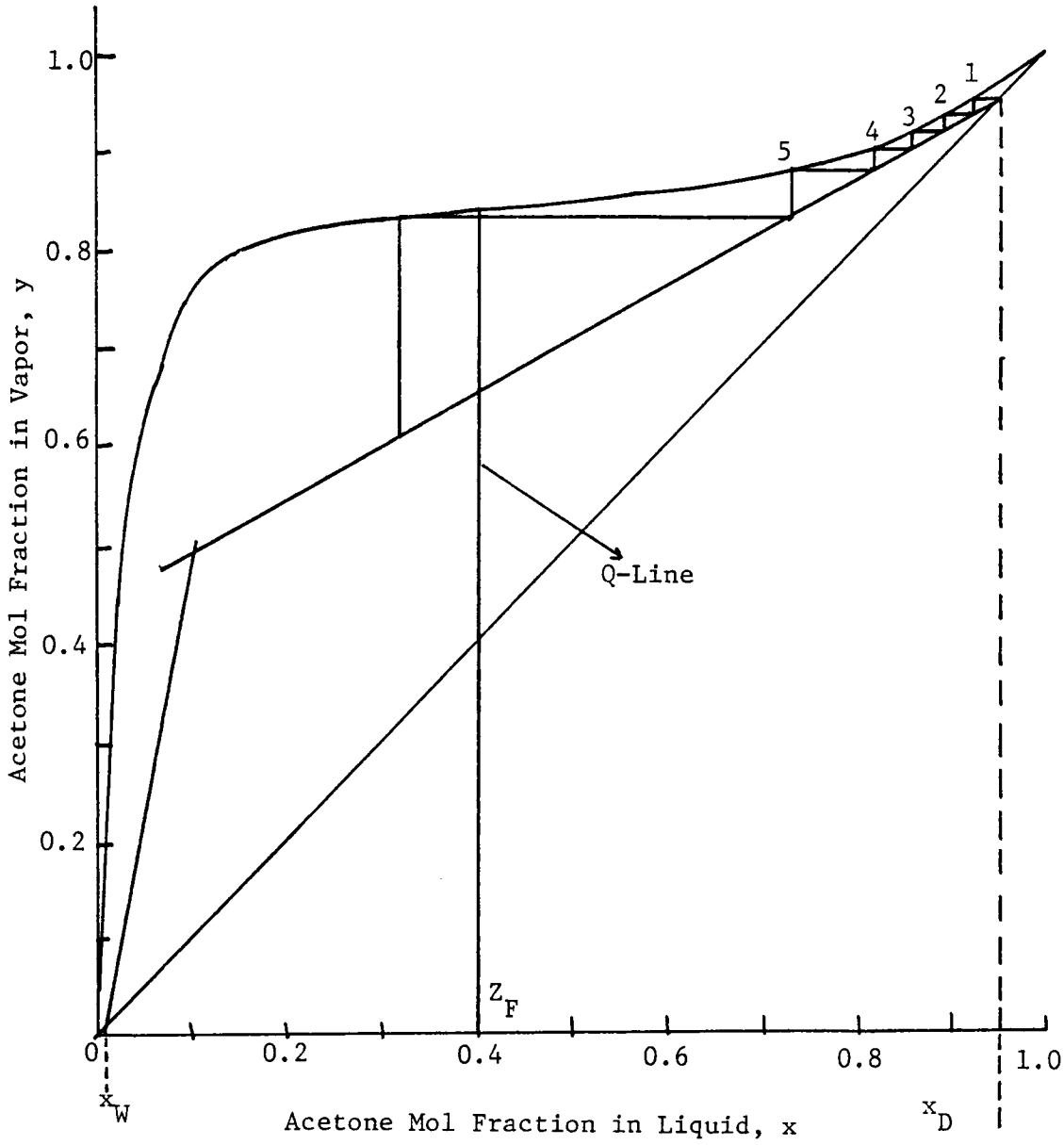


Figure 2.4. Continued.

equilibrium curve, Equation (2.1) is rearranged to the form

$$x = \frac{1}{\alpha(\frac{1}{y} - 1) + 1} \quad . \tag{2.17}$$

The equation of operating line is given as

$$y = \frac{L}{V} x + (1 - \frac{L}{V}) x_D \quad . \tag{2.18}$$

The number of plates are calculated by calculating the concentration at each plate by stepping down from the equilibrium curve to the operating line. For varying alpha Prahl suggested a method for calculating alpha by the vapor pressure i.e.,

$$\alpha = p_B / p_T \quad . \tag{2.19}$$

The vapor pressure may be estimated by the use of Antoine equation, for example:

$$l_n(p_V) = A - B/(T+C) \quad . \tag{2.20}$$

Where p_V = Vapor pressure in mmHg

T = Temperature in °F

A, B and C = Antoine constant.

Henry H. Chein, in his paper "A Rigorous Method for Calculating Minimum Reflux Rate in Distillation" (AIChE Journal, Vol. 24, July 1978) has given a method for convergence to find the pinch zone. In the design of a simple distillation column, as the reflux is reduced, a specified separation can be maintained by increasing the number of stages in the column. The minimum reflux for the

specified separation is reached when the stage requirement becomes infinite. At the minimum reflux, a column should have one or two pinch zones, usually one above and one below the feed. A pinch zone is a section of the column with infinite number of stages having identical liquid compositions, vapor compositions, pressures, temperatures and molal overflows. The important assumption in this method is that pinch zone is not at a point where operating line is tangent to equilibrium curve. A lot of work has been done in other countries on this topic and a number of papers are found in other languages as well--some are listed in Table 2.3.

2.2 Multicomponent Distillation

Practical distillation design problems generally involve multicomponent mixtures. The general principals of design of multicomponent fractionators are the same in many respects as those for binary systems (Treybal, 1979) but the dearth of adequate vapor liquid equilibrium data imposes severe restriction on their application. Since the design calculations involve extensive trial and error procedures, it is useful to use computers for the calculations. It is not impossible to carry them out by hand, and can be done when only few designs are to be made. The short cut method has a number of advantages over the rigorous method and a lot of work has been carried out in this connection.

The most reliable design procedure is that of Thiele and Geddes (1933). The method assumes that for a given feed the

Table 2.3. Papers on Computer Assisted Binary Distillation.

Title	Author	Journal
Computation & Simulation of Distillation Columns using Minicomputer. Romanian	Pamfil, Virgil	Rev. Chim (Bueharcst) 33(1), 1982
Economic Optimization in Design of Rectification Column by Computer. Spanish	Armenjou, Rojo	Ing Quim (Madrid) 12(131), 1980
Distillation Column Design. Polish	Nygleda, Renata	Przem Chem (Poland) 59(4), 1980
Calculation for Batch Fractionation with a Digital Computer. Polish	Fieg, Jenzy	Ing. Apar Chem (Poland) 18(5), 1979
Design Distillation Columns, The Computer Way. English	Daoo V.S.	Indian Chem. Manuf (India) 15(12), 1977

number of trays, position of feed tray, temperature for each tray and liquid vapor ratio is known and it computes the resulting distillate and residue products. Many methods of estimating the minimum reflux ratio have been proposed, most of which are tedious to use and not very accurate. Underwood (1948) uses constant average alphas and assumes constant L/V, it is not very accurate except for systems which are essentially ideal. The basic equation developed by Underwood is given as:

$$\frac{\alpha_3 Z_{3,F}}{\alpha_3 - \phi} + \frac{\alpha_2 Z_{2,F}}{\alpha_2 - \phi} + \frac{\alpha_1 Z_{1,F}}{\alpha_1 - \phi} = (1-Q) \quad . \tag{2.21}$$

Where $Z_{1,F}$, $Z_{2,F}$, $Z_{3,F}$ represent the composition of the feed, α_1, α_2, α_3 are the respective relative volatilities and Q represents the thermal condition of the feed, that is, the total heat required to vaporize one mole of feed divided by the latent heat of vaporization. Multiplying Equation (2.21) by F, the feed rate and summing for all J components in the feed gives the Equation:

$$\Sigma \frac{\alpha_J Z_{JF} F}{\alpha_J - \phi} = F(1-Q) \quad . \tag{2.22}$$

Equation (2.22) is solved for that value of ϕ which lies between the relative volatilities of the key components, i.e.,

$$1 \cdot 0 < \phi < \alpha_{LK} \quad .$$

The value of ϕ chosen is such that

$$\frac{\alpha_3 \alpha_3}{\alpha_3 - \phi} + \frac{\alpha_2 \alpha_2}{\alpha_2 - \phi} + \frac{\alpha_1 \alpha_1}{\alpha_1 - \phi} = 1.0 \quad . \tag{2.23}$$

The value of ϕ so found is substituted in the equation to give R_m which is minimum reflux ratio

$$\frac{\alpha_3 x_{3D}}{\alpha_3 - \phi} + \frac{\alpha_2 x_{2D}}{\alpha_2 - \phi} + \frac{\alpha_1 x_{1D}}{\alpha_1 - \phi} = R_m + 1 \quad . \tag{2.24}$$

Multiplying Equation (2.24) by D, the distillate rate and summing for all J components in distillate gives

$$\Sigma \frac{\alpha_J x_{JD} D}{\alpha_J - \phi} = D(R_m + 1) \quad . \tag{2.25}$$

The Underwood equations are not good for wide boiling mixtures.

The Fenske (1932) equation can be applied to key components to determine minimum number of plates i.e.,

$$N_m = \frac{\log[((X_{LKD}D)/(X_{HKD}D)(X_{HK}W/X_{LKW}W)]}{\log\alpha_{LK,av}} \tag{2.26}$$

Winn (1958) suggested a modified Fenske equation that accounts for variation of relative volatility:

$$\ln K = A + \frac{B}{T} \quad . \tag{2.27}$$

Where A and B are constant, T is absolute temperature in °K and K is the equilibrium constant (K = y/x). The feed tray location can be calculated by a number of methods. It can be calculated by trial and error in Thiele-Geddes (1933) calculation. This method is a plate-to-plate calculation procedure, working with composition ratios and computing products for assumed plates and reflux. The procedure is to calculate down from the condenser to the feed plate. At the feed plate the appropriate ratios are matched and

the quality of the two product streams (distillate and bottoms) are calculated. The location of feed tray is given by

$$\left(\frac{X_{LK}}{X_{HK}}\right)_{\text{stage above feed}} > \left(\frac{X_{LK}}{X_{HK}}\right)_{\text{feed liquid}} > \left(\frac{X_{LK}}{X_{HK}}\right)_{\text{feed stage}}. \tag{2.28}$$

The Kirkbride method (1944) is given by the equation

$$\frac{\log N_A}{N_B - 1} = 0.206 \log\left[\frac{D}{B}\left(\frac{f_{HK}}{f_{LK}}\right)\left(\frac{b_{LK}}{d_{HK}}\right)^2\right] . \tag{2.29}$$

Where N_A and N_B stages above and below feed entry points respectively.

D and B Moles distillate and bottom respectively.

f_{LK} and f_{HK} Moles light key and heavy key in feed respectively.

b_{LK} Moles light key in bottom.

d_{HK} Moles heavy key in distillate.

Another method involves the use of Fenske equation i.e.,

$$N_{BM} = \ln\left[\left(\frac{f_{LK}}{f_{HK}}\right)\left(\frac{b_{HK}}{b_{LK}}\right)\right] / \ln(\alpha_{LK}) . \tag{2.30}$$

N_{BM} stages below feed for total reflux.

A number of methods have been presented for the relation between the number of stages and reflux ratio. Gilliland (1940) gave a correlation by plotting on the abscissa and ordinate the following variables:

$$\frac{R - R_m}{R+1} \text{ and } \frac{N - N_m}{N+1} .$$

He calculated N_m by Fenske equation and R_m by his own method. For

a given R, R_m can be calculated and N can be read from graph. Erbar Maddox used a different plotting method. The abscissa was N_m/N and ordinate value was L_o/V_1 which is related to R as

$$\frac{L_o}{V_1} = \frac{L_o}{L_o+D} = \frac{L_o/D}{L_o/D+1} = \frac{R}{R+1} \quad . \tag{2.31}$$

Parametric values of (L_o/V_1) are calculated by

$$\left(\frac{L_o}{V_1}\right)_m = \frac{R_m}{R_m+1} \quad . \tag{2.32}$$

The above method has been grouped together for calculating minimum reflux, feed plate and number of theoretical plates. Dimitrious (1981) has given a method in which he calculates minimum reflux by Underwood equation, minimum number of plates by Fenske equation, the number of plates by Erbar Maddox diagram and feed plate by Kirkbridge method. The composition of top and bottom products are calculated by Thiele-Geddes equation.

Huan Chang (1980) has also developed a computer code using short cut technique. The code assumes that the feed composition and the average values of the relative volatility are known. It starts with a set of guessed values of the recoveries of the key component in the distillate and bottoms. The distribution of the non keys are estimated by the Hengstebeck-Geddes equation:

$$\ln(d_i/b_i) = c_1+c_2\ln\alpha_i \quad . \tag{2.33}$$

Where b = number of moles of component in bottom

d = number of moles of component in distillate

c_1, c_2 = constants in Hengstebeck-Geddes equation.

The main program solves distribution of the keys in the distillate and the bottom by the Newton-Raphson iteration technique. It then establishes distribution of the non-keys by the Hengstebeck-Geddes equation (Equation (2.33)). The minimum number of theoretical plates is based on Fenske's equation. Subroutine UWD calculates minimum reflux ratio by the Underwood's equation. Finally, subroutine GLLD calculates number of theoretical plates at operating reflux ratio by Gilliland's correlation. Some of the other methods developed for multicomponent distillation are given in Table 2.4.

2.3 Curve Fitting Techniques for Property Data

In the binary system when alpha is not constant, the equilibrium data plotted as y vs. x, have some very peculiar shapes. A number of curve fitting techniques may be applied to get a close fit to the experimental data in order to have a good result. In multicomponent distillation too, the procedure requires the 'K' values such as those provided by De Priestor's nomograph for hydrocarbons (Treybal, 1979). A technique should be applied to have a good fit to the curve in order to have a good approximation. Hence, curve fitting techniques are very important in the designing of a distillation column by computer methods. A number of techniques are available and lots of methods have been developed. For example, George and Malcolm (1977) have discussed a number of curve fitting

Table 2.4. Papers on Multicomponent Distillation.

Title	Author	Journal
Computerized Design of Multicomp. Dist. Columns using Unifac Group Contribution Method for Calculation of Activity Coefficients	Fredenslund, Age	Ind. Eng. Chem. Proc. Vol. 16n4 Oct. 1977
A Method for Solving Design Problems of Multicomponent Distillation	Hiraoka, Selsuro Yamada, Ikuho	J. Chem. Eng. Jpn. 15(4), 1982
Rigorous Calculation Methods for Minimum Stages in Multicomponent Distillation	Chien, Henry	Chem. Eng. Sci. V28n11, Nov. 1973
Short Cut Method for Multicomponent Distillation	Marinos, Kouris	Chem. Eng. N.Y., 88(5), 1981

techniques, some of them are polynomial interpolation which is given as

$$y(x) = a_o + a_1 x + a_2 x^2 + \text{------} + a_n x^n \quad . \tag{2.34}$$

These polynomials have the advantage of being easy to evaluate directly and are known to approximate for a given set of data. Another method is the spline interpolation. This method puts a different cubic between every two successive data points such that the curve pass exactly through each data point and that the first two derivatives of the curve on the right hand side of a data point are equal, respectively, to the first two derivatives of the curve on the left hand side of the data point, all derivatives evaluated at the data point (Kalus and Van Ness, 1967). The method of least square can be used to determine the coefficients of any form of interpolation. George and Malcolm (1977) have developed a number of subroutines for the application of these techniques.

The data can be plotted by using different plotting subroutines. V.A. Dyck (1979) in his book "Introduction to Computing" has given some subroutines for plotting the function. As subroutines, they cannot be used on their own but must be referenced by other programmes. There are four subroutines given, each routine is invoked by a CALL statement. Subroutine SETPLT initializes the other plotting subroutines. It must be the first of the subroutines called and is executed only once for each complete graph. The subroutine SETSIZ is used to change the default size of the plotting surface. The STOPNT routine is used to retain or store points for

future plotting to a maximum of one thousand points. Finally, PLOTC subroutine causes the stored points to be printed. It is executed after all points have been given to the STOPNT routine. Yehuda and Abraham (1938) have developed a method for correlating data by means of cubic polynomial. The correlation is obtained by minimizing the sum of squares of deviations between the experimental data and the analytic representation, subject to constraint of continuity of the first derivative. Antoher method for fitting the data are the different forms of model equations like polynomials:

$$y = a+bx+cx^2+dx^3 \quad . \tag{2.35}$$

An equation in exponential form e.g.,

$$y = a+bx+c(1-e^{-dx}) \quad . \tag{2.36}$$

An equation in logarithm form e.g.,

$$y = a+bx+c\ln(x+d) \quad . \tag{2.37}$$

The constants in these equations can be determined by linear regression analysis. The regression can be quickly done by using a computer code such as STATPACK.

2.4 Cost Estimation Methods for Distillation Columns

One method of optimizing a distillation operation is by minimizing the total annual operating cost. Peters and Timmerhaus (1980) have discussed a method for calculating the total annual cost by determining the optimum reflux. The optimum reflux ratio

occurs at the point where the sum of fixed cost and operating cost is minimum. They have given a graphical interpolation to determine the annual operating cost. Once the fixed charges are known, then the operating cost can be determined for selected range of reflux ratio. The fixed charges can be calculated graphically by calculating purchase cost of the material of construction in $/plate for a known diameter of the column, using the cost data provided by Peters and Timmerhaus (1980).

CHAPTER 3

COMPUTER CODE FOR BINARY DISTILLATION

The binary distillation problem is generally posed as follows: Given a feed rate, its composition and thermodynamic state, establish the economic column size (number of plates and diameter), the optimum reflux ratio, and feed tray location required to produce distillate of a specified purity. The "economic column size" here is taken to be that size which yields the minimum total annual cost (fixed + operating charges). The optimum reflux ratio is that corresponding to the minimum total annual cost.

The usual approach to the development of a solution to this problem may be outlined as follows:

1. Establish the minimum reflux ratio required to effect the separation by use of the equilibrium data for the system. The McCabe-Thiele method is usually adequate for this purpose, for systems which are reasonably ideal and for columns which are well insulated. The McCabe-Thiele method is also often used for estimating purpose for those systems which are highly non-ideal because of the lack of ethalpy-composition data.
2. Establish the number of theoretical trays required to effect the separation for a realistic value of the operating reflux ratio of say, 1.5 times the minimum.
3. Establish the column diameter required to produce a

specified distillate/bottom split.

4. Establish the optimum reflux ratio by varying the ratio of the operating to minimum reflux. This would give the reflux ratio which yields the minimum total annual cost. Optimum reflux ratio is usually 1.1 to 1.5 times the minimum reflux.

Two classes of binary systems are considered. The first class contains systems whose vapor-liquid equilibrium (VLE) data can be represented reasonably well by a single, constant value of relative volatility, α. This approximation holds reasonably well for ideal mixtures. An example of a system which is approximately ideal is Benzene-Toulene mixture. The second class of binary systems considered is that whose members exhibit an inflexion point when their VLE data are plotted as x vs. y (mole fraction in liquid phase, x, vs., mole fraction in vapor phase, y). This behavior is somewhat representative of relatively highly non-ideal systems. Examples of these systems are the aqueous solutions of Acetone or of Ethanol. In addition to representing relatively large classes of solutions of interest with respect to distillation, a reason for considering these two classes of binary solutions is that each class presents to the computer programmer a different problem with respect to determining the minimum reflux ratio required for achieving a specified separation of a given feed. The computer codes in both cases are based on the McCabe-Thiele method of determining the number of theoretical plates required for the specified separation for a specified reflux ratio.

3.1 Models for the Equilibrium Curve and Data Fitting

3.1.1 Systems which are nearly ideal. The McCabe-Thiele method requires the VLE data in the form of y vs. x. In the development of the computer code based on this design method, an analytic equation is developed which is representative of the VLE data, with y given explicity as a function of x. For the nearly ideal systems whose relative volatility (α) is approximately constant, the defining equation for α is rearranged to the form (see, for example, Treybal, 1979),

$$\text{Model A:} \quad y = \frac{\alpha x}{1+(\alpha-1)x} \tag{3.1}$$

which is used as a model equation for fitting the VLE data for a given binary nearly ideal system. The experimental equilibrium curve along with the fitted model (model A) is shown in Figure 3.1 for the Benzene-Toulene system. The correlation coefficient (r) was found to be 0.9961, which indicates that the model equation fitted very well for the Benzene-Toulene system. The fitted model (model A) is shown in Figure 3.2 along with the experimental equilibrium data for the Benzene-Ethylenedichloride system. A very high correlation coefficient ($r = 0.9996$) indicates that the model quation fits extremely well.

3.1.2 Non ideal systems. For those binary systems whose VLE data exhibit an inflexion point, the data were fitted by regression analysis, once a suitable form for a model equation had been established. Several candidate model equations were tested against

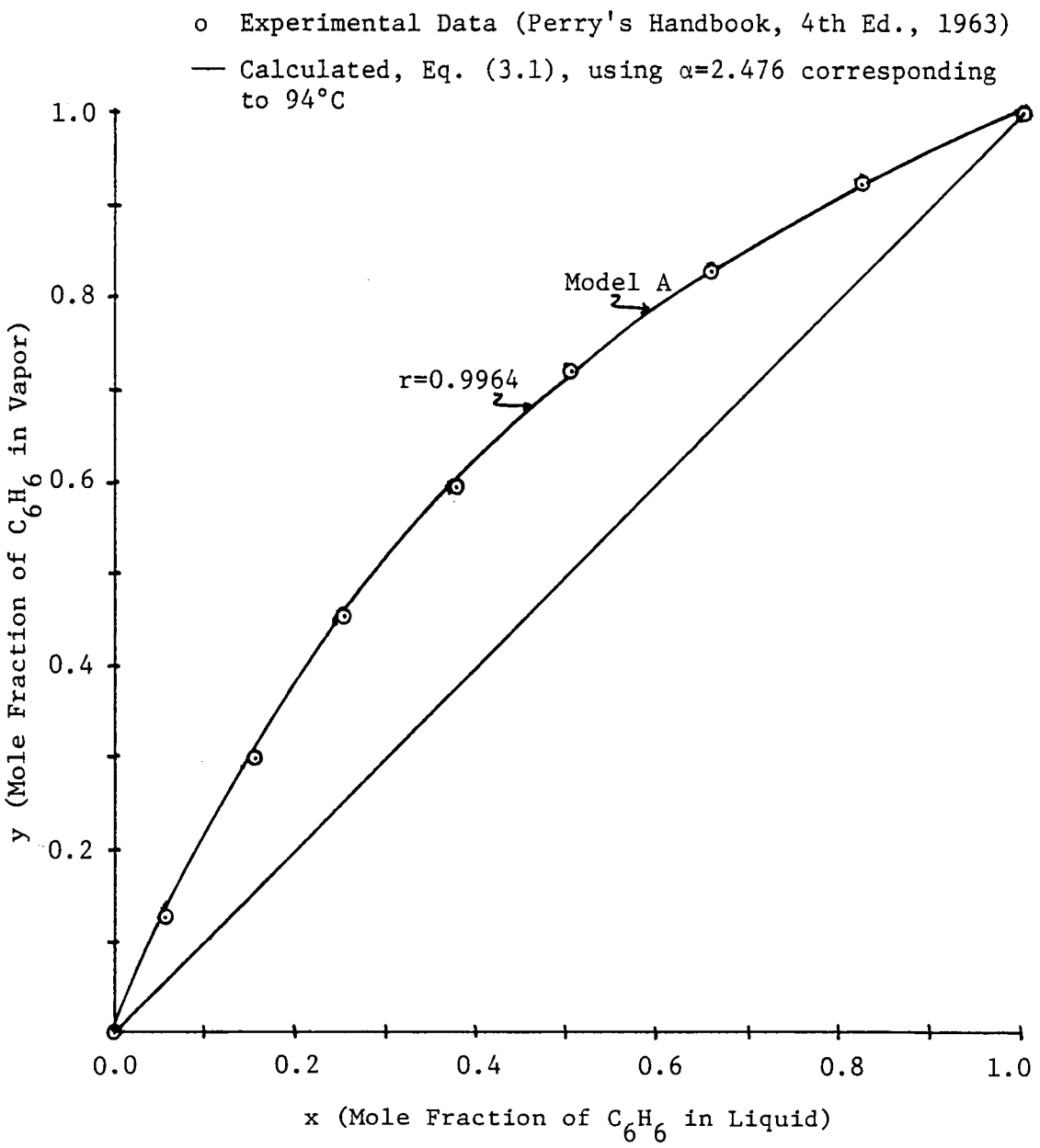


Figure 3.1. Equilibrium Data for Benzene-Toulene System at one Atmosphere.

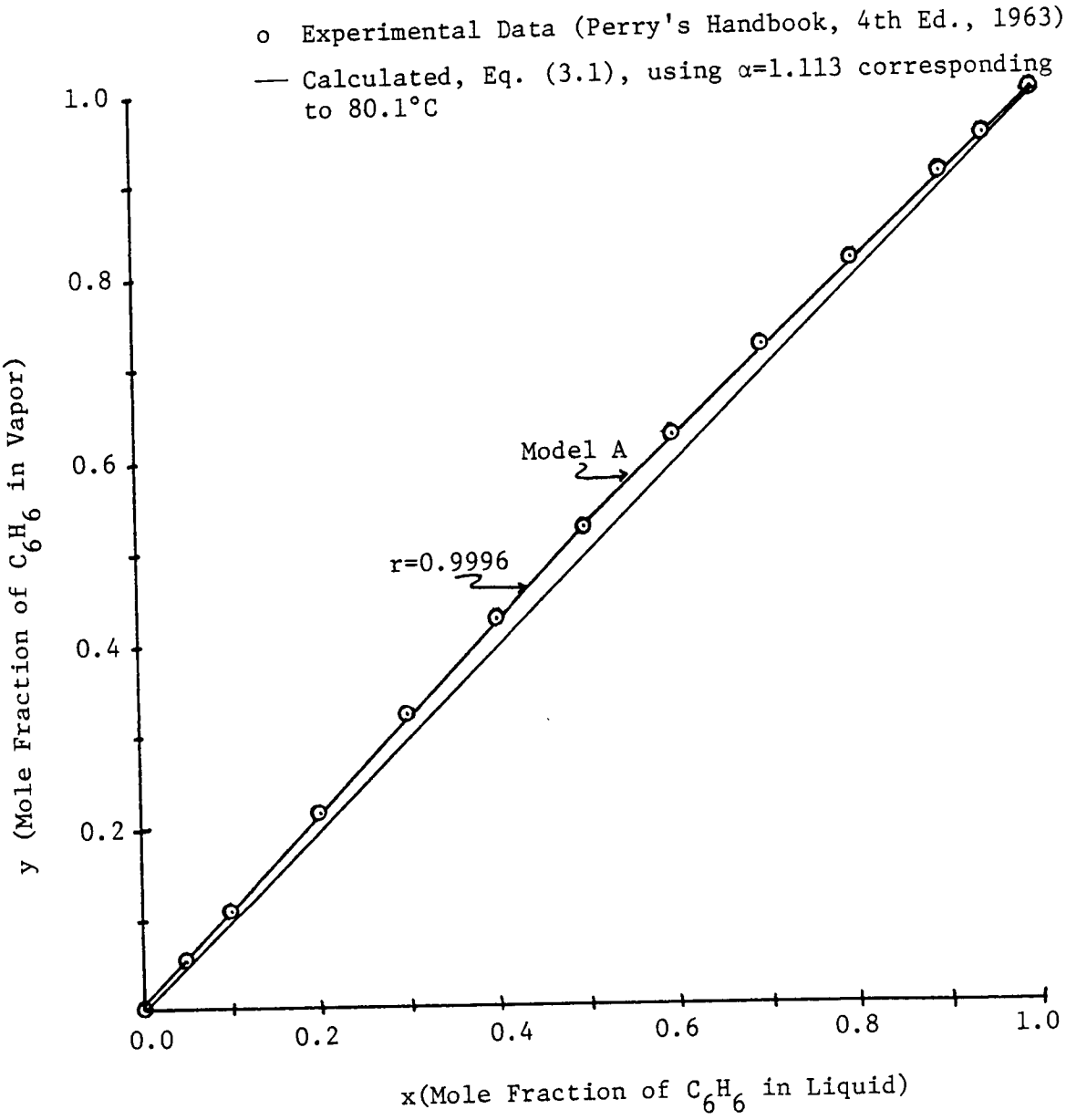


Figure 3.2. Equilibrium Data for Benzene-Ethylene Dichloride System at One Atmosphere.

known VLE data, in an effort to establish a suitable equation. For the binary system of Ethanol-Water several forms of α were tried in order to fit the data, some of them are as follows:

$$\text{Model C:} \quad \alpha = a+bx+c(1-e^{-dx}) \tag{3.2}$$

$$\text{Model D:} \quad \alpha = a+bx+cx^2+dx^3 \tag{3.3}$$

$$\text{Model E:} \quad \alpha = a+bx^n \tag{3.4}$$

The values of y (mole fraction in vapor phase) were determined using the equation (3.1). Equation (3.2) and Equation (3.3) are shown as models C and D respectively, in Figure 3.3 along with the experimental data. Another type of model equations tested for the Ethanol-Water system were different forms of K (K=y/x), e.g.,

$$\text{Model F:} \quad K = a+bx+c\ln(x+d) \tag{3.5}$$

$$\text{Model G:} \quad K = a+bx+c(1-e^{-dx}) \tag{3.6}$$

$$\text{Model H:} \quad K = a+bx+cx^2 \tag{3.7}$$

These equations are shown in Figures 3.4 and 3.5 as models F, G and H respectively. The values of y were calculated by the equation

$$y = Kx \tag{3.8}$$

Equation (3.2) (a combination of linear terms in x with a negative exponential) was found to be the best model form for fitting VLE

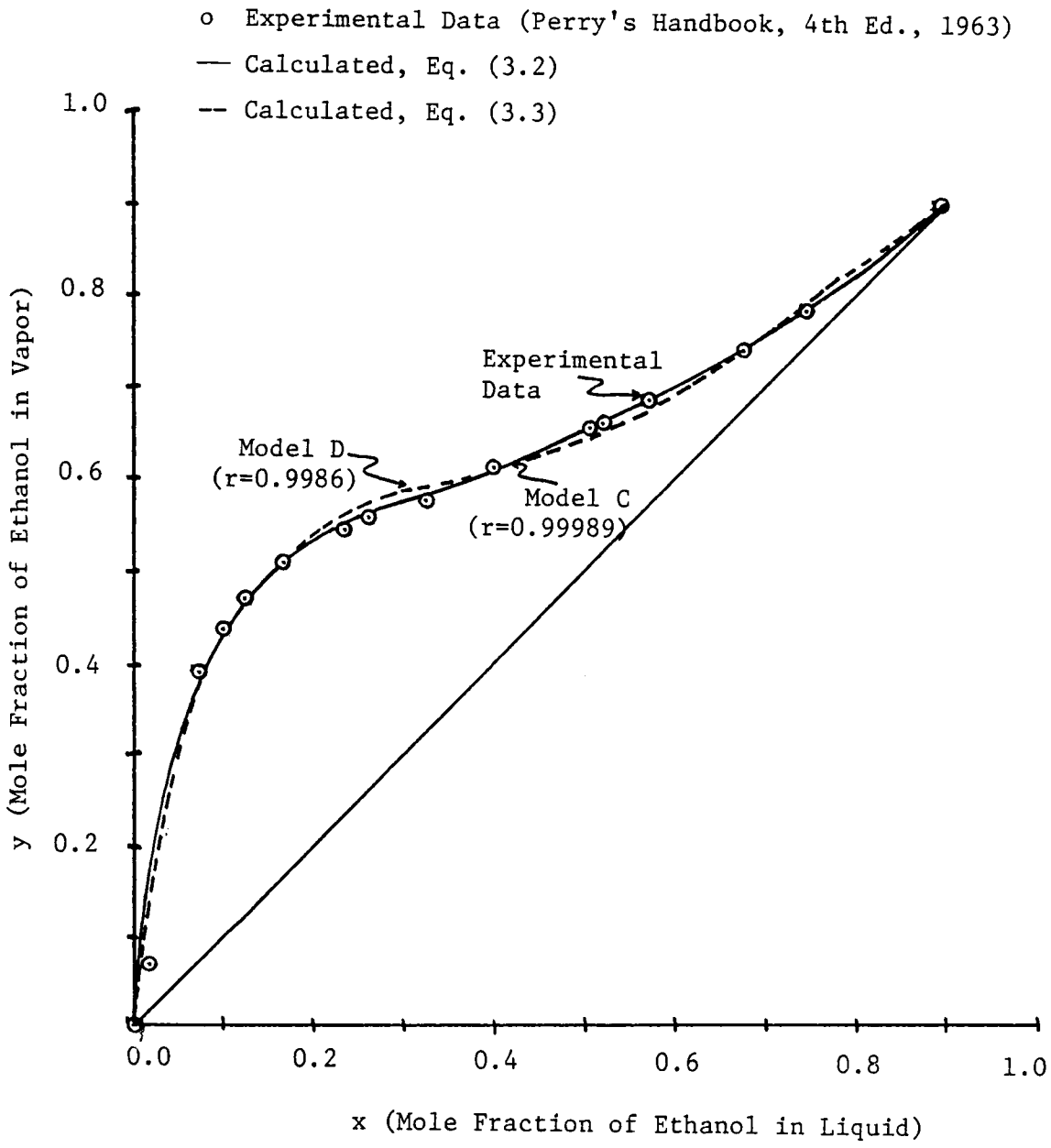


Figure 3.3. Equilibrium Data for Ethanol-Water System at One Atmosphere, Models C and D.

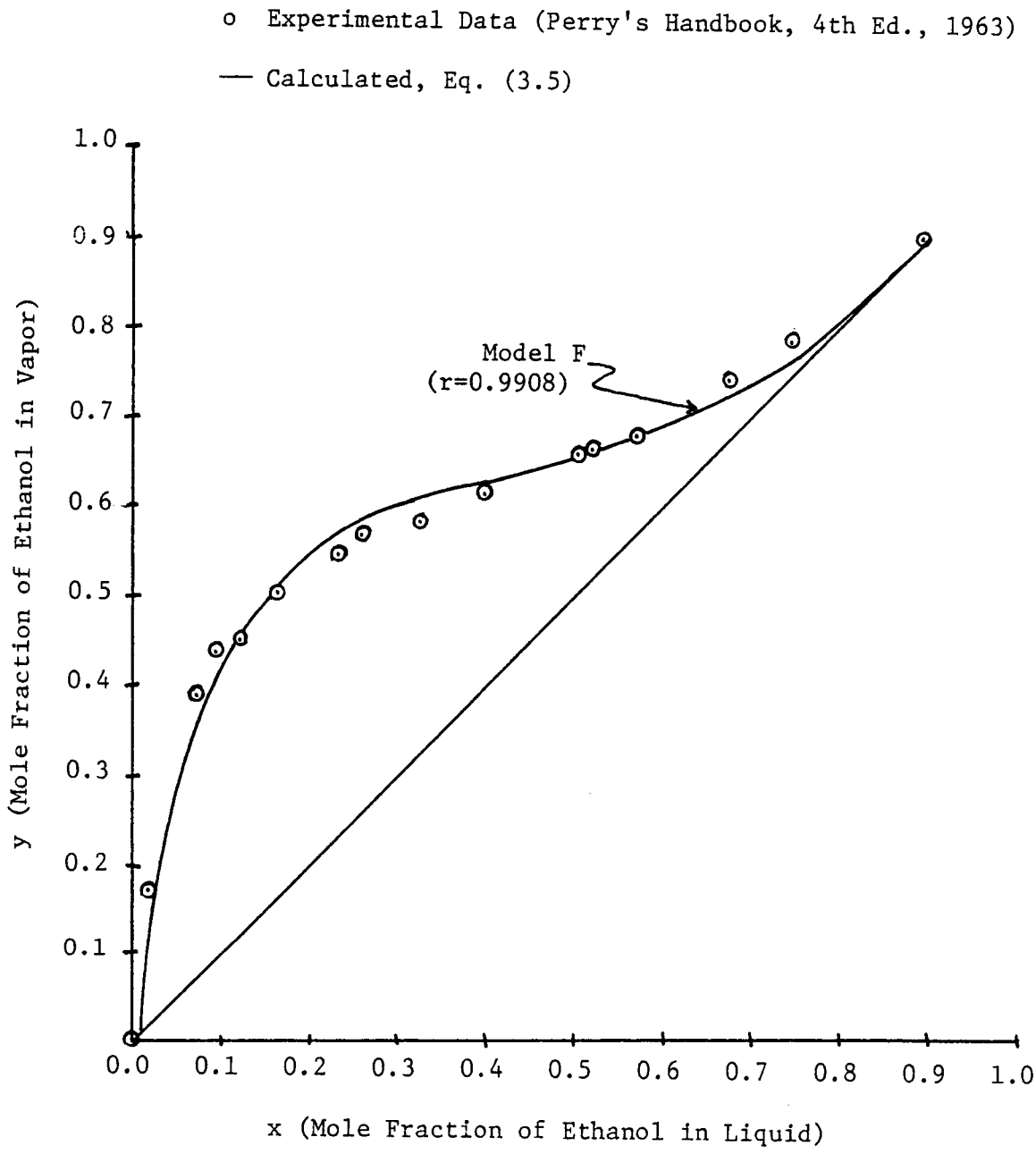


Figure 3.4. Equilibrium Data for Ethanol-Water System at One Atmosphere, Model F.

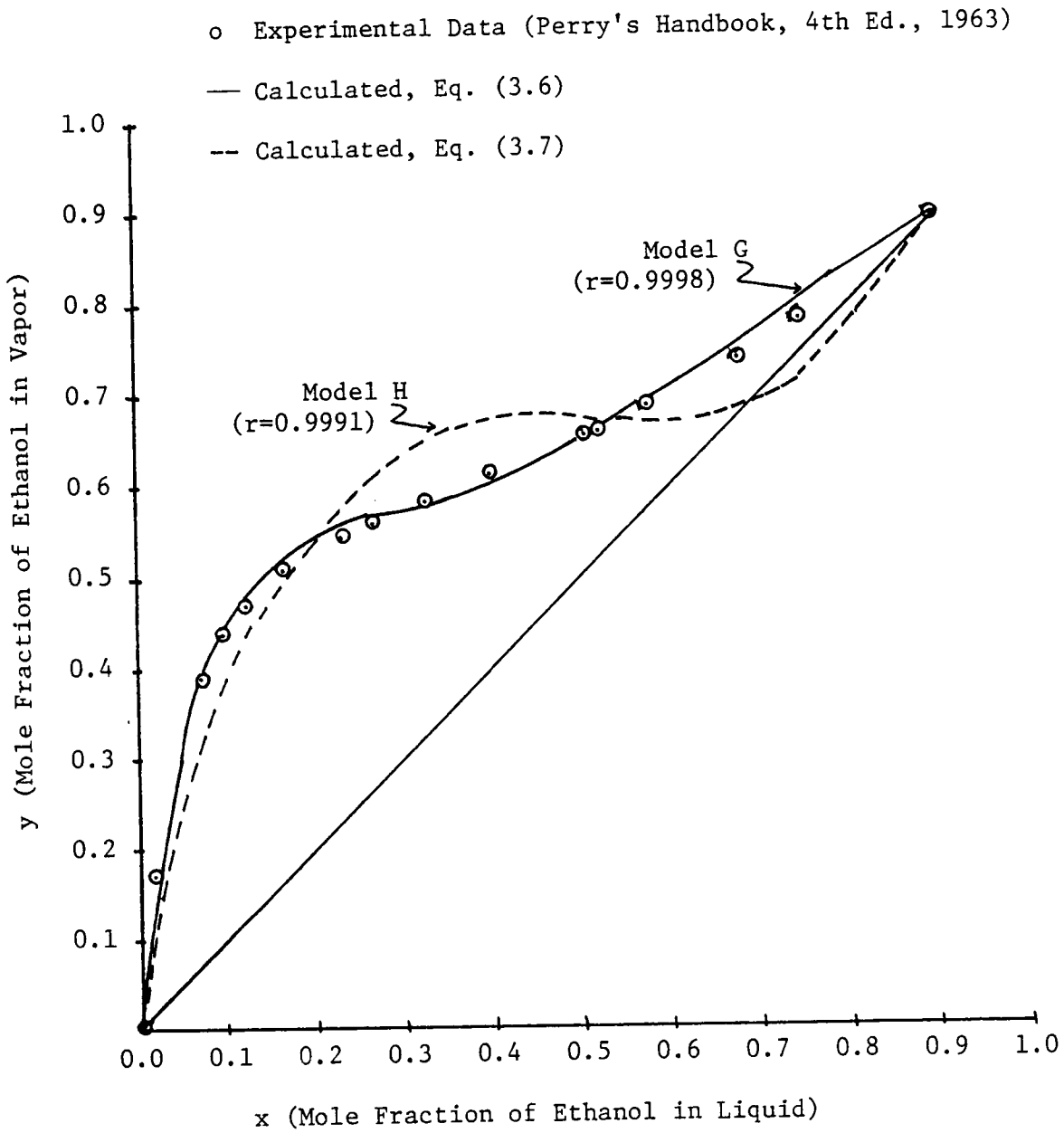


Figure 3.5. Equilibrium Data for Ethanol-Water System at One Atmosphere, Models G and H.

data of Ethanol-Water system. The parameters a, b, c and d are determined by regression analysis, which were found to be 1.929, -1.089, -9.431 and 6.0 respectively. The regression coefficient was found to be 0.99989 indicating a very good fit to the data. The model equations were also tested for the VLE data of aqueous solutions of Methanol and Acetone. Figure 3.6 and 3.7 shows the fitted curves along with the experimental data for both of the systems.

The different model equations tried for fitting the VLE data of the three systems are shown in Table 3.1 with the corresponding values of the regression coefficients. For the Ethanol-Water system, the correlation coefficient for model C was found to be the best among the other models tried indicating the fact that the model is very good to fit the VLE data for the system. The correlation coefficients were not good for the models tried for the Methanol-Water system, hence the models did not give a good fit to the VLE data. For Acetone-Water system, model C had a good correlation coefficient, but the model only fitted well for a distillate composition of less than 0.85, hence the model is not good for high purity distillate.

3.2 Code For Column Design

A computer code has been developed to design a tray type distillation column for the separation of certain binary systems. The code takes into account two types of systems, i.e., ideal and non-ideal systems. The program also takes into account the different thermal feed conditions, e.g., saturated feed, partially vaporized

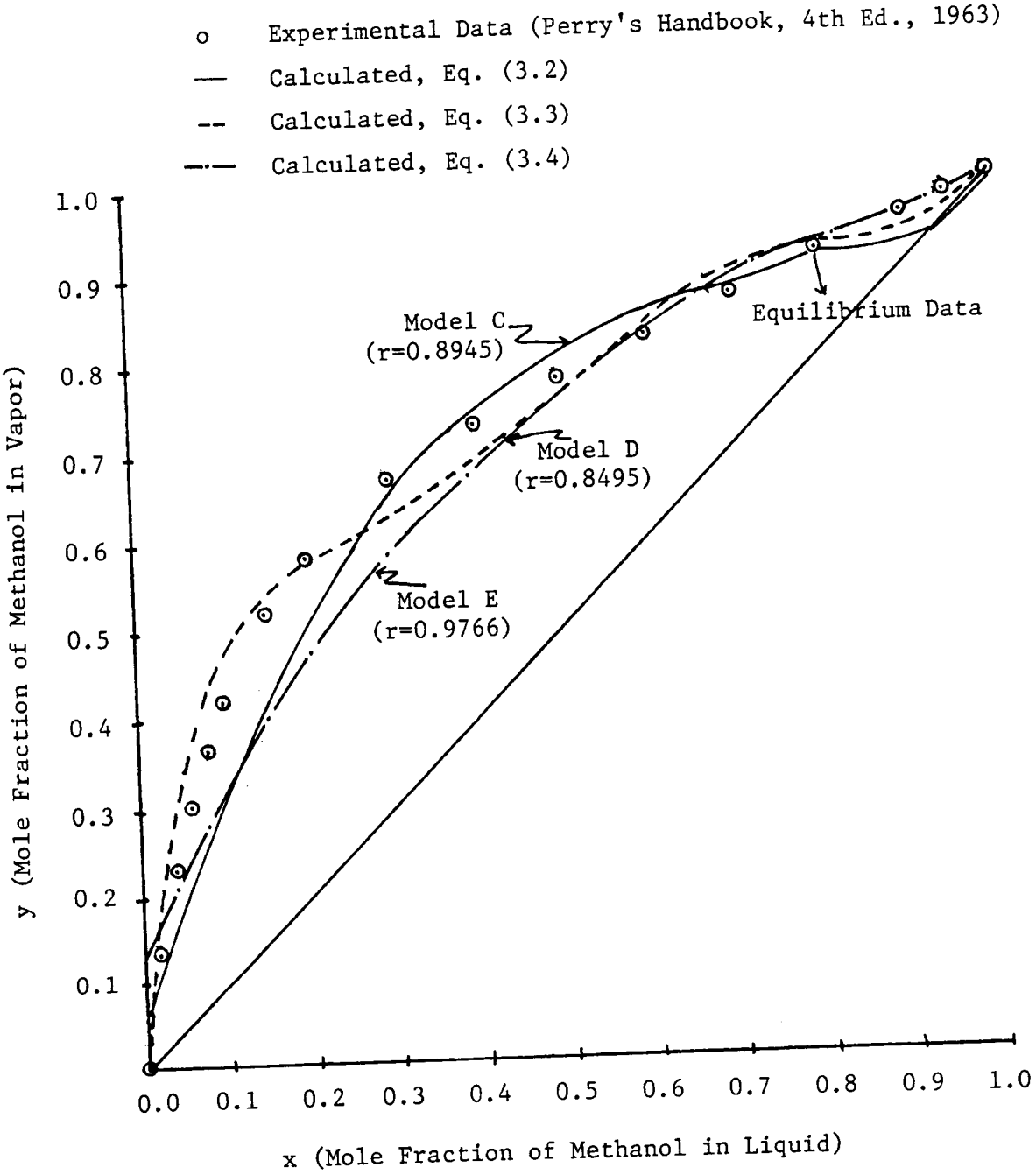


Figure 3.6. Equilibrium Data for Methanol-Water System at One Atmosphere, Models C, D and E.

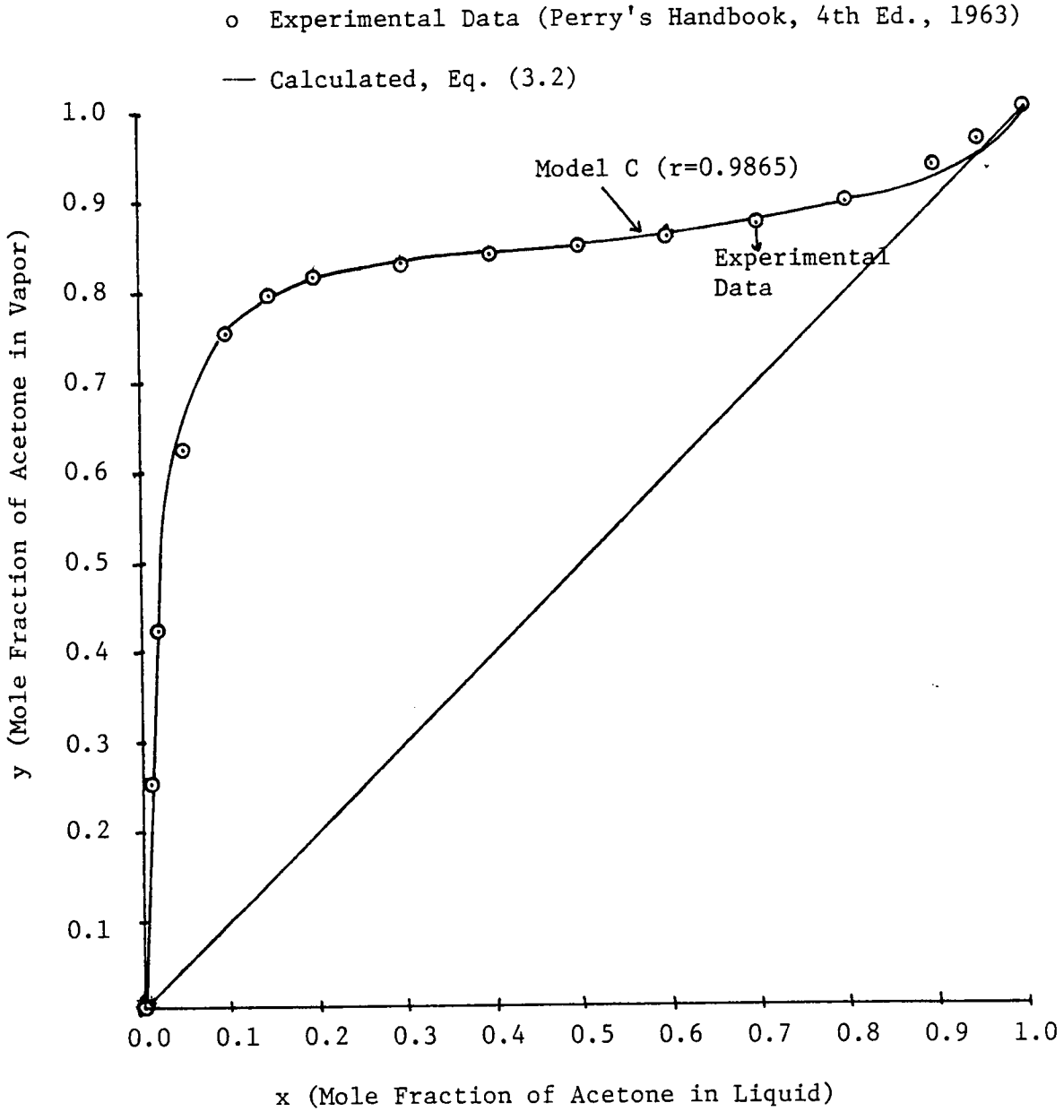


Figure 3.7. Equilibrium Data for Acetone-Water System at One Atmosphere, Model C.

Table 3.1. Summary of Binary Equilibrium Data as fit by Six Models by Regression Analysis.

Model	System	Correlation Coefficient (r)
C	Ethanol-Water	0.99989
D	Ethanol-Water	0.9986
F	Ethanol-Water	0.9908
G	Ethanol-Water	0.9998
H	Ethanol-Water	0.9941
C	Methanol-Water	0.8945
D	Methanol-Water	0.8495
E	Methanol-Water	0.9766
C	Acetone-Water	0.9865

feed and subcooled feed. Once the thermal condition of feed, composition of a component in feed, distillate and bottoms, and the ratio of operating and minimum reflux has been specified, the code calculates the minimum reflux, the operating reflux, the feed plate, the total number of plates and the diameter of the column.

The minimum reflux for ideal systems is obtained by the intersection of Q-line and equilibrium curve, whereas for non-ideal systems it is obtained by drawing a tangent to the curve, if the tangency is not found then it is obtained by the manner similar to the ideal systems. The method has been discussed in Section 3.2.1. The equilibrium curve for ideal systems is obtained by the model equation (equation 3.1) for a given value of α. For non-ideal systems it is determined by the model equation obtained by fitting the VLE data of a system by regression. The number of theoretical plates is obtained by the McCabe-Thiele method. The composition at each plate is determined by stepping down from the equilibrium curve to the operating line, and hence the number of plates is counted. The method has been described in Section 3.2.1. Section 3.2.2 describes the method for calculating the diameter of column. The procedure discussed by Treybal (1979) is used as a basis for sizing the tower. An iterative approach is used to converge to the true diameter. The initial estimate of the diameter is based upon the maximum allowable vapor velocity.

The cost data and cost as a function of tower size curve as provided by Peters and Timmerhaus (1980) is used to optimize the design

with an objective function of minimizing total annual cost. By varying the reflux ratio the optimum reflux is obtained at which the annual cost is minimum. The method is described in Section 3.3.

3.2.1 Establishing the number of theoretical plates. The number of theoretical plates is determined by translating the McCabe-Thiele method into digital mode. The data is read from a file and a flag is set up to take into account the case for constant or non-constant alpha, e.g., a zero flag indicates the case for non-constant alpha. The technique is shown in flow chart (Figure 3.8). Another flag is set up for the thermal condition of feed, and the value of one indicates that the feed is saturated, i.e., Q=1.0. For ideal systems (constant alpha case), the minimum reflux is calculated by the formula (McCabe and Smith, 1976)

$$Rm = (x_D - YP)/(YP - XP) \tag{3.9}$$

XP and YP are the intersection points of the equilibrium curve and Q-line equation which is given as (Treybal, 1979)

$$y = \frac{Q}{Q-1} x - \frac{Z_F}{Q-1} \tag{3.10}$$

The equilibrium curve is obtained by rearranging equation (3.1), for a given value of alpha as,

$$x = \frac{1}{\alpha(1/y-1) + 1} \tag{3.11}$$

The intersection points of equilibrium curve and Q-line are determined in a straight forward manner for the saturated feed, but

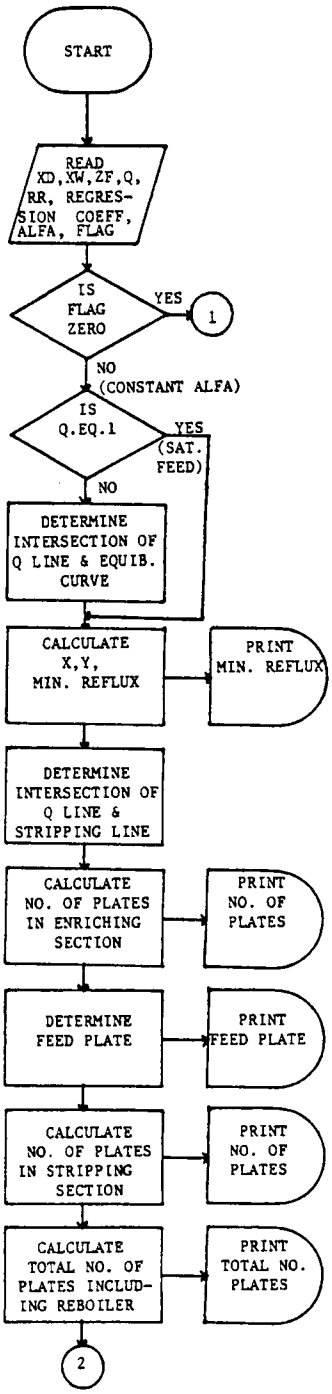


Figure 3.8. Flow Chart for Estimating Number of Theoretical Plates for Ideal Systems.

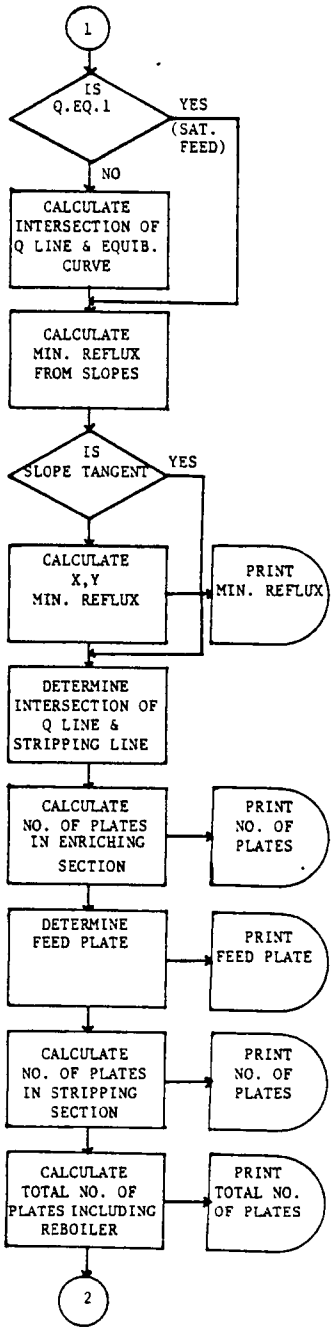


Figure 3.8. (Continued)

for other conditions the points are obtained by solving equation (3.1) and equation (3.10) simultaneously, and calculating their roots. A hand calculation was done to find the solution of the two equations and an equation was obtained of the form:

$$\left(\frac{Q}{Q-1}(\alpha-1)\right)x^2 + \left(\frac{Q}{Q-1} - \alpha - \frac{Z_F}{Q-1}(\alpha-1)\right)x - \frac{Z_F}{Q-1} = 0 \qquad (3.12)$$

This is a quadratic equation, i.e.,

$$AX^2+BX+C = 0 \qquad (3.13)$$

The code calculates the coefficients A, B and C obtained from equation (3.12), and the roots are determined by the relation

$$X = \frac{-B \pm \sqrt{B^2-4AC}}{2A} \qquad (3.14)$$

Once the reflux ratio has been calculated, the number of plates in the enriching section are determined by stepping down from the equilibrium curve starting from the distillate composition, x_D, to the enriching section operating line which is given as

$$y = \frac{R}{R+1}x + \frac{x_D}{R+1} \qquad (3.15)$$

The stepping off is carried out until the feed composition is reached. The feed plate is located at point of intersection of the operating line and Q-line. The plates in the stripping section are determined by stepping down from the equilibrium curve to the stripping section operating line given by the relation

$$y = a+bx \qquad (3.16)$$

where 'a' and 'b' are the intercept and slope of the stripping section operating line, and are calculated by

$$b = (YI-x_W)/(Z_F-x_W) \tag{3.17}$$

$$a = YI-bXI \tag{3.18}$$

XI and YI are the intersection points of the Q-line and operating line, and are obtained by solving the Q-line equation (equation (3.10)) and the operating line equation (equation (3.15)), the solution was obtained by hand claculation and is given as

$$XI = \left(\frac{Z_F}{Q-1} + \frac{X_D}{R+1}\right)/\left(\frac{R}{R+1} - \frac{Q}{Q-1}\right) \tag{3.19}$$

$$YI = \frac{RXI + X_D}{R+1} \tag{3.20}$$

The calculations are carried on until the composition of the bottoms, x_W, is reached. The number of plates are counted by the number of times the operating line is intercepted. Additional plate is counted in the total number of plates to take into account the plate for reboiler. The flow chart for the code is shown in Figure 3.8, and the section of the code is shown in Table 3.2.

The example 19-4 (page 560), provided by McCabe and Smith (1976) was solved graphically to check the code, the problem is as follows: A continuous fractionating column is to be designed to separate 30,000 lb/h of a mixture of 40% benzene and 60% toluene into an overhead product containing 97% benzene and a bottom product containing 98% toluene. These percentages are by weight. A reflux ratio of 3.5

Table 3.2. Code For Estimation of Number of Theoretical Plates.

```
C
C
      REAL INT,M1,M2,MG,ML,MD,MB,MF,LR,LAMV,LAMC,LAMW
      INTEGER P,T
      DIMENSION X(2500),Y(2500),FUNC(2500)
      OPEN(FILE='DIST.DAT',ACCESS='SEQIN',UNIT=1)
C CHECK FOR ALFA
      WRITE(5,1)
1     FORMAT(' IS ALFA CONSTANT,TYPE 0 FOR NO,1 FOR YES')
      READ(5,*)F
      IF(F.EQ.0)GOTO300
      READ(1,*)MF,ZF,XW,XD,TT,RA,SIGMA,VFL,DL,ML,MG,RR,VMAX,LAMV,PFC,
     1 UC,TW,CC,LAMC,TB,TF,TS,CW,CR,LAMW,DELTW,OPT,CS,HC,UR,Q,ALFA,PO
      WRITE(5,2)
2     FORMAT(' IS FEED SATURATED,TYPE 1 FOR YES,0 FOR NO')
      READ(5,*)QF
      IF(QF.NE.1)GOTO10
C CALCULATING MINIMUM REFLUX
      XP=ZF
5     YP=(ALFA*XP)/(1.0+((ALFA-1.0)*XP))
      RM=(XD-YP)/(YP-XP)
      WRITE(5,6)RM
6     FORMAT(' THE MINIMUM REFLUX IS',F10.5)
      WRITE(20,6)RM
      R=RR*RM
      WRITE(5,7)R
7     FORMAT(' THE OPERATING REFLUX IS',F10.5)
      WRITE(20,7)R
      GOTO40
10    A=(Q/(Q-1.0))*(ALFA-1.0)
      B=Q/(Q-1.0)-ALFA-((ZF/(Q-1.0))*(ALFA-1.0))
      C=-ZF/(Q-1.0)
      DISC=(B**2)-(4.0*A*C)
      IF(DISC.LT.0.0)GOTO15
      GOTO20
15    WRITE(5,16)
16    FORMAT(5X,/,' THERE IS NO REAL SOLUTION FOR THE INTERSECTION
     1 OF EQUIB.CURVE AND Q-LINE')
      WRITE(20,16)
      GOTO999
20    X1=(-B+(DISC**0.5))/(2.0*A)
      X2=(-B-(DISC**0.5))/(2.0*A)
      IF(X1.GE.1.0)GOTO30
      IF(X1.LE.0.0)GOTO30
      XP=X1
      GOTO5
30    IF(X2.GE.1.0)GOTO35
```

Table 3.2. Continued.

```
      IF(X2.LE.0.0)GOTO35
      XP=X2
      GOTO5
35    WRITE(5,36)
36    FORMAT(5X,/,' THERE IS NO SOLUTION FOR THE INTERSECTION OF
     1 EQUIB.CURVE AND Q-LINE')
      WRITE(20,36)
      GOTO999
C INTERSECTION OF Q-LINE AND OPERATING LINE
40    IF(QF.NE.1)GOTO50
      XI=ZF
45    YI=((R*XI)+XD)/(R+1.0)
      GOTO55
50    XNU=(ZF/(Q-1.0))+(XD/(R+1.0))
      XDE=(R/(R+1.0))- (Q/(Q-1.0))
      XI=-XNU/XDE
      GOTO45
C CALCULATING SLOPE AND INTERCEPT OF STRIPPING SECTION OPERATING LINE
55    SLP=(YI-XW)/(ZF-XW)
      INT=YI-SLP*XI
C CALCULATING NUMBER OF PLATES
      IF(QF.NE.1)GOTO180
      Y1=XD
      DO 100  I= 1,50
      X(I)  =Y1/(ALFA-(Y1*(ALFA-1.0)))
      K=I+1
      Y(K)=((R*X(I))+XD)/(R+1.0)
      Y1=Y(K)
      IF(X(I).LE.ZF)GOTO60
      GOTO100
60    XS=X(I)
      N=I
      GOTO110
100   CONTINUE
110   WRITE(5,112)N
112   FORMAT(' THE NUMBER OF PLATES IN ENRICHING SECTION ARE',I5)
      WRITE(20,112)N
      WRITE(5,113)N
113   FORMAT(' THE FEED IS AT PLATE',I5)
      WRITE(20,113)N
      DO150J=1,50
      Y(J)=INT+SLP*XS
      M=J+1
      X(M)=Y(J)/(ALFA-(Y(J)*(ALFA-1.0)))
      XS=X(M)
      IF(XS.LE.XW)GOTO120
      GOTO150
120   P=M
      GOTO160
150   CONTINUE
160   WRITE(5,162)P
162   FORMAT(' THE NUMBER OF PLATES IN STRIPPING SECTION ARE',I5)
      WRITE(20,162)P
      GOTO280
180   Y1=XD
      DO200I=1,50
      X(I)=Y1/(ALFA-(Y1*(ALFA-1.0)))
      K=I+1
      Y(K)=((R*X(I))+XD)/(R+1.0)
      Y1=Y(K)
      IF(X(I).LE.XI)GOTO190
```

Table 3.2. Continued.

```
      GOTO200
190   XS=X(I)
      N=I
      GOTO210
200   CONTINUE
210   WRITE(5,112)N
      WRITE(20,112)N
      WRITE(5,113)N
      WRITE(20,113)N
      DO250J=1,50
      Y(J)=INT+SLP*XS
      M=J+1
      X(M)=Y(J)/(ALFA-(Y(J)*(ALFA-1.0)))
      XS=X(M)
      IF(XS.LE.XW)GOTO240
      GOTO250
240   P=M
      GOTO260
250   CONTINUE
260   WRITE(5,162)P
      WRITE(20,162)P
280   T=N+P+1
      WRITE(5,282)T
282   FORMAT(' THE TOTAL NUMBER OF PLATES INCLUDING REBOILER ARE',I5)
      WRITE(20,282)T
      GOTO750
300   READ(1,*)MF,ZF,XW,XD,TT,RA,SIGMA,VFL,DL,ML,MG,RR,VMAX,LAMV,
     1 PFC,UC,TW,CC,LAMC,TB,TF,TS,CW,CR,LAMW,DELTW,OPT,CS,HC,UR,Q,
     2 AP,B,C,D,PO
      WRITE(5,301)
301   FORMAT(' IS FEED SATURATED,TYPE 1 FOR YES,0 FOR NO')
      READ(5,*)QF
      IF(QF.NE.1)GOTO400
C CALCULATING MINIMUM REFLUX
      XQ=ZF
      XO=ZF
310   E=0.01
      JJ=1
      DELXQ=(XD-XQ)/100.
      DO350IJ=1,200
      YN=(1.0-XQ+AP*XQ+B*(XQ**2)-(C*XQ*EXP(-D*XQ)))
      YQ=(AP*XQ+B*(XQ**2)-(C*XQ*EXP(-D*XQ)))/YN
      YM=((1.0-XQ+AP*XQ+B*(XQ**2)-(C*XQ*EXP(-D*XQ)))**2)
      M1=(AP+2.*B*XQ-B*(XQ**2)-((C*EXP(-D*XQ))*(1.0-D*XQ+D*(XQ**2))))/
     1 YM
      M2=(XD-YQ)/(XD-XQ)
      IF(ABS((M1-M2)/M1).LE.E)GOTO320
      XQ=XQ+DELXQ
      GOTO350
320   IF(JJ.EQ.2)GOTO360
      XQ=XQ-DELXQ
      DELXQ=DELXQ/100.
      JJ=2
350   CONTINUE
360   IF(XQ.GE.XD)GOTO380
      YP=YQ
      XP=XQ
365   RM=(XD-YP)/(YP-XP)
      WRITE(5,6)RM
      WRITE(20,6)RM
      R=RR*RM
```

Table 3.2. Continued.

```
      GOTO480
380   WRITE(5,382)
382   FORMAT(' TANGENCY OF EQUIB.CURVE AND OPERATING LINE NOT FOUND')
      WRITE(20,382)
      XP=XO
      YDE=(1.0-XP+AP*XP+B*(XP**2)-(C*XP*EXP(-D*XP)))
      YP=(AP*XP+B*(XP**2)-(C*XP*EXP(-D*XP)))/YDE
      GOTO365
400   XO=0.01
      ER=0.01
      DELXO=0.005
      DO450KK=1,200
      Y(KK)=(-Q/(1.0-Q))*XO+(ZF/(1.0-Q))
      YDE=(1.0-XO+AP*XO+B*(XO**2)-(C*XO*EXP(-D*XO)))
      YZ=(AP*XO+B*(XO**2)-(C*XO*EXP(-D*XO)))/YDE
      IF(ABS(YZ-Y(KK)).LE.ER)GOTO460
      XO=XO+DELXO
450   CONTINUE
460   XQ=XO
      GOTO310
C INTERSECTION OF Q-LINE AND OPERATING LINE
480   IF(QF.NE.1)GOTO500
      XI=ZF
490   YI=((R*XI)+XD)/(R+1.0)
      GOTO510
500   XNU=(ZF/(Q-1.0))+(XD/(R+1.0))
      XDE=(R/(R+1.0))-(Q/(Q-1.0))
      XI=-XNU/XDE
      GOTO490
C CALCULATING SLOPE AND INTERCEPT OF STRIPPING SECTION OPERATING LINE
510   SLP=(YI-XW)/(ZF-XW)
      INT=YI-SLP*XI
C CALCULATING NUMBER OF PLATES
      IF(QF.NE.1)GOTO630
      X1=XD
      Y1=XD
      K=1
520   ERR=0.0005
      DELX1=0.0001
      DO550 I=1,2500
      FUNC(I)=(AP+B*X1-(C*EXP(-D*X1)))*X1*(1.0-Y1)-Y1*(1.0-X1)
      IF(FUNC(I).LE.ERR)GOTO560
      X1=X1-DELX1
550   CONTINUE
560   IF(X1.LE.ZF)GOTO580
      K=K+1
      Y1=((R*X1)+XD)/(R+1.0)
      GOTO520
580   N=K
      WRITE(5,112)N
      WRITE(20,112)N
      WRITE(5,113)N
      WRITE(20,113)N
      M=1
590   Y1=INT+SLP*X1
      ERR=0.0005
      DELX1=0.0001
      DO600 J=1,2500
      FUNC(J)=(AP+B*X1-(C*EXP(-D*X1)))*X1*(1.0-Y1)-Y1*(1.0-X1)
      IF(FUNC(J).LE.ERR)GOTO610
      X1=X1-DELX1
```

Table 3.2. Continued.

```
600     CONTINUE
610     IF(X1.LE.XW)GOTO620
        M=M+1
        GOTO590
C THE NUMBER OF PLATES ARE COUNTED BY THE NUMBER OF TIMES THE OPERATING
C LINE IS INTERCEPTED.TRANSICTION FROM ONE OPERATING TO ANOTHER IS SUCH
C THAT THE FIRST TIME THE BOTTOM OPERATING LINE IS INTERCEPTED THE TRAY
C IS COUNTED FOR ENRICHING SECTION.HENCE THE NUMBER OF TRAYS ARE ONE
C LESS THAN THE COUNTER FOR THE STRIPPING SECTION.
620     P=M-1
        WRITE(5,162)P
        WRITE(20,162)P
        GOTO720
630     X1=XD
        Y1=XD
        K=1
640     ERR=0.0005
        DELX1=0.0001
        DO650 I=1,2500
        FUNC(I)=(AP+B*X1-(C*EXP(-D*X1)))*X1*(1.0-Y1)-Y1*(1.0-X1)
        IF(FUNC(I).LE.ERR)GOTO660
        X1=X1-DELX1
650     CONTINUE
660     IF(X1.LE.XI)GOTO670
        K=K+1
        Y1=((R*X1)+XD)/(R+1.0)
        GOTO640
670     N=K
        WRITE(5,112)N
        WRITE(20,112)N
        WRITE(5,113)N
        WRITE(20,113)N
        M=1
680     Y1=INT+SLP*X1
        ERR=0.0005
        DELX1=0.0001
        DO690 J=1,2500
        FUNC(J)=(AP+B*X1-(C*EXP(-D*X1)))*X1*(1.0-Y1)-Y1*(1.0-X1)
        IF(FUNC(J).LE.ERR)GOTO700
        X1=X1-DELX1
690     CONTINUE
700     IF(X1.LE.XW)GOTO710
        M=M+1
        GOTO680
710     P=M-1
        WRITE(5,162)P
        WRITE(20,162)P
720     T=N+P+1
        WRITE(5,282)T
        WRITE(20,282)T
```

moles to 1 mol of product is to be used. The molal latent heats of benzene and toulene are 7360 and 7960 cal/gmol respectively.

1. Calculate the moles of overhead product and bottoms per hour.
2. Determine the number of ideal plates and the position of the feed plate.
    i) if the feed is liquid and at its boiling point
    ii) if the feed is liquid and at 20°C (specific heat = 0.44);
    iii) if the feed is a mixture of two-thirds vapor and one third liquid.

The example was solved with the following quantities specified:

$x_D = 0.974$; $x_W = 0.0235$; $Z_F = 0.44$; $R/Rm = 3.5$; $\alpha = 2.34$.

The graphical solutions of part i) and part ii) for Q = 1.0 and Q = 1.37 are shown in Figure 2.2 (page 11) and Figure 3.9 respectively. A comparison of the solution obtained by solving the example graphically with that obtained by the computer code is shown in Table 3.3 and 3.4 for the parts i) and ii) respectively. It is seen that the results obtained by the code are very close to the ones obtained by the graphical solution of the example, which clearly indicate the correctness of the code.

For non-ideal systems the minimum reflux is calculated by two ways. The first method is based on drawing a tangent on the equilibrium curve, and determining the intersection of the tangent and the curve as shown in Figure 3.10. This approach is solved in the code by comparing the slope of the tangent and equilibrium curve, and the

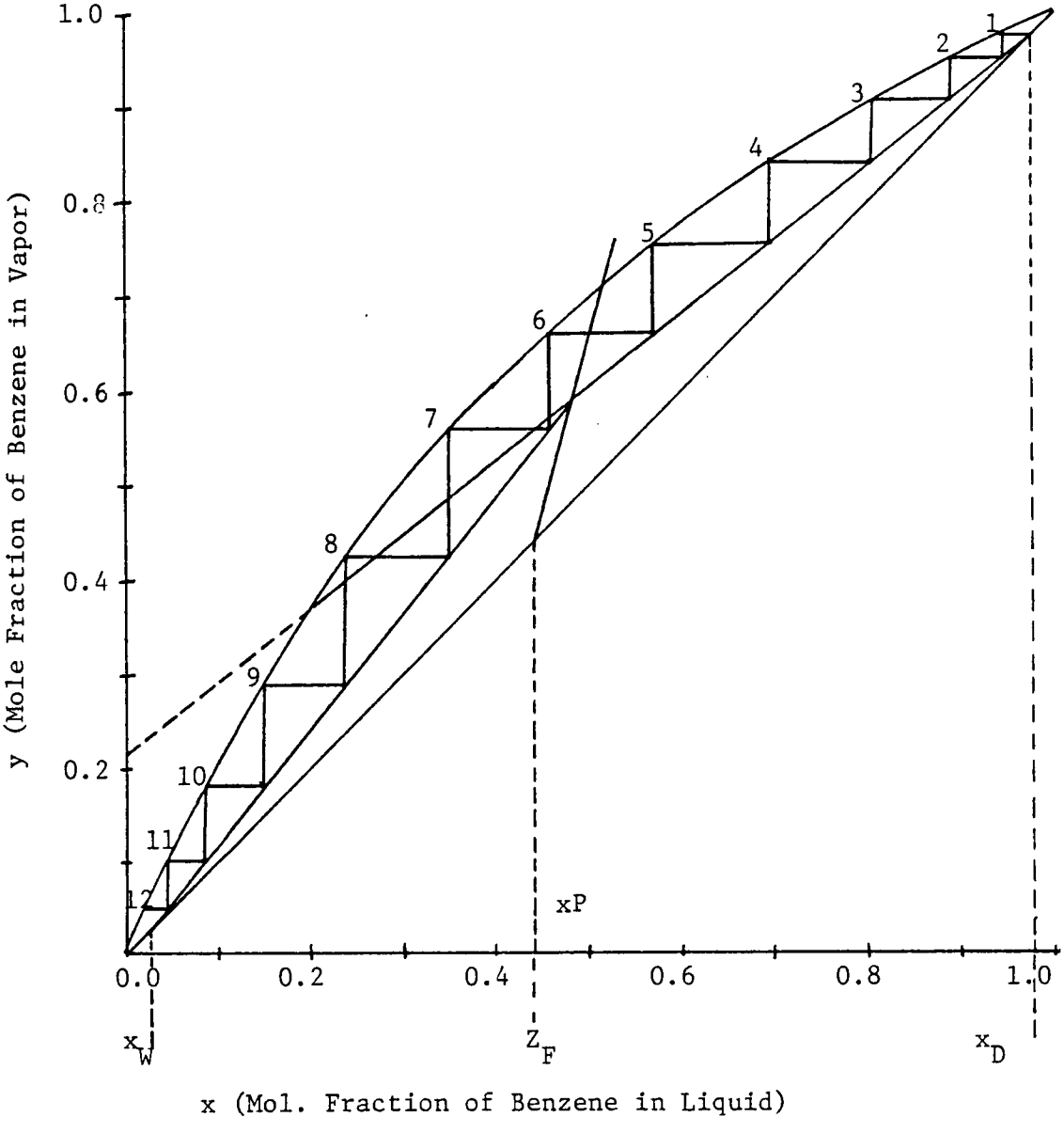


Figure 3.9. Estimating Number of Theoretical Plates for Benzene-Toulene System.

Table 3.3. Comparison of Results of a Benzene-Toluene Separation Example Problem for Q = 1.0.

Quantity	Results	
	Graphical Solution[a]	Computer Solution
Minimum reflux	1.57	1.57
Number of Theoretical plates,		
Enriching section	6	6
Stripping section	6	6
Feed Tray Location	6	6
Total number of plates including reboiler	13	13

[a]Data Source: Example 19-4, page 560, McCabe and Smith, 1976, See Figure 2.2 (page 11).

Table 3.4. Comparison of Results for a Benzene-Toluene Separation Example Problem for Q = 1.37.

Quantity	Results	
	Graphical Solution[a]	Computer Solution
Minimum reflux	1.37	1.32
Number of theoretical plates,		
Enriching section	6	6
Stripping section	5	5
Feed Tray Location	6	6
Total number of plates including reboiler	12	12

[a]Data Source: Example 19-4, page 560, McCabe and Smith, 1976, See Figure 3.9 (page 56).

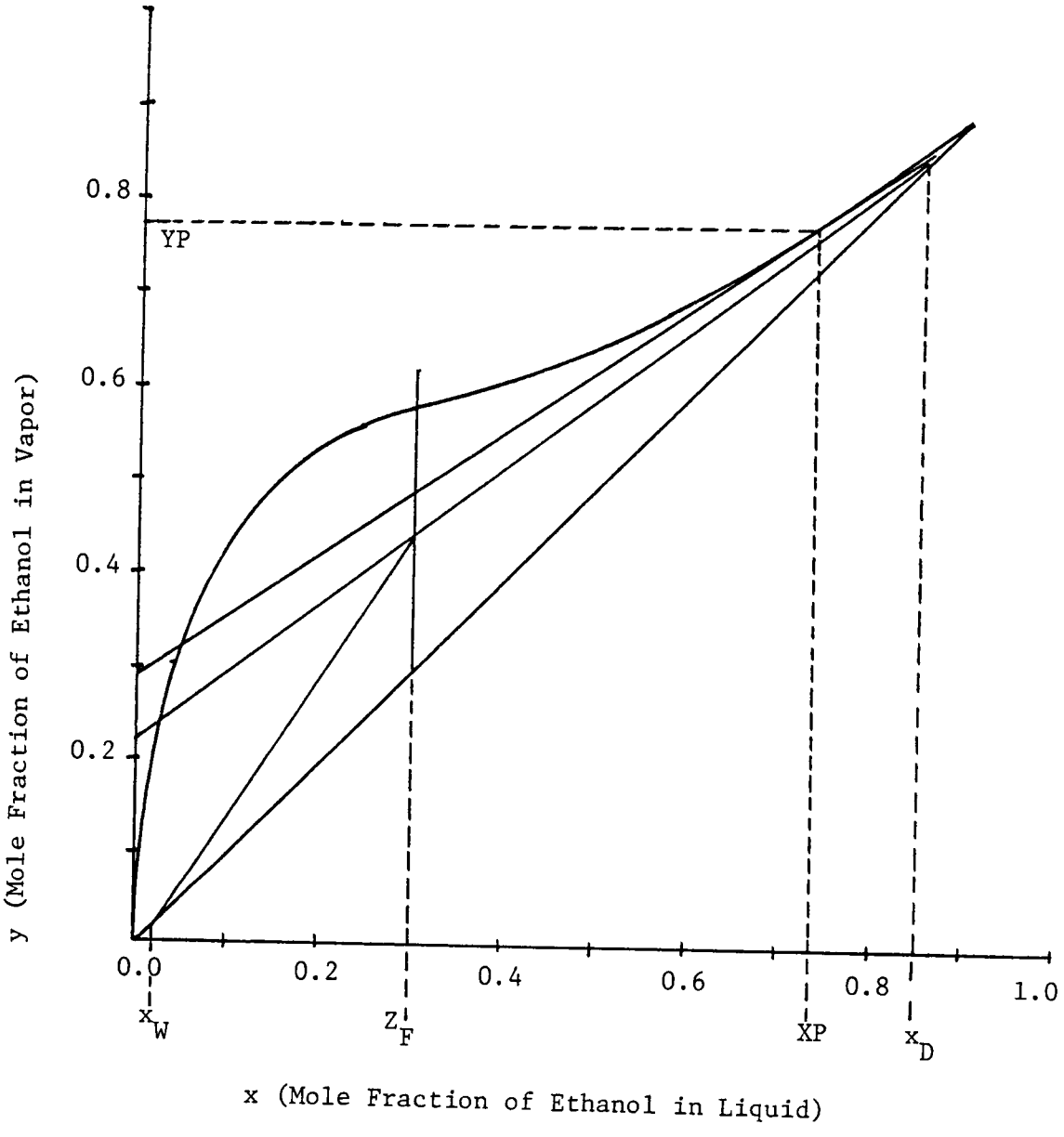


Figure 3.10. Calculating Minimum Reflux by Tangent for Ethanol-Water System.

intersection point is determined when the slopes are equal. The equilibrium curve is obtained for the Ethanol-Water system by substituting the model equation of α (model C, equation (3.2)) into the equation (3.1), the resulting equation is given as

$$y = \frac{ax+bx^2-cxe^{-dx}}{1-x+ax+bx^2-cxe^{-dx}} \tag{3.21}$$

The slope of the equilibrium curve is obtained by taking the derivative of equation (3.21) which is given by

$$M_1 = \frac{dy}{dx} = \frac{a+2bx-bx^2-ce^{-dx}(1-dx+dx^2)}{(1-x+ax+bx^2-cxe^{-dx})^2} \tag{3.22}$$

The slope of the tangent is given by the relation

$$M_2 = \frac{(x_D-y)}{(x_D-x)} \tag{3.23}$$

An iterative approach is used to compare the slopes M_1 and M_2 starting from the feed point towards the distillate composition. An error limit of 0.01 was found to be satisfactory for the convergence criterion.

If the tangency is not found then the minimum reflux is calculated by intersection of Q-line and equilibrium curve as shown in Figure 3.11. An iterative method was used to compare the composition in vapor phase at a specified composition in liquid phase from the Q-line equation (equation (3.10)) and equilibrium curve equation, (equation (3.21)). The convergence criterion was satisfied when both the compositions matched. An error limit of 0.01 was found suitable to meet the convergence criterion. The number of plates

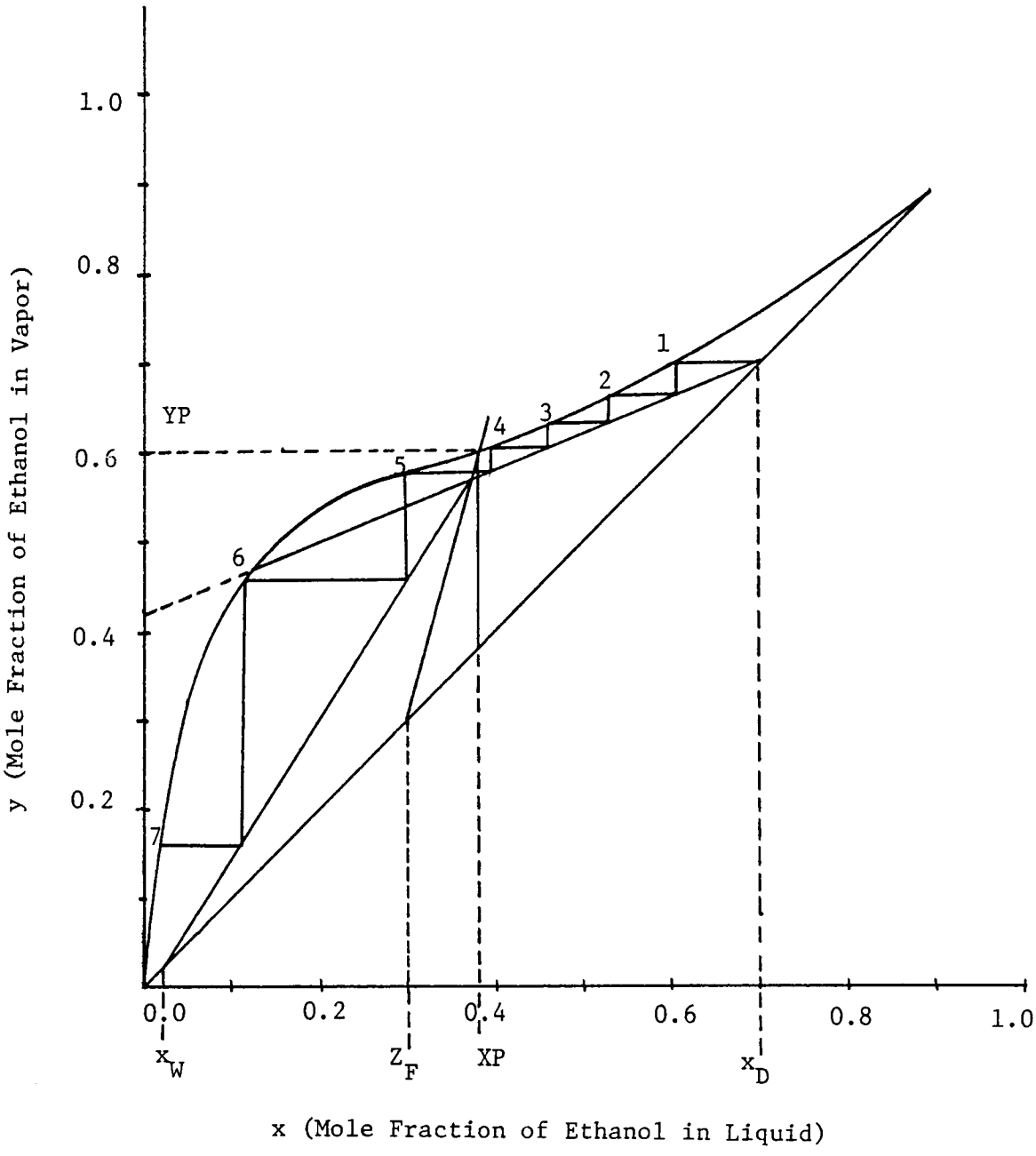


Figure 3.11. Calculating Minimum Reflux by Intersection of Q-Line and Equilibrium Curve for Ethanol-Water System.

are calculated by the method described previously. Figure 3.8 shows the flow chart of the code for estimating the number of plates, and the section of the code is shown in Table 3.2.

A problem was solved graphically for the Ethanol-Water system to check the correctness of code, with the following specified quantities:

$x_D = 0.7$; $x_W = 0.02$; $Z_F = 0.3$; R/Rm = 1.5; Q = 1.37 .

The graphical solution to the problem is shown in Figure 3.11, and a comparison with the solution obtained by the computer code is shown in Table 3.5. The closeness of the two solutions indicates the fact that the code works equally well for the non-ideal systems too, once a good model to the VLE data of the system to be considered is provided.

3.2.2 Establishing the column diameter. The column is sized by the procedure as provided by Treybal (1979). An iterative approach is used in order to converge to the true diameter. An initial estimate of the diameter is made based upon a specified maximum allowable vapor velocity, VMAX, by the relation

$$TD = \frac{4QT}{\sqrt{\pi VMAX}} \tag{3.24}$$

where QT is the volumetric flowrate of the gas in ft^3/sec and is determined by

$$QT = \frac{VD \times 359(TT+460)}{492 \times 3600} \times \frac{14.7}{P_o} \tag{3.25}$$

TT is the temperature at the top of the tower in °F, P_o is the operating pressure in psia, and VD is the moles of vapor per hour at the top of column, and is calculated by the equation

Table 3.5. Comparison of Results for an Ethanol-Water Separation Example Problem for Q = 1.37.

Quantity	Results	
	Graphical Solution[a]	Computer Solution
Minimum reflux	0.455	0.434
Number of theoretical plates,		
Enriching section	5	5
Stripping section	1	1
Feed Plate Location	5	5
Total number of plates including reboiler	7	7

[a]Data Source: Figure 3.11 (page 61).

$$VD = MD(R+1) \tag{3.26}$$

where MD is the moles of distillate per hour. The method is shown in the attached flow chart (Figure 3.12). The tray spacing based upon the tower diameter is determined by regressing upon the data provided by Treybal (1979), and the equation of the form,

$$\text{Model I:} \quad t = a+b(TD)+C(TD)^2 \tag{3.27}$$

was found to be a suitable fit to the data. The values of the parameters were found to be as a = 16.146, b = 1.54 and c = -0.027. The correlation coefficient was not very high (r = 0.9468), the F-statistic for the variables were found to be 21.81 and 4.39 respectively which is not very significant indicating the fact that the model 'I' did not fit very well to the data. Figure 3.13 shows the actual data along with the fitted curve (Model I).

The diameter of the tower is calculated by determining the area of cross section of the tower which is given by the relation

$$A = QT/V \tag{3.28}$$

where 'V' is the superficial velocity based upon the flooding velocity. The flooding conditions are checked at the top tray. For a given type of tray at flooding the superficial velocity is given as

$$V_F = C_F \left(\frac{\rho_L - \rho_G}{\rho_G}\right)^{1/2} \tag{3.29}$$

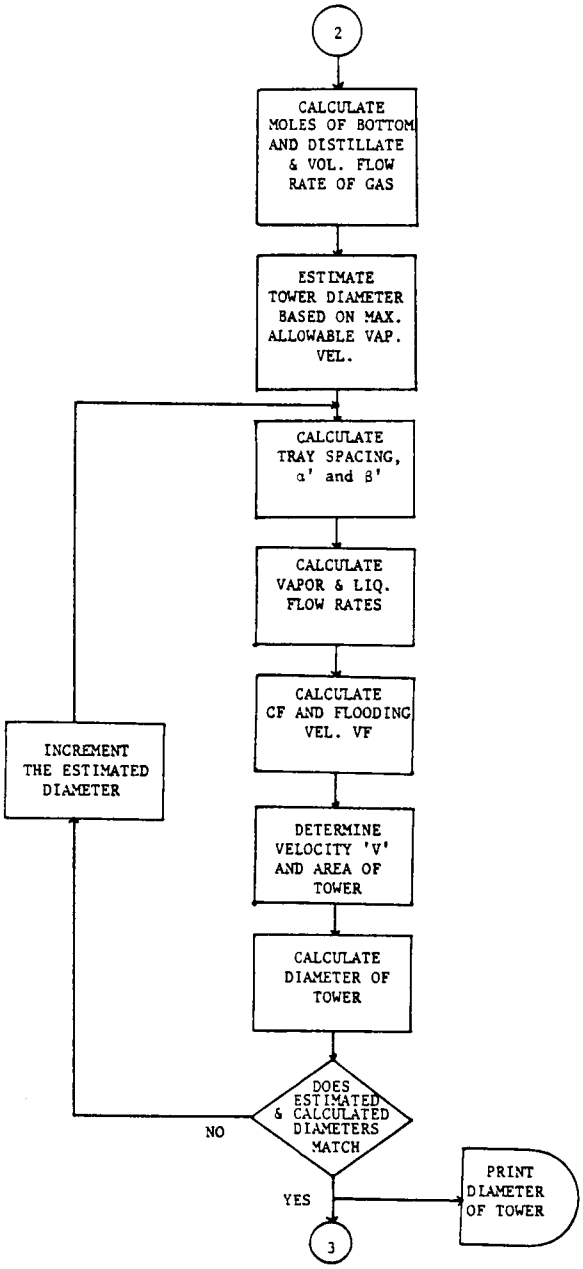


Figure 3.12. Flow Chart for Estimating Tower Diameter.

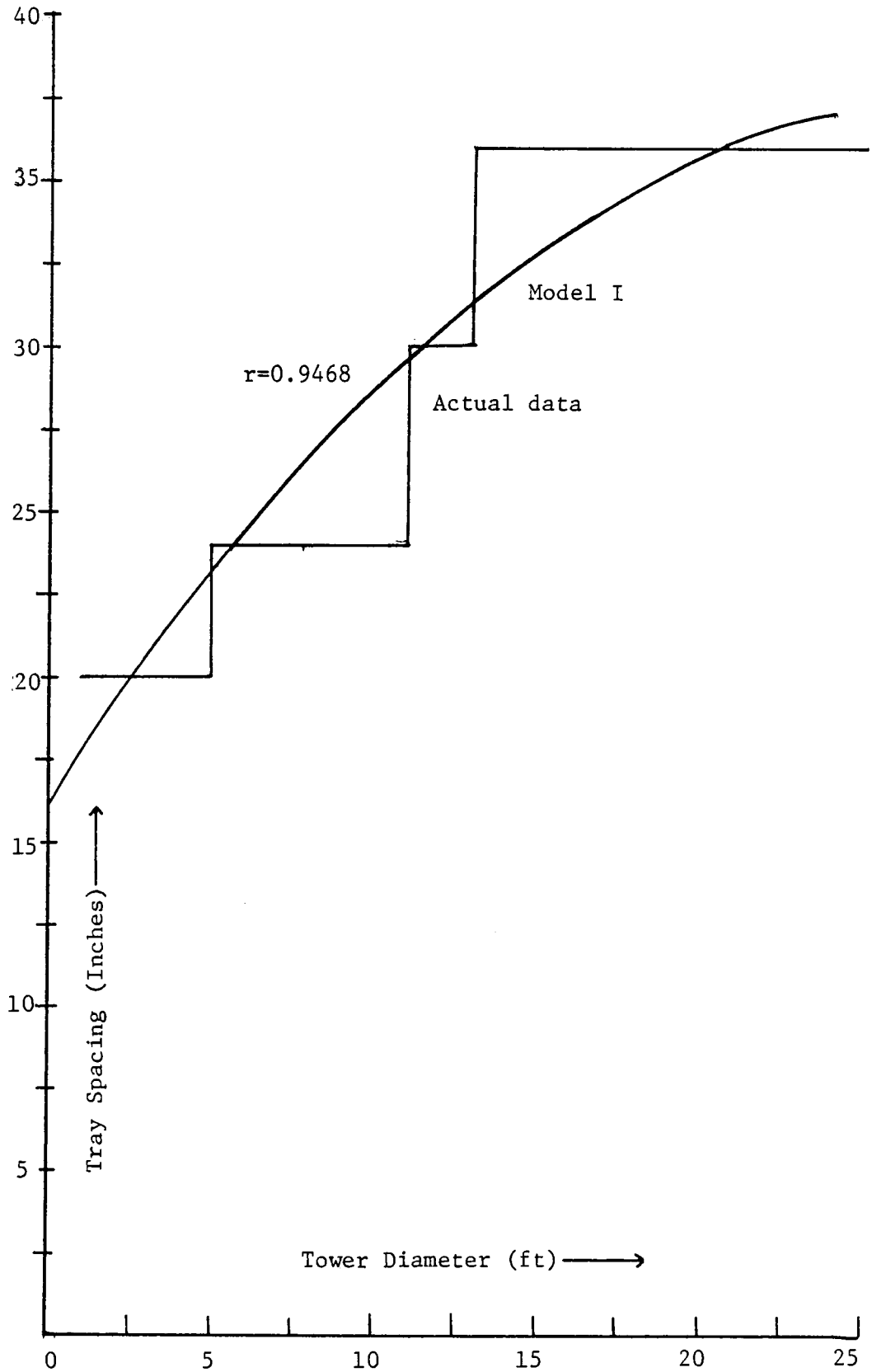


Figure 3.13. Tray Spacing as a Function of Tower Diameter.

Where ρ_L and ρ_G are the densities of liquid and gas respectively, and C_F is the flooding constant correlated by

$$C_F = [\alpha' \log \frac{1}{(L'/G')(\rho_G/\rho_L)^{0.5}} + \beta'](\frac{\sigma}{0.02})^{0.2} \qquad (3.30)$$

The values of the empirical constants α' and β' are dependent upon the tray spacing. The convergence criterion for the diameter is satisfied when the estimated and calculated diameters match, the error of convergence being 0.05 ft, which is about 5% for a tower of 1 ft diameter and 1% for a tower of 5 ft diameter. Table 3.6 shows the section of the code which calculates the diameter of the tower.

3.3 Optimizing The Design

The cost data as provided by Peters and Timmerhaus (1980) is used to optimize the design based upon minimizing the total annual cost. Once the diameter of the tower is determined by the use of the computer code, the cost as a function of tower size curves as given by Peters and Timmerhaus (1980), and shown in Figure 3.14, is used to calculate the annual cost of the column. The curve for the sieve tray tower (steel shell, stainless steel trays) is chosen as an example in order to compare the results with the example discussed by Peters & Timmerhaus (1980). A model equation is found to fit the cost data curve. A cubic equation is found to give a good fit to the data, i.e.,

$$\log(\text{cost}) = a+b(\log(\text{dia})) + c(\log(\text{dia}))^2 + d(\log(\text{dia}))^3 \qquad (3.20)$$

The parameters a, b, c and d were determined by regression analysis and were found to be a = 5.165, b = -0.064, c = 0.176 and d = -0.004.

Table 3.6. Code for Calculating Tower Diameter.

```
750     MD=(MF*(ZF-XW))/(XD-XW)
        MB=MF-MD
        VD=MD*(R+1.0)
        QT=(VD*359.*(TT+460.)*14.7)/(492.*3600.*PO)
        TD=((4.*QT)/(VMAX*3.1416))**0.5
C
C
C
        DO 800 I=1,100
        IF(TD.GT.4.0)GOTO760
        SMT=20.0

        GOTO770
760     SMT=16.14636+1.54*TD-0.02754*(TD**2.)
770     IF(RA.GE.0.1)GOTO780
        ALFA1=(0.0062*SMT+0.0385)*((5.*RA)+0.5)
        BETA1=(0.00253*SMT+0.05)*((5.*RA)+0.5)
        GOTO790
780     ALFA1=0.0062*SMT+0.0385
        BETA1=0.00253*SMT+0.05
790     YG=XD
        YL=1.0-YG
        AMWG=(YG*MG)+(YL*ML)
        XG=XW
        XL=1.0-XG

        AMWL=1.0/((XG/MG)+(XL/ML))
        DG=(AMWG*492.)/(359.*(TT+460.))
        VR=(MD*359.*(TT+460.))/(492.*3600.)
        LR=(MB*AMWL)/(DL*3600.)
        DEN=((LR*DL)/(VR*DG))*((DG/DL)**0.5)
        CF=(ALFA1*(ALOG10(1.0/DEN))+BETA1)*((SIGMA/0.02)**0.2)
C THE FLOODING CONDITIONS ARE CHECKED AT TOP OF THE COLUMN.
        VF=CF*(((DL-DG)/DG)**0.5)
        V=VF*(VFL/100.)
        AREA=QT/V
        DIA=((4.*AREA)/3.1416)**0.5
        ERR=0.05
        IF(ABS(TD-DIA).LE.ERR)GOTO810
        DELTD=0.1
        TD=TD+DELTD
800     CONTINUE
810     IF(I.EQ.100)GOTO820
        WRITE(5,815)DIA
        WRITE(20,815)DIA
815     FORMAT(' THE DIAMETER OF TOWER IS',F8.6)
        GOTO830
820     WRITE(5,825)
        WRITE(20,825)
825     FORMAT(' THE VALUES OF ASSUMED AND CALCULATED DIAMETERS DO
     1 NOT CONVERGE')
        GOTO999
```

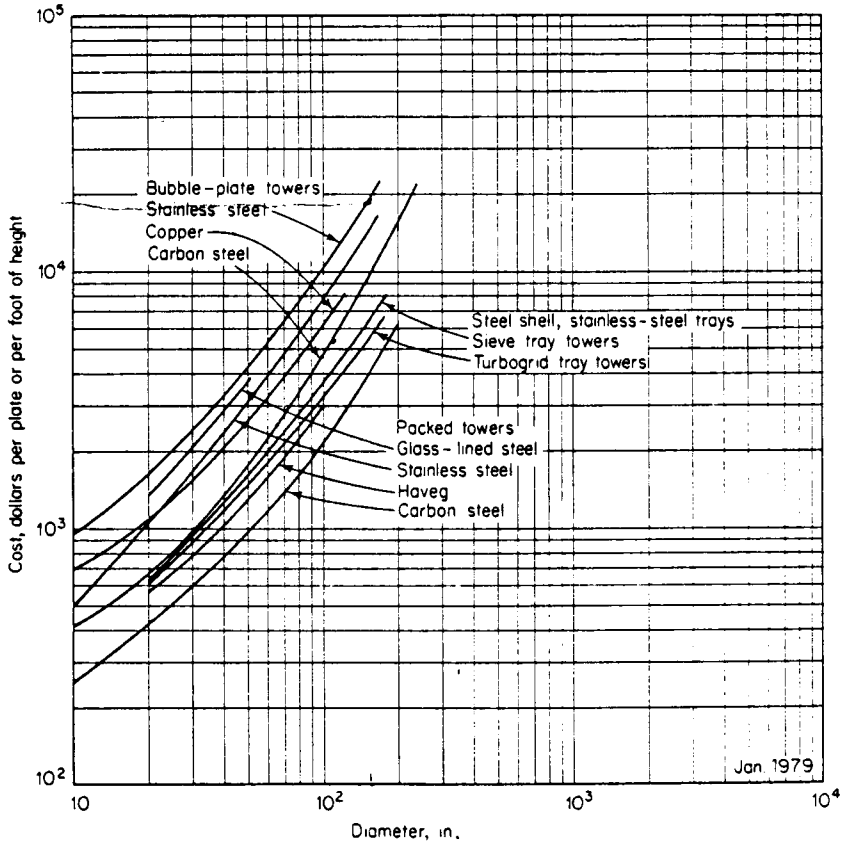


Figure 3.14. Cost of Towers Including Installation and Auxiliaries.

Source: Fig. 15-28, Peters and Timmerhaus, (1980)

The correlation coefficient is found good (r = 0.9972), the F-statistic is also good (F = 1377.58) indicating a good fit to the data. Once the annual cost of the column is determined, the heat transfer rate and area of the condenser and reboiler are calculated to determine the annual costs for condenser, reboiler, cooling water and steam. By summing these costs the total annual cost is determined at a specified reflux ratio. By varying the reflux ratio the optimum conditions are determined, i.e., the optimum reflux which yields the minimum total annual cost. The example 6, page 388, discussed by Peters and Timmerhaus (1980) is used to check the code; the problem is stated below:

A sieve-plate distillation column is being designed to handle 700 lb mol of feed per hour. The unit is to operate continuously at a total pressure of 1 atm. The feed contains 45 mol% benzene and 55 mol% toluene, and the feed enters at its boiling temperature. The overhead product from the distillation tower must contain 92 mol% benzene, and the bottoms must contain 95 mol% toluene. Determine the following:

1. The optimum reflux ratio as moles liquid returned to tower per mole of distillate product withdrawn.
2. The ratio of the optimum reflux ratio to the minimum reflux ratio.
3. The percent of the total variable cost due to steam consumption at the optimum conditions.

The following data apply:

Vapor-liquid equilibrium data for benzene-toluene mixture at

atmospheric pressure. The molal heat capacity for liquid mixtures of benzene and toluene in all proportions may be assumed to be 40 Btu/lb mol.°F. The molal heat of vaporization of benzene and toluene may be taken as 13,700 Btu/lb mol. Effects of change in temperature on heat capacity and heats of vaporization are negligible. Heat losses from the column are negligible. Effects of pressure drop over the column may be neglected. The overall coefficient of heat transfer is 80 Btu/hr ft^2 °F in the reboiler and 100 Btu/hr ft^2 °F in the condenser.

The boiling temperature is 201°F for the feed, 179°F for the distillate, and 227°F for the bottoms. The temperature-difference driving force in the reflux condenser may be based on an average cooling water temperature of 90°F, and the change in cooling water temperature is 50°F for all cases. Saturated steam at 60 psia is used in reboiler. At this pressure, the temperature of the condensing steam is 292.7°F and the heat of condensation is 915.5 Btu/lb. No heat-saving devices are used.

The column diameter is to be based on a maximum allowable vapor velocity of 2.5 ft/sec at the top of the column. The overall plate efficiency may be assumed to be 70%. The unit is to operate 8500 hr per year.

Cost data:

Steam = \$0.75/1000 lb

Cooling Water = \$0.054/10,000 lb

The sum of costs for piping, insulation, and instrumentation can be

estimated to be 60% of the cost for the installed equipment. Annual fixed charges amount to 15% of the total cost for installed equipment, piping, instrumentation and insulation.

The example is solved by Peters and Timmerhaus (1980) by first calculating the reflux ratio, and the number of plates by McCabe-Thiele method. The diameter of the column is calculated based upon the maximum allowable vapor velocity of 2.5 ft/sec at top of the tower. The cost per plate of the column is obtained by the cost as a function of tower size curve, and the annual cost of the column is obtained for the total number of plates. The annual cost of condenser and reboiler are determined by calculating the heat transfer area and rate of heat transfer for the condenser and reboiler respectively. The annual costs are then determined based on cost per square foot for the condenser and reboiler. The cost data as a function of heat transfer area is shown in Table 3.7 and 3.8 for condenser and reboiler respectively. The annual cost for cooling water and steam are determined based on the cost data provided. The total annual cost is obtained by summing all the costs at the specified reflux ratio.

A similar approach has been followed in developing the program for optimizing the column, and the results of the example are shown in Figure 3.15 along with the results obtained from the computer code (model A). Figure 3.16 shows the flow chart for the optimization code, and Table 3.9 shows the section of the corresponding code. The cost as a function of tower size curves and the cost data for

Table 3.7. Cost Data for Condenser--Tube and Shell Heat Exchanger.

Heat-Transfer Area (Ft^2)	Cost ($)
800	9,750
1000	11,250
1200	12,600
1400	13,800
1600	14,850

Data Source: Plant Design and Economics for Chemical Engineers, Peters and Timmerhaus (1980).

Table 3.8. Cost Data for Reboiler--Tube and Shell Heat Exchanger.

Heat Transfer Area (Ft^2)	Cost ($)
1000	17,250
1400	21,150
1800	24,600
2200	27,750
2600	30,300

Data Source: Plant Design and Economics for Chemical Engineers, Peters and Timmerhaus (1980).

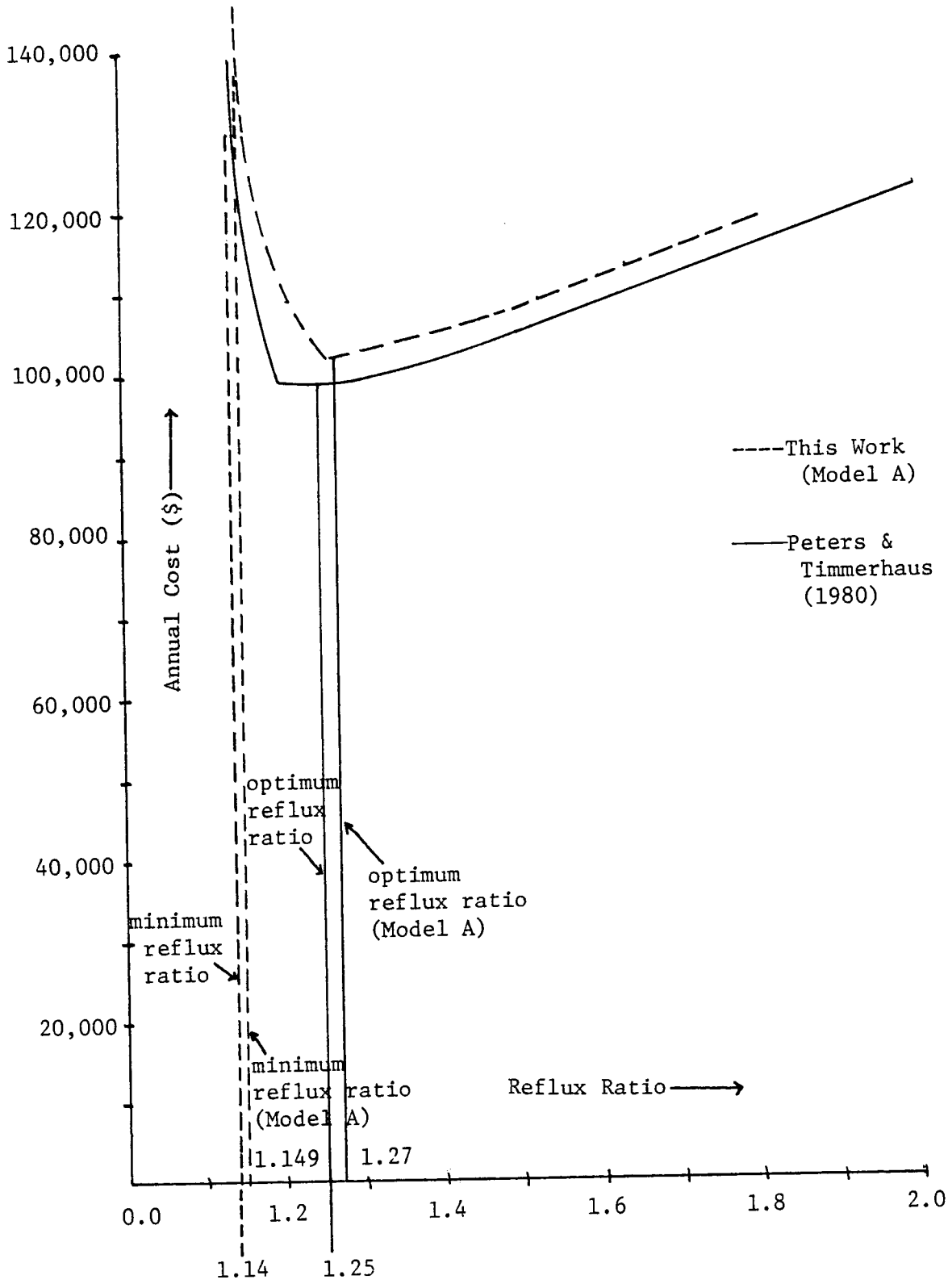


Figure 3.15. Optimum Reflux Ratio in Distillation Operation.

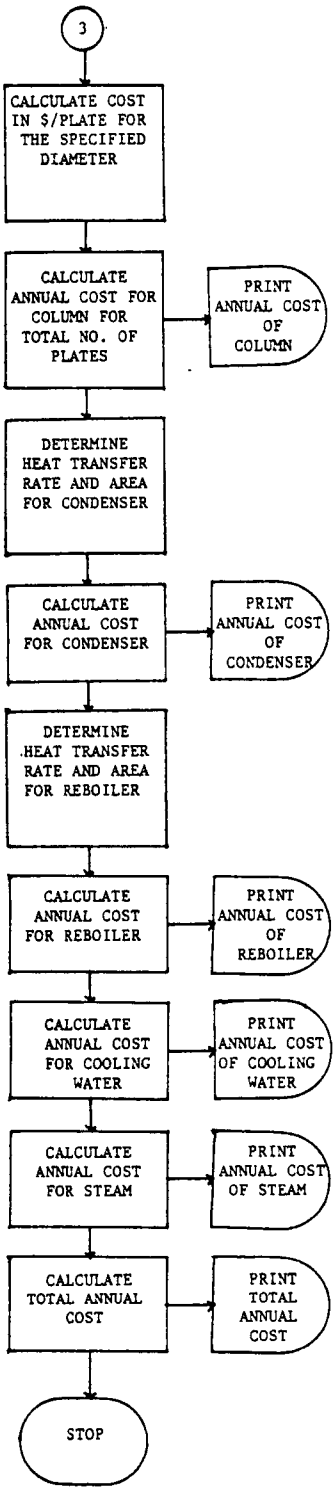


Figure 3.16. Flow Chart for Calculating Total Annual Cost.

Table 3.9. Code for Calculating Total Annual Cost.

```
830     DIAIN=DIA*12.0
        COST=EXP(5.16474-0.06366*(ALOG(DIAIN))+0.1755*((ALOG(DIAIN))**
       1 2)-0.004*((ALOG(DIAIN))**3))
        SLOPE =R/(R+1.0)
        ACOST=COST*T*(1.+SLOPE)*(PFC/100.)
        WRITE(5,835)ACOST
        WRITE(20,835)ACOST
835     FORMAT(' ANNUAL COST OF DIST.COLUMN IS',F8.2)
        QC=VD*LAMV
        HAC=QC/(UC*(TT-TW))
        AC=(CC/HAC)*HAC*(1.+SLOPE)*(PFC/100.)
        WRITE(5,840)AC
        WRITE(20,840)AC
840     FORMAT(' ANNUAL COST OF CONDENSER IS',F8.2)
        QR=QC+MB*LAMC*(TB-TT)-MF*LAMC*(TF-TT)
        HAR=QR/(UR*(TS-TB))
        AR=(CR/HAR)*HAR*(1.+SLOPE)*(PFC/100.)
        WRITE(5,845)AR
        WRITE(20,845)AR
845     FORMAT(' ANNUAL COST OF REBOILER IS',F10.2)
        AW=(QC*CW*OPT)/(LAMW*DELTW)

        WRITE(5,850)AW
        WRITE(20,850)AW
850     FORMAT(' ANNUAL COST OF COOLING WATER IS',F10.2)
        AS=(QR*CS*OPT)/HC
        WRITE(5,900)AS
        WRITE(20,900)AS
900     FORMAT(' ANNUAL COST OF STEAM IS',F10.2)
        TAC=ACOST+AC+AR+AW+AS
        WRITE(5,910)TAC
        WRITE(20,910)TAC
910     FORMAT(' TOTAL ANNUAL COST IS',F10.2)
999     STOP
        END
```

the cooling water, steam condenser and reboiler are based on the cost of January 1979. While solving the example the same costs were used in order to compare the results obtained with the results obtained by Peters and Timmerhaus (1980), however, the cost data should be updated for a specific design as required using an inflationary index such as the Marshall and Swift equipment cost index (see for example, Peters and Timmerhaus, 1980).

It is clear from Figure 3.15, that the results obtained from the computer code are close enough with those obtained by Peters and Timmerhaus (1980), for the example previously discussed. The difference in the values for the minimum reflux between the code and that obtained by Peters and Timmerhaus (1980), is less than 1%, and similarly for the optimum reflux it is about 1.5%, whereas for the total annual cost it is about 3% which is reasonable considering the error in the cost data. Hence, we can satisfactorily state that the code is quite effective for optimizing the design of a tower for the separation of binary systems. Table 3.10 shows a comparison between the results obtained by the code with those provided by Peters and Timmerhaus (1980).

Table 3.10. Comparison of Results for an Example to Determine Total Annual Cost at Optimum Reflux Ratio.

Quantity	Results	
	Peters and Timmerhaus Solution[a]	Computer Solution
Minimum reflux ratio	1.14	1.149
Optimum reflux ratio	1.25	1.264
Diameter of tower (ft)	6.9	7.142
Number of theoretical plates required	18	19
Total annual cost ($)	99,000	102,095.01

[a]Data Source: Example 6, page 388, Peters and Timmerhaus, (1980).

CHAPTER 4

COMPUTER CODE FOR MULTICOMPONENT DISTILLATION

In this type of system only those systems are considered which are reasonably ideal, such as mixture of certain hydrocarbons. For the development of the computer code the short cut design method as provided by Treybal (1979) in Chapter 9, is taken as the basis. This method requires VLE data in the form of K-values (K=y/x) as a function of temperature, and it computes the number of theoretical trays required for the separation and also the composition of bottoms and distillate, for specified values of column pressure, reflux ratio, and thermal condition of feed (e.g., saturated liquid or partially vaporized feed, etc.) The method also requires an initial estimate of the average column temperature in order to determine the average volatility of each component of the mixture. A computer code using this short cut method has been developed by Chang (1980). His code is based on the assumption that the true average column temperature is known at the outset, and hence the relative volatilities are known. The code calculates the minimum number of plates by Fenske's (1932) equation, minimum reflux by Underwood's (1948) equation, number of theoretical plates by Gilliland's (1940) method, and the composition in bottoms and distillate by Hengstebeck (1946)--Geddes (1958) method.

Chang's code is extended here to the case where the only quantity known at the outset (in addition to the feed composition, column

pressure, specified split in the two components, etc.) is the thermal condition of feed. An initial estimate of the average column temperature is made, and an iterative approach is used to converge to the true average column temperature. Regression analysis is done to develop analytic equations based on the De-Priester's nomograph to determine K-values for selected light hydrocarbons at a pressure of 150 psia. The data was fitted using a quadratic or polynomial equation of the form:

$$\text{Model M:} \quad \ln(K) = a+bT+CT^2 \tag{4.1}$$

$$\text{Model N:} \quad \ln(K) = a+bT+CT^2+dT^3 \tag{4.2}$$

Where T is the average column temperature in °C. Figure 4.1 shows the experimental and fitted models for VLE relationships for selected light hydrocarbons at 150 psia. Table 4.1 shows the values of the coefficients and the correlation coefficients of the fitted models for the selected light hydrocarbons. The high values of correlation coefficients indicates the good fit to the data. The vapor composition for each component in feed is calculated by the relation:

$$y_F = \frac{x_F + (L_F/G_F+1.0)}{(1.0 + L_F/G_F \times K)} \tag{4.3}$$

where x_F is the mole fraction of component in feed. L_F and G_F are the liquid and vapor rates respectively, for a specified thermal condition of feed. The convergence criterion is satisfied when the sum of the vapor compositions of the components is unity, and hence

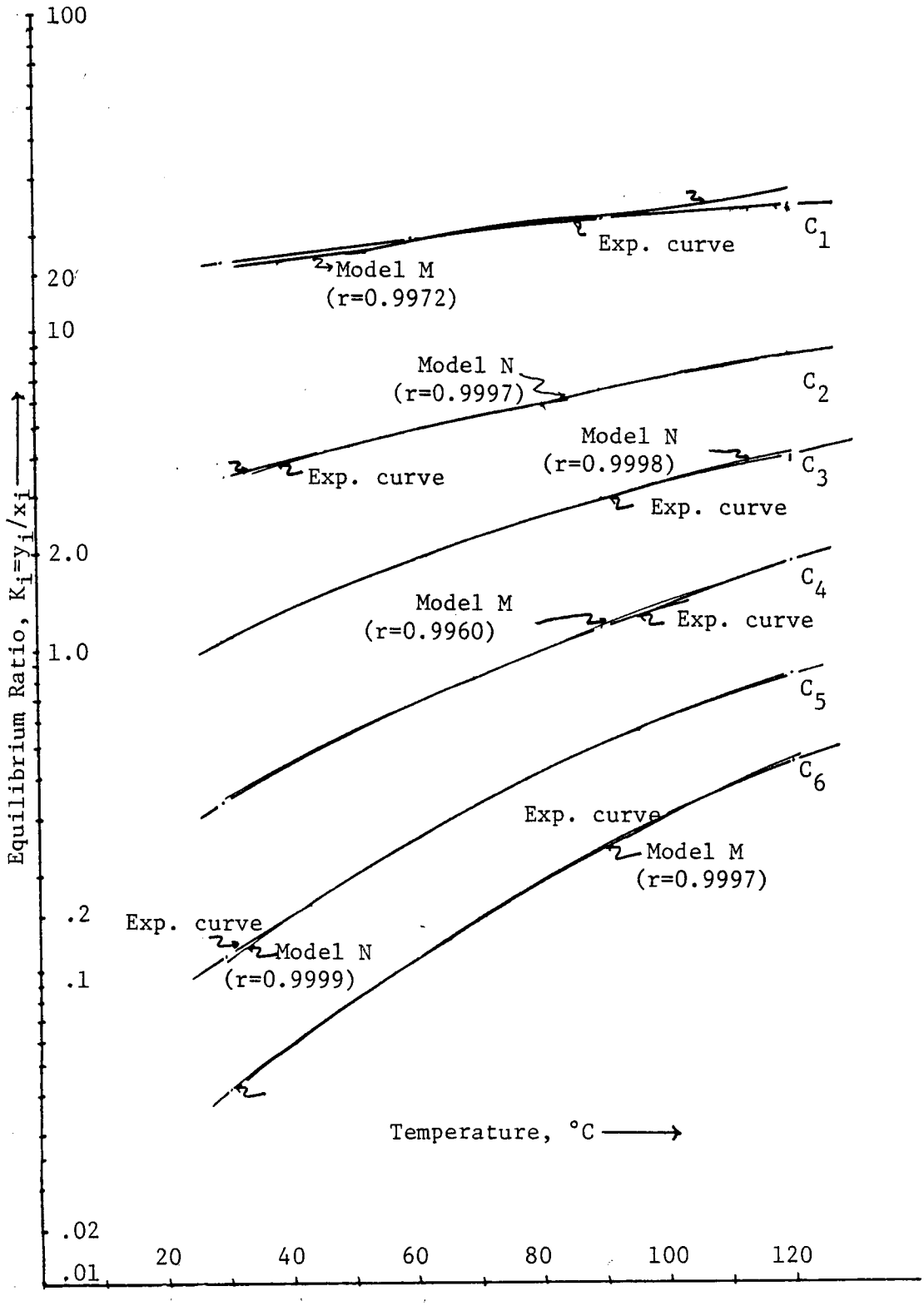


Figure 4.1. VLE Relationships for Selected Light Hydrocarbons.

Source: Treybal, Illustration 9.13, and De Priester's K-Value Nomograph, Pressure = 150 psia.

Table 4.1. Summary of VLE Relationship for Selected Light Hydrocarbons at 150 psia as Fitted by a Model by Regression Analysis.

Type of Hydrocarbon	Model	Correlation Coefficient (r)	Values of Parameters			
			a	b	c	d
C_1	M	0.9972	2.577	0.0066	-1.1×10^{-7}	-
C_2	N	0.9997	1.011	0.0068	5.42×10^{-5}	-3.0×10^{-7}
C_3	N	0.9998	-0.668	0.0297	-1.625×10^{-4}	4.8×10^{-7}
C_4	M	0.9960	-1.843	0.0285	-6.977×10^{-5}	-
C_5	N	0.9999	-3.336	0.0425	-1.772×10^{-4}	3.5×10^{-7}
C_6	M	0.9997	-4.302	0.0401	-9.1×10^{-5}	-

the assumed temperature is correct. The error of convergence is taken as 0.01, which is about 1%. The relative volatility (α) of each component is determined at the average column temperature using the relation:

$$\alpha_J = K_J/K_{HK} \tag{4.4}$$

where J is any component and HK is the heavy key. The estimated keys are checked by using the Shiras equation which is given as

$$\frac{x_{J,D}{}^D}{Z_{J,F}{}^F} = \frac{\alpha_J - 1}{\alpha_{LK} - 1} \frac{x_{LK,D}{}^D}{Z_{LK,F}{}^F} + \frac{\alpha_{LK} - \alpha_J}{\alpha_{LK} - 1} \frac{x_{HK,D}{}^D}{Z_{HK,F}{}^F} \quad . \tag{4.5}$$

The components between the keys are said to distribute for $x_{J,D}{}^D/Z_{J,F}{}^F$ between 0.01 and 0.99. If the keys are guessed wrong then an error message is indicated.

The number of moles of the keys are calculated by the following relations:

$$d_{LK} = (df)_{LK}/f_{LK} \tag{4.6}$$

$$b_{LK} = f_{LK} - d_{LK} \tag{4.7}$$

$$d_{HK} = (1-(bf)_{HK})f_{HK} \tag{4.8}$$

$$b_{HK} = f_{HK} - d_{HK} \tag{4.9}$$

where $(df)_{LK}$ and $(bf)_{HK}$ are the initial guesses of the light and heavy key in distillate and bottoms respectively. The distribution of the non-keys are estimated by the Hengstebeck-Geddes equation which is given as

$$\ln(d_i/b_i) = C_1+C_2\ln\alpha_i \tag{4.10}$$

substituting LK and HK for i in equation (4.10) we obtain two equations in two unknowns, which can be solved simultaneously as

$$C_1 = \ln(d_{HK}/b_{HK}) \tag{4.11}$$

and

$$C_2 = \ln[(d_{LK}/b_{LK})(b_{HK}/d_{HK})]/\ln\alpha_{LK} \quad . \tag{4.12}$$

The material balance for component i is given as

$$f_i = d_i + b_i \tag{4.13}$$

Eliminating d_i between equation (4.13) and equation (4.10) we get

$$b_i = \frac{f_i}{1+\text{Exp}(C_1+C_2\ln\alpha_i)} \tag{4.14}$$

and

$$d_i = f_i - b_i \tag{4.15}$$

The mole fractions of each component in the distillate and bottoms are computed by the relations:

$$x_{Di} = d_i/\Sigma d_i \tag{4.16}$$

and

$$x_{Bi} = b_i/\Sigma b_i \tag{4.17}$$

The two functions g_1 and g_2 are defined as:

$$g_1(s_1,s_2) = (x_{D,HK})_{CAL} - x_{D,HK} \tag{4.18}$$

and

$$g_2(s_1,s_2) = (x_{B,LK})_{CAL} - x_{B,LK} \tag{4.19}$$

where s_1 and s_2 are equivalent to $(df)_{LK}$ and $(bf)_{HK}$ respectively. $(x_{D,HK})_{CAL}$ and $(x_{B,LK})_{CAL}$ are the mole fractions of the key components calculated by equations (4.16) and (4.17) based on the assumed values of s_1 and s_2, while $x_{D,HK}$ and $x_{B,LK}$ are the specified mole fractions. The objective is to find s_1 and s_2, so the functions g_1 and g_2 are zero, this is done by Newton-Raphson Method. The values of s_1 and s_2 are updated by the relations:

$$s_{1,new} = s_{1,old} + \Delta s_1 \tag{4.20}$$

and

$$s_{2,new} = s_{2,old} + \Delta s_2 \tag{4.21}$$

The values of Δs_1 and Δs_2 are evaluated by solving the following relation

$$\begin{bmatrix} g'_{1,1} & g'_{1,2} \\ g'_{2,1} & g'_{2,2} \end{bmatrix} \begin{bmatrix} \Delta s_1 \\ \Delta s_2 \end{bmatrix} = \begin{bmatrix} -g_1 \\ -g_2 \end{bmatrix} \tag{4.22}$$

where $g'_{i,j} = \partial g_i / \partial s_j$ (4.23)

The value of $g'_{i,j}$ is obtained by the finite-difference approximation method which is given by

$$\frac{\partial g_i}{\partial s_1} = \frac{g_i(s_1+\delta, s_2) - g_i(s_1, s_2)}{\delta} \tag{4.24}$$

and

$$\frac{\partial g_i}{\partial s_2} = \frac{g_i(s_1, s_2+\delta) - g_i(s_1, s_2)}{\delta} \tag{4.25}$$

The value of δ is found satisfactory as 10^{-5}. The convergence criterion is satisfied for an error value of ±0.0001.

The minimum number of plates are calculated by the Fenske's equation given as

$$N_{min} = \ln[(x_{D,LK}/x_{B,LK})(x_{B,HK}/x_{D,HK})] \; / \ln\alpha_{LK} \tag{4.26}$$

The N_{min} is equivalent to C_2 in equation (4.12). The minimum reflux is calcualted by the Underwood equations given by

$$1-Q = \Sigma \frac{\alpha_i x_{Fi}}{\alpha_i - \phi} \tag{4.27}$$

and

$$R_{min}+1 = \Sigma \frac{\alpha_i x_{Di}}{\alpha_i - \phi} \tag{4.28}$$

The equation (4.27) is solved for $\alpha_{HK}<\phi<\alpha_{LK}$ by the bisection method, and the value of ϕ obtained is substituted in equation (4.28) to obtain R_{min}.

The Gilliland's equation is used to determine the number of theoretical plates at operating reflux ratio. Molokanov, Korabline, Mazurine, and Nikiforov (1972), have fitted Gilliland's correlation curve into the following equations:

$$X = \frac{R-R_{min}}{R+1} \tag{4.29}$$

$$Y = 1-\text{Exp}\left[\frac{(1+54.4X)(X-1)}{(11+117.2X)\sqrt{X}}\right] \tag{4.30}$$

and

$$N = (Y+N_{min})/(1-Y) \tag{4.31}$$

Figure 4.2 shows a flow chart of the code for the multicomponent system and the code is shown in Appendix B. In order to check the correctness of the code, example 9.13, page 436, as provided by Treybal (1979) was done. The problem is stated as follows:
The following feed at 82°C, 1035 KN/m^2 (150 psia) is to be fractionated at that pressure so that the vapor distillate contains 98% of the C_3H_8 but only 1% of the C_5H_{12}:

Component	CH_4	C_2H_6	n-C_3H_8	n-C_4H_{10}	n-C_5H_{12}	n-C_6H_{14}
Z_F, mole fraction	0.03	0.07	0.15	0.33	0.30	0.12

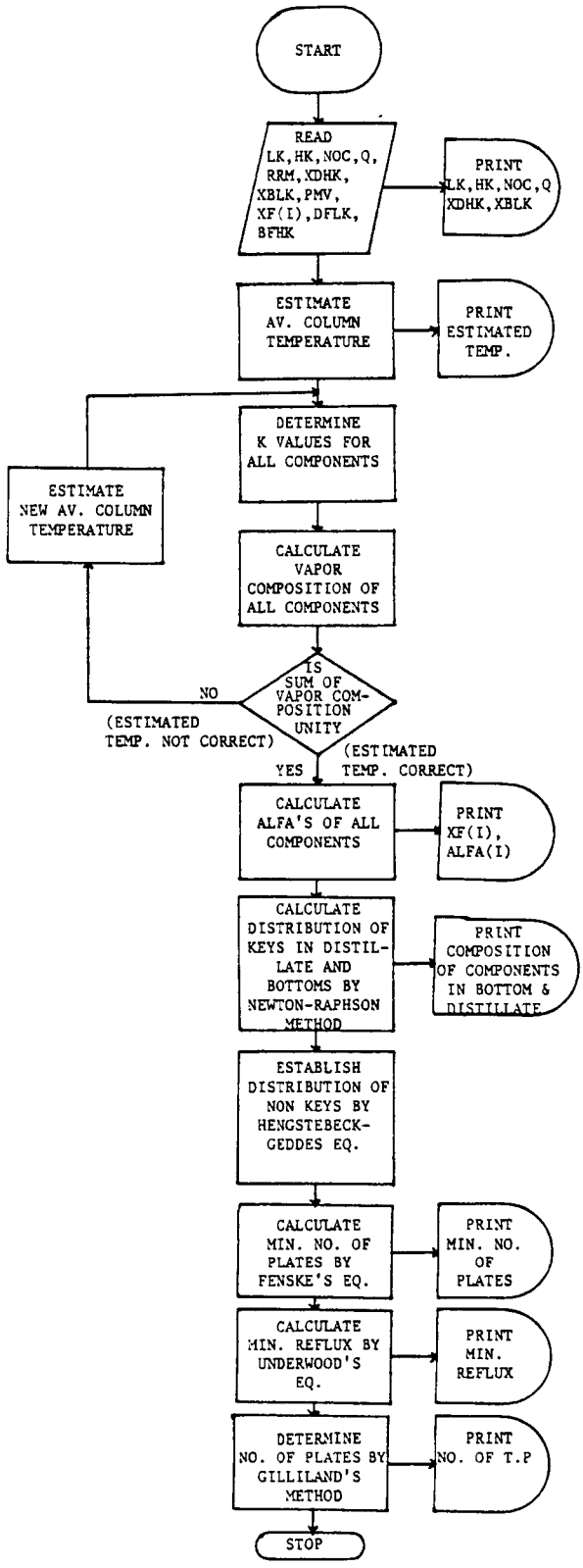


Figure 4.2. Flow Chart for Short Cut Method for Multi-component System.

While solving the problem by code the value of Q is specified as 0.67. Table 4.2 shows the comparison of the results provided by Treybal (1979) with those obtained by the code. The closeness in the two solutions indicates the fact that the code works pretty well for the separation problem of ideal multicomponent systems.

Table 4.2. Comparison of the Results for a Multicomponent Separation Example Problem.

Quantity	Results	
	Treybal's Solution[a]	Computer Solution
Average column temperature	80°C	80°C
ALFA (C_1)	53.2	53.939
ALFA (C_2)	14.94	14.01
ALFA (C_3)	6.30	6.07
ALFA (C_4)	2.405	2.42
ALFA (C_5)	1.0	1.0
ALFA (C_6)	0.456	0.454
PHI (ϕ)	1.4177	1.42
Minimum reflux ratio	0.58	0.47
Minimum number of plates	4.55	3.79
Total number of theoretical plates	10.05	9.54

[a]Data Source: Example 9.13, page 436, Treybal (1979).

CHAPTER 5

SUMMARY AND CONCLUSIONS

Two computer codes have been developed for the design of distillation column for two types of systems, i.e.,

(a) Binary systems

(b) Multicomponent systems.

(a) Two classes of binary systems are considered. The first class contains systems whose vapor-liquid equilibrium (VLE) data can be represented reasonably well by a single, constant value of the relative volatility, α. This approximation holds reasonably well for ideal mixtures. An example of a system considered which is approximately ideal is Benzene-Toulene System. The second class of binary systems considered are those whose members exhibit an inflexion point when their VLE data are plotted as x vs. y (mole fraction in liquid phase, x, vs. mole fraction in vapor phase, y). This behavior is somewhat representative of relatively highly non-ideal systems. An example of this class of system is the Ethanol-Water System. The established desgin procedure of McCabe-Thiele is used in both cases to determine the number of theoretical plates required for the specified separation for a specified reflux ratio. Once the number of theoretical plates have been established, the tower is sized by the usual procedure, as provided by Treybal (1979).

A program has also been developed for optimizing the column design based upon minimizing the total annual cost. The cost data

and the cost as a function of tower size curves provided by Peters and Timmerhaus (1980) were used to establish the optimum reflux ratio which yields the minimum total annual cost.

(b) For the multicomponent case only those systems are considered which are reasonably ideal, such as mixtures of certain light hydrocarbons. The code is based upon the short cut method as discussed by Treybal (1979) and a published computer code of Change (1980), who assumes prior knowledge of the average column temperature. This assumption was relaxed in this work, so that the only prior knowledge required is the feed composition and the thermodynamic condition.

The task common to both the programs was the development of analytical equations to provide reasonable fits to the property data, especially to the VLE data of the systems. This task is accomplished by using a published regression analysis routine.

The conclusions drawn from this work may be stated as follows:

1. For binary systems which are reasonably ideal, a model equation in terms of a single constant value for the relative volatility, α, given as

$$y = \frac{\alpha x}{1+(\alpha-1)x} \qquad (5.1)$$

can fit the vapor-liquid equilibrium data with correlation coefficients as high as 0.9996. For example for the Benzene-Toulene System, with $\alpha = 2.476$, the correlation coefficient is 0.9961.

2. For non-ideal binary systems whose VLE data exhibit an inflexion point in the x-y space, such as the Ethanol-Water

System, a four parameter model equation of the form

$$y = (ax+bx^2-cxe^{-dx}) / (1-x+ax+bx^2-cxe^{-dx}) \quad (5.2)$$

fits the VLE data with correlation coefficient as high as 0.99989.

3. Vapor-liquid equilibrium constant, K = y/x, as a function of temperature for multicomponent light hydrocarbon mixtures can be fitted by model equations of the form

$$\ln(K) = a+bT+cT^2 \quad (5.3)$$

and

$$\ln(K) = a+bT+cT^2+dT^3 \quad (5.4)$$

in the temperature range of 0 to 120°C, and correlation coefficient as high as 0.9999.

4. A computer code based on the McCabe-Thiele method for binary systems gives results for the number of theoretical plates required for a specified separation for a specified reflux ratio, was tested against the two systems: Benzene-Toulene, and Ethanol-Water, with different thermodynamic feed conditions, Q, which provided results in agreement with results obtained by the traditional graphical method. For example:

		Number of Theoretical Plates		Feed Plate Location	
System	Q	Graphical Solution	Computer Solution	Graphical Solution	Computer Solution
Benzene-Toulene	1.0	13	13	6	6
Benzene-Toulene	1.37	12	12	6	6
Ethanol-Water	1.37	7	7	5	5

5. The cost data as provided by Peters and Timmerhaus (1980) was used to optimize the design based upon minimizing the total annual cost. An example discussed by Peters and Timmerhaus (1980) for the Benzene-Toulene System was used to check the code, and the results were in good agreement with the results obtained by Peters and Timmerhaus (1980). For example:

	Results		
Quantity	Peters and Timmerhaus Solution	Computer Solution	% Error
Minimum reflux ratio	1.14	1.149	0.79%
Optimum reflux ratio	1.25	1.264	1.5%
Total annual cost ($)	99,000	102,095.01	3%

6. For multicomponent systems the code was based on the short cut method provided by Treybal (1979), and a published code of Chang (1980). An example published by Treybal (1979), for a mixture of six light hydrocarbons (CH_4, C_2H_6, n-C_3H_8, n-C_4H_{10}, n-C_5H_{12}, n-C_6H_{14}), was used to test the code and the results obtained were in agreement with the ones obtained by Treybal (1979). For example:

	Results	
Quantity	Treybal's Solution	Computer Solution
Minimum reflux ratio	0.58	0.47
Minimum number of plates	4.55	3.79
Total number of theoretical plates	10.05	9.54

CHAPTER 6

RECOMMENDATIONS FOR FUTURE WORK

The two computer codes developed for binary and multicomponent systems, can be used for designing and optimizing distillation systems which otherwise is very tedious and time consuming. Some of the possible recommendations for using the codes are discussed below:

1. For binary systems which are rasonably ideal, the vapor-liquid equilibrium (VLE) data can be fitted reasonably well by using the suggested model for a given single, constant value of relative volatility.
2. For non-ideal binary systems such as aqueous solutions of Ethanol or Acetone, a model equation was discovered which represents the VLE data well over most of the mole fraction range of the light component in the liquid phase. However, the model equation generally did not fit the VLE data particularly well in the liquid phase mole fraction range, x, of greater than about 0.9. The VLE model equations used in this work are, therefore, not well suited to the design of distillation columns for production of high purity product. It is therefore recommended that additional effort in future work be directed toward the development of model equations which are well suited to fitting binary VLE data in the range of $x \geq 0.9$, more or less.

3. The McCabe-Thiele method is used to determine the number of theoretical plates. The assumptions used in this method breaks down for highly non-ideal systems, and when there are heat losses in the column. The Ponchon-Savarit method is more rigorous under such conditions. However, this method requires detailed enthalpy data which is difficult to obtain. It is therefore recommended that consideration be given to develop a computer code which is based on this reasonably rigorous design method, in future work.
4. For optimizing the design based upon minimizing the total annual cost, the cost curve of a sieve tray tower was used to develop the code. The other tower size curves provided by Peters and Timmerhaus (1980) can be used by fitting the curve by regression analysis. The cost data should be updated for a specific design as required using an inflationary index, such as Marshall and Swift equipment cost index.
5. The short cut method for multicomponent separation used in this work is suitable for preliminary distillation column design. A plate-to-plate calculation is more precise and is generally recommended for the final design of a column for a multicomponent system. It is therefore suggested that further computer codification work in this area be based on a plate-to-plate design procedure.

6. Extend the code to check the flooding condition at locations other than on the top tray. For example, on the feed tray and bottom tray as well as the top tray.
7. Consider using step wize data of tray spacing vs. tower size so that results obtained will be more readily consistent with standard tower sizes.

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APPENDICES

APPENDIX A

CODE FOR BINARY DISTILLATION

```
C   PROGRAM :   BINARY DISTILLATION
C   PROGRAMMER :   MANZOOR, Q.HARIS                    JANUARY 20,1984
C
C      THIS PROGRAM DESIGNS A TRAY TYPE DISTILLATION COLUMN FOR
C   SEPERATION OF CERTIAN BINARY SYSTEMS. THE CODE COMPUTES THE
C   MINIMUM REFLUX, THE FEED PLATE, THE NUMBER OF THEORETICAL PLATES
C   AND THE DIAMETER OF THE COLUMN FOR A SPECIFIED SEPERATION OF A
C   BINARY SYSTEM. THE COMPUTATION IS BASED ON THE MCCABE-THIELE
C   METHOD. THE PROGRAM NAME IS "DIST.FOR".
C      IN DEVELOPING THE PROGRAM TWO TYPES OF SYSTEMS ARE CONSIDERED.
C   SYSTEMS WHOSE VLE DATA CAN BE REPRESENTED REASONABLY WELL BY A
C   SINGLE, CONSTANT VALUE OF THE RELATIVE VOLATILITY, ALPHA, AND
C   SYSTEMS WHOSE VLE DATA EXHIBIT AN INFLEXION POINT IN X-Y SPACE.
C   THAT IS, IT CONSIDERS BOTH THE IDEAL AND NON-IDEAL SYSTEMS.
C      THE PROGRAM IS ALSO DEVELOPED FOR OPTIMIZING THE DESIGN BASED
C   UPON MINIMIZING THE TOTAL ANNUAL OPERATING COST. BY VARYING THE
C   REFLUX RATIO THE OPTIMUM REFLUX IS OBTAINED WHICH YIELDS THE
C   MINIMUM TOTAL ANNUAL OPERATING COST.
C      THE PARAMETERS WHICH ARE SPECIFIED AS INPUT TO THE PROGRAM
C   ARE AS FOLLOWS:
C         ALFA  THE VALUE OF THE RELATIVE VOLATILITY FOR IDEAL
C               SYSTEMS.
C      AP,B,C,D  PARAMETERS OF THE MODEL EQ.FITTED TO THE VLE DATA
C               OF A NON-IDEAL SYSTEM.
C           CC  COST OF CONDENSER IN $/FT**2.
C           CR  COST OF REBOILER IN  $/FT**2.
C           CS  COST OF STEAM IN $/LB.
C           CW  COST OF COOLING WATER IN $/LB.
C         DELTW  CHANGE IN COOLING WATER TEMPERATURE IN °F.
C            DL  DENSITY OF LIQUID IN LB/FT**3.
C           HC  HEAT OF CONDENSATION IN BTU/LB.
C         LAMC  MOLAL HEAT CAPACITY OF MIXTURE IN BTU/LBMOL-°F.
C         LAMV  MOLAL HEAT OF VAPORIZATION OF MIX.IN BTU/LBMOL.
C         LAMW  MOLAL HEAT CAPACITY OF WATER IN BTU/LBMOL-°F.
C            MF  FEED RATE IN LBMOL/HR.
C           MG  MOL. WEIGHT OF GAS.
C            ML  MOL. WEIGHT OF LIQUID.
C           OPT  OPERATING TIME IN HR/YR.
C          PFC  PERCENTAGE OF FIXED CHARGES.
C            PO  OPERATING PRESSURE IN LB/IN**2.
C            Q  THERMAL CONDITION OF FEED. Q MAY BE LESS THAN, EQUAL
C                TO, OR GREATER THAN UNITY.
C            RA  RATIO OF HOLE AREA TO ACTIVE AREA.
C           RR  RATIO OF THE OPERATING REFLUX RATIO, R, TO THE MIN.
C               REFLUX RATIO, RM.
C         SIGMA  SURFACE TENSION IN DYN/CM*(10**-3)
C            TB  TEMPERATURE AT BOTTOM OF THE COLUMN IN °F.
C            TF  TEMPERATURE OF THE FEED IN °F.
C            TS  TEMPERATURE OF THE STEAM IN °F.
C            TT  TEMPERATURE AT TOP OF THE COLUMN IN °F.
C            TW  TEMPERATURE OF WATER IN °F.
C            UC  HEAT TRANSFER COEFF.IN CONDENSER IN BTU/HR-°F-FT**2.
C           UR  HEAT TRANSFER COEFF.IN REBOILER IN  BTU/HR-°F-FT**2.
C          VMAX  MAXIMUM ALLOWABLE VAPOR VELOCITY.
C            XD  MOL.FRACTION OF THE MORE VOLATILE COMPONENT IN
C               DISTILLATE.
C            XW  MOL.FRACTION OF THE MORE VOLATILE COMPONENT IN BOTTOM.
C            ZF  MOL.FRACTION OF THE MORE VOLATILE COMPONENT IN FEED.
C
C   THE INPUT DATA ARE CONTAINED IN A SINGLE FILE, NAMED "DIST.DAT".
C
```

```
C   OUTPUT FROM THE PROGRAM INCLUDES THE FOLLOWING QUANTITIES:
C          1. THE MINIMUM REFLUX RATIO, RM, AND THE OPERATING REFLUX,
C             R, FOR THE SPECIFIED SEPERATION.
C          2. THE NUMBER OF PLATES IN ENRICHING SECTION, N, THE FEED
C             PLATE, NUMBER OF PLATES IN STRIPPING SECTION, P,AND THE
C             TOTAL NUMBER OF THEORETICAL PLATES INCLUDING REBOILER, T
C             FOR EACH VALUE OF RR SPECIFIED.
C           3. THE DIAMETER OF THE COLUMN IN FT.
C          4. THE ANNUAL COST OF COLUMN, ACOST, THE ANNUAL COST OF
C             CONDENSER, AC, THE ANNUAL COST OF REBOILER, AR, THE
C             ANNUAL COST OF COOLING WATER, AW, THE ANNUAL COST OF
C             STEAM, AS, AND THE TOTAL ANNUAL OPERATING COST, TAC, FOR
C              A SPECIFIED VALUE OF RR.
C
C
C
      REAL INT,M1,M2,MG,ML,MD,MB,MF,LR,LAMV,LAMC,LAMW
      INTEGER P,T
      DIMENSION X(2500),Y(2500),FUNC(2500)
      OPEN(FILE='DIST.DAT',ACCESS='SEQIN',UNIT=1)
C CHECK FOR ALFA
      WRITE(5,1)
1     FORMAT(' IS ALFA CONSTANT,TYPE 0 FOR NO,1 FOR YES')
      READ(5,*)F
      IF(F.EQ.0)GOTO300
      READ(1,*)MF,ZF,XW,XD,TT,RA,SIGMA,VFL,DL,ML,MG,RR,VMAX,LAMV,PFC,
     1 UC,TW,CC,LAMC,TB,TF,TS,CW,CR,LAMW,DELTW,OPT,CS,HC,UR,Q,ALFA,PO
      WRITE(5,2)
2     FORMAT(' IS FEED SATURATED,TYPE 1 FOR YES,0 FOR NO')
      READ(5,*)QF
      IF(QF.NE.1)GOTO10
C CALCULATING MINIMUM REFLUX
      XP=ZF
5     YP=(ALFA*XP)/(1.0+((ALFA-1.0)*XP))
      RM=(XD-YP)/(YP-XP)
      WRITE(5,6)RM
6     FORMAT(' THE MINIMUM REFLUX IS',F10.5)
      WRITE(20,6)RM
      R=RR*RM
      WRITE(5,7)R
7     FORMAT(' THE OPERATING REFLUX IS',F10.5)
      WRITE(20,7)R
      GOTO40
10    A=(Q/(Q-1.0))*(ALFA-1.0)
      B=Q/(Q-1.0)-ALFA-((ZF/(Q-1.0))*(ALFA-1.0))
      C=-ZF/(Q-1.0)
      DISC=(B**2)-(4.0*A*C)
      IF(DISC.LT.0.0)GOTO15
      GOTO20
15    WRITE(5,16)
16    FORMAT(5X,/,' THERE IS NO REAL SOLUTION FOR THE INTERSECTION
     1 OF EQUIB.CURVE AND Q-LINE')
      WRITE(20,16)
      GOTO999
20    X1=(-B+(DISC**0.5))/(2.0*A)
      X2=(-B-(DISC**0.5))/(2.0*A)
      IF(X1.GE.1.0)GOTO30
      IF(X1.LE.0.0)GOTO30
      XP=X1
      GOTO5
30    IF(X2.GE.1.0)GOTO35
```

```
      IF(X2.LE.0.0)GOTO35
      XP=X2
      GOTO5
35    WRITE(5,36)
36    FORMAT(5X,/,' THERE IS NO SOLUTION FOR THE INTERSECTION OF
     1 EQUIB.CURVE AND Q-LINE')
      WRITE(20,36)
      GOTO999
C INTERSECTION OF Q-LINE AND OPERATING LINE
40    IF(QF.NE.1)GOTO50
      XI=ZF
45    YI=((R*XI)+XD)/(R+1.0)
      GOTO55
50    XNU=(ZF/(Q-1.0))+(XD/(R+1.0))
      XDE=(R/(R+1.0))- (Q/(Q-1.0))
      XI=-XNU/XDE
      GOTO45
C CALCULATING SLOPE AND INTERCEPT OF STRIPPING SECTION OPERATING LINE
55    SLP=(YI-XW)/(ZF-XW)
      INT=YI-SLP*XI
C CALCULATING NUMBER OF PLATES
      IF(QF.NE.1)GOTO180
      Y1=XD
      DO 100  I= 1,50
      X(I)  =Y1/(ALFA-(Y1*(ALFA-1.0)))
      K=I+1
      Y(K)=((R*X(I))+XD)/(R+1.0)
      Y1=Y(K)
      IF(X(I).LE.ZF)GOTO60
      GOTO100
60    XS=X(I)
      N=I
      GOTO110
100   CONTINUE
110   WRITE(5,112)N
112   FORMAT(' THE NUMBER OF PLATES IN ENRICHING SECTION ARE',I5)
      WRITE(20,112)N
      WRITE(5,113)N
113   FORMAT(' THE FEED IS AT PLATE',I5)
      WRITE(20,113)N
      DO150J=1,50
      Y(J)=INT+SLP*XS
      M=J+1
      X(M)=Y(J)/(ALFA-(Y(J)*(ALFA-1.0)))
      XS=X(M)
      IF(XS.LE.XW)GOTO120
      GOTO150
120   P=M
      GOTO160
150   CONTINUE
160   WRITE(5,162)P
162   FORMAT(' THE NUMBER OF PLATES IN STRIPPING SECTION ARE',I5)
      WRITE(20,162)P
      GOTO280
180   Y1=XD
      DO200I=1,50
      X(I)=Y1/(ALFA-(Y1*(ALFA-1.0)))
      K=I+1
      Y(K)=((R*X(I))+XD)/(R+1.0)
      Y1=Y(K)
      IF(X(I).LE.XI)GOTO190
```

```
      GOTO200
190   XS=X(I)
      N=I
      GOTO210
200   CONTINUE
210   WRITE(5,112)N
      WRITE(20,112)N
      WRITE(5,113)N
      WRITE(20,113)N
      DO250J=1,50
      Y(J)=INT+SLP*XS
      M=J+1
      X(M)=Y(J)/(ALFA-(Y(J)*(ALFA-1.0)))
      XS=X(M)
      IF(XS.LE.XW)GOTO240
      GOTO250
240   P=M
      GOTO260
250   CONTINUE
260   WRITE(5,162)P
      WRITE(20,162)P
280   T=N+P+1
      WRITE(5,282)T
282   FORMAT(' THE TOTAL NUMBER OF PLATES INCLUDING REBOILER ARE',I5)
      WRITE(20,282)T
      GOTO750
300   READ(1,*)MF,ZF,XW,XD,TT,RA,SIGMA,VFL,DL,ML,MG,RR,VMAX,LAMV,
     1 PFC,UC,TW,CC,LAMC,TB,TF,TS,CW,CR,LAMW,DELTW,OPT,CS,HC,UR,Q,
     2 AP,B,C,D,PO
      WRITE(5,301)
301   FORMAT(' IS FEED SATURATED,TYPE 1 FOR YES,0 FOR NO')
      READ(5,*)QF
      IF(QF.NE.1)GOTO400
C CALCULATING MINIMUM REFLUX
      XQ=ZF
      XO=ZF
310   E=0.01
      JJ=1
      DELXQ=(XD-XQ)/100.
      DO350IJ=1,200
      YN=(1.0-XQ+AP*XQ+B*(XQ**2)-(C*XQ*EXP(-D*XQ)))
      YQ=(AP*XQ+B*(XQ**2)-(C*XQ*EXP(-D*XQ)))/YN
      YM=((1.0-XQ+AP*XQ+B*(XQ**2)-(C*XQ*EXP(-D*XQ)))**2)
      M1=(AP+2.*B*XQ-B*(XQ**2)-((C*EXP(-D*XQ))*(1.0-D*XQ+D*(XQ**2))))/
     1 YM
      M2=(XD-YQ)/(XD-XQ)
      IF(ABS((M1-M2)/M1).LE.E)GOTO320
      XQ=XQ+DELXQ
      GOTO350
320   IF(JJ.EQ.2)GOTO360
      XQ=XQ-DELXQ
      DELXQ=DELXQ/100.
      JJ=2
350   CONTINUE
360   IF(XQ.GE.XD)GOTO380
      YP=YQ
      XP=XQ
365   RM=(XD-YP)/(YP-XP)
      WRITE(5,6)RM
      WRITE(20,6)RM
      R=RR*RM
```

```
      GOTO480
380   WRITE(5,382)
382   FORMAT(' TANGENCY OF EQUIB.CURVE AND OPERATING LINE NOT FOUND')
      WRITE(20,382)
      XP=XO
      YDE=(1.0-XP+AP*XP+B*(XP**2)-(C*XP*EXP(-D*XP)))
      YP=(AP*XP+B*(XP**2)-(C*XP*EXP(-D*XP)))/YDE
      GOTO365
400   XO=0.01
      ER=0.01
      DELXO=0.005
      DO450KK=1,200
      Y(KK)=(-Q/(1.0-Q))*XO+(ZF/(1.0-Q))
      YDE=(1.0-XO+AP*XO+B*(XO**2)-(C*XO*EXP(-D*XO)))
      YZ=(AP*XO+B*(XO**2)-(C*XO*EXP(-D*XO)))/YDE
      IF(ABS(YZ-Y(KK)).LE.ER)GOTO460
      XO=XO+DELXO
450   CONTINUE
460   XQ=XO
      GOTO310
C INTERSECTION OF Q-LINE AND OPERATING LINE
480   IF(QF.NE.1)GOTO500
      XI=ZF
490   YI=((R*XI)+XD)/(R+1.0)
      GOTO510
500   XNU=(ZF/(Q-1.0))+(XD/(R+1.0))
      XDE=(R/(R+1.0))-(Q/(Q-1.0))
      XI=-XNU/XDE
      GOTO490
C CALCULATING SLOPE AND INTERCEPT OF STRIPPING SECTION OPERATING LINE
510   SLP=(YI-XW)/(ZF-XW)
      INT=YI-SLP*XI
C CALCULATING NUMBER OF PLATES
      IF(QF.NE.1)GOTO630
      X1=XD
      Y1=XD
      K=1
520   ERR=0.0005
      DELX1=0.0001
      DO550 I=1,2500
      FUNC(I)=(AP+B*X1-(C*EXP(-D*X1)))*X1*(1.0-Y1)-Y1*(1.0-X1)
      IF(FUNC(I).LE.ERR)GOTO560
      X1=X1-DELX1
550   CONTINUE
560   IF(X1.LE.ZF)GOTO580
      K=K+1
      Y1=((R*X1)+XD)/(R+1.0)
      GOTO520
580   N=K
      WRITE(5,112)N
      WRITE(20,112)N
      WRITE(5,113)N
      WRITE(20,113)N
      M=1
590   Y1=INT+SLP*X1
      ERR=0.0005
      DELX1=0.0001
      DO600 J=1,2500
      FUNC(J)=(AP+B*X1-(C*EXP(-D*X1)))*X1*(1.0-Y1)-Y1*(1.0-X1)
      IF(FUNC(J).LE.ERR)GOTO610
      X1=X1-DELX1
```

```
600     CONTINUE
610     IF(X1.LE.XW)GOTO620
        M=M+1
        GOTO590
C THE NUMBER OF PLATES ARE COUNTED BY THE NUMBER OF TIMES THE OPERATING
C LINE IS INTERCEPTED.TRANSICTION FROM ONE OPERATING TO ANOTHER IS SUCH
C THAT THE FIRST TIME THE BOTTOM OPERATING LINE IS INTERCEPTED THE TRAY
C IS COUNTED FOR ENRICHING SECTION.HENCE THE NUMBER OF TRAYS ARE ONE
C LESS THAN THE COUNTER FOR THE STRIPPING SECTION.
620     P=M-1
        WRITE(5,162)P
        WRITE(20,162)P
        GOTO720
630     X1=XD
        Y1=XD
        K=1
640     ERR=0.0005
        DELX1=0.0001
        DO650 I=1,2500
        FUNC(I)=(AP+B*X1-(C*EXP(-D*X1)))*X1*(1.0-Y1)-Y1*(1.0-X1)
        IF(FUNC(I).LE.ERR)GOTO660
        X1=X1-DELX1
650     CONTINUE
660     IF(X1.LE.XI)GOTO670
        K=K+1
        Y1=((R*X1)+XD)/(R+1.0)
        GOTO640
670     N=K
        WRITE(5,112)N
        WRITE(20,112)N
        WRITE(5,113)N
        WRITE(20,113)N
        M=1
680     Y1=INT+SLP*X1
        ERR=0.0005
        DELX1=0.0001
        DO690 J=1,2500
        FUNC(J)=(AP+B*X1-(C*EXP(-D*X1)))*X1*(1.0-Y1)-Y1*(1.0-X1)
        IF(FUNC(J).LE.ERR)GOTO700
        X1=X1-DELX1
690     CONTINUE
700     IF(X1.LE.XW)GOTO710
        M=M+1
        GOTO680
710     P=M-1
        WRITE(5,162)P
        WRITE(20,162)P
720     T=N+P+1
        WRITE(5,282)T
        WRITE(20,282)T
750     MD=(MF*(ZF-XW))/(XD-XW)
        MB=MF-MD
        VD=MD*(R+1.0)
        QT=(VD*359.*(TT+460.)*14.7)/(492.*3600.*PO)
        TD=((4.*QT)/(VMAX*3.1416))**0.5
C
C
C
        DO 800 I=1,100
        IF(TD.GT.4.0)GOTO760
        SMT=20.0
```

```
      GOTO770
760   SMT=16.14636+1.54*TD-0.02754*(TD**2.)
770   IF(RA.GE.0.1)GOTO780
      ALFA1=(0.0062*SMT+0.0385)*((5.*RA)+0.5)
      BETA1=(0.00253*SMT+0.05)*((5.*RA)+0.5)
      GOTO790
780   ALFA1=0.0062*SMT+0.0385
      BETA1=0.00253*SMT+0.05
790   YG=XD
      YL=1.0-YG
      AMWG=(YG*MG)+(YL*ML)
      XG=XW
      XL=1.0-XG

      AMWL=1.0/((XG/MG)+(XL/ML))
      DG=(AMWG*492.)/(359.*(TT+460.))
      VR=(MD*359.*(TT+460.))/(492.*3600.)
      LR=(MB*AMWL)/(DL*3600.)
      DEN=((LR*DL)/(VR*DG))*((DG/DL)**0.5)
      CF=(ALFA1*(ALOG10(1.0/DEN))+BETA1)*((SIGMA/0.02)**0.2)
C THE FLOODING CONDITIONS ARE CHECKED AT TOP OF THE COLUMN.
      VF=CF*(((DL-DG)/DG)**0.5)
      V=VF*(VFL/100.)
      AREA=QT/V
      DIA=((4.*AREA)/3.1416)**0.5
      ERR=0.05
      IF(ABS(TD-DIA).LE.ERR)GOTO810
      DELTD=0.1
      TD=TD+DELTD
800   CONTINUE
810   IF(I.EQ.100)GOTO820
      WRITE(5,815)DIA
      WRITE(20,815)DIA
815   FORMAT(' THE DIAMETER OF TOWER IS',F8.6)
      GOTO830
820   WRITE(5,825)
      WRITE(20,825)
825   FORMAT(' THE VALUES OF ASSUMED AND CALCULATED DIAMETERS DO
     1 NOT CONVERGE')
      GOTO999
830   DIAIN=DIA*12.0
      COST=EXP(5.16474-0.06366*(ALOG(DIAIN))+0.1755*((ALOG(DIAIN))**
     1 2)-0.004*((ALOG(DIAIN))**3))
      SLOPE =R/(R+1.0)
      ACOST=COST*T*(1.+SLOPE)*(PFC/100.)
      WRITE(5,835)ACOST
      WRITE(20,835)ACOST
835   FORMAT(' ANNUAL COST OF DIST.COLUMN IS',F8.2)
      QC=VD*LAMV
      HAC=QC/(UC*(TT-TW))
      AC=(CC/HAC)*HAC*(1.+SLOPE)*(PFC/100.)
      WRITE(5,840)AC
      WRITE(20,840)AC
840   FORMAT(' ANNUAL COST OF CONDENSER IS',F8.2)
      QR=QC+MB*LAMC*(TB-TT)-MF*LAMC*(TF-TT)
      HAR=QR/(UR*(TS-TB))
      AR=(CR/HAR)*HAR*(1.+SLOPE)*(PFC/100.)
      WRITE(5,845)AR
      WRITE(20,845)AR
845   FORMAT(' ANNUAL COST OF REBOILER IS',F10.2)
      AW=(QC*CW*OPT)/(LAMW*DELTW)
```

```
      WRITE(5,850)AW
      WRITE(20,850)AW
850   FORMAT(' ANNUAL COST OF COOLING WATER IS',F10.2)
      AS=(QR*CS*OPT)/HC
      WRITE(5,900)AS
      WRITE(20,900)AS
900   FORMAT(' ANNUAL COST OF STEAM IS',F10.2)
      TAC=ACOST+AC+AR+AW+AS
      WRITE(5,910)TAC
      WRITE(20,910)TAC
910   FORMAT(' TOTAL ANNUAL COST IS',F10.2)
999   STOP
      END
```

APPENDIX B

CODE FOR MULTICOMPONENT SYSTEM

```
C      PROGRAM : MULTICOMPONENT DISTILLATION
C       PROGRAMMER: MANZOOR,Q.HARIS                JANUARY 20,1984.
C      HENGSTEBECK-GEDDES-FENSKE-UNDERWOOD-GILLILAND SHORT-CUT
C      DISTILLATION METHOD
C      ALL INPUT ENTRIES ARE FORMAT FREE
C      THE INPUT CONSISTS OF THE FOLLOWING:
C         1. LK,HK,NOC,Q,RRM,XDHK,XBLK
C         2. XF(I)
C         3. DFLK,BFHK
C      DEFINATIONS:
C         LK=NO.ASSIGNED TO THE LIGHT KEY COMPONENT
C         HK=NO.ASSIGNED TO THE HEAVY KEY COMPONENT
C         NOC=TOTAL NO. OF COMPONENTS
C         Q=FEED THERMAL CONDITION
C         RRM=R/RMIN,WHERE R=OPERATING REFLUX RATIO AND
C         RMIN=MINIMUM REFLUX RATIO
C         XDHK=MOLE FRACTION OF THE HEAVY KEY IN THE DISTILLATE
C         XBLK=MOLE FRACTION OF THE LIGHT KEY IN THE BOTTOM
C         XF(I)=MOL. FRAC.OF A COMPONENT IN THE FEED
C         PMV=PERCENTAGE MOLE VAPORIZED.
C         ALFA(I)=AV.VALUE OF THE RELATIVE VOLATILITY OF A COMP.
C         DFLK=INITIAL GUESS OF FRACTION RECOVERY OF THE LIGHT
C              KEY COMPONENT IN THE DISTILLATE
C         BFHK=INITIAL GUESS OF FRACTION RECOVERY OF THE HEAVY
C              KEY COMPONENT IN THE BOTTOM
C      FLOW RATES ARE BASED ON F=100 MOLES
C      THE OUTPUT PRINTS OUT THE FOLLOWING:
C         1. THE VALUES OF THE RELATIVE VOLATILITIES OF THE COMPONENTS.
C        2. NO.OF ITERATIONS IN THE NEWTON-RAPHSON METHOD
C        3. CONVERGED VALUES OF DFLK & BFHK
C        4. DISTILLATE AND BOTTOM COMPOSITIONS
C        5. NMIN BY THE FENSKE'S EQ.
C        6. PHI AND RMIN BY THE UNDERWOOD'S EQ.
C        7. NO.OF T.P.AT SPECIFIED R BY GILLILAND'S CORRELATION
C
       REAL N,NMIN,K,LF
       INTEGER LK,HK
       DIMENSION FUNC(2),S(2),G(2),DG(2,2),K(15),YF(15),RATIO(15)
       COMMON/BLOCK1/XF(15),XD(15),ALFA(15)
       COMMON/BLOCK2/FD,SUMB,SUMD,D(15),B(15),F(15),XB(15)
       COMMON NOC,LK,HK
       EQUIVALENCE (C2,NMIN),(S(1),DFLK),(S(2),BFHK)
C
C      DATA INPUT AND PRINT OUT
C
       OPEN(FILE='MULTI.DAT',ACCESS='SEQIN',UNIT=1)
       READ(1,*)LK,HK,NOC,Q,RRM,XDHK,XBLK,PMV
       READ(1,*)(XF(I),I=1,NOC)
       READ(1,*)DFLK,BFHK
       WRITE(24,900)
       WRITE(24,901)NOC
       WRITE(24,902)LK,HK
       WRITE(24,903)Q
       WRITE(24,920)RRM
       WRITE(24,906)XDHK,XBLK
       WRITE(24,907)DFLK,BFHK
C
C
C
C
       FD=100.0
```

```
1       WRITE(5,2)
2       FORMAT(' PLEASE ENTER ESTIMATED VALUE OF AV.COLUMN TEMP')
        READ(5,*)TF
        WRITE(24,915)TF
        K(1)=EXP(2.57723+0.00656*TF-0.00000011*(TF**2))
        K(2)=EXP(1.011147+0.00686*TF+0.0000542*(TF**2)-0.0000003*(
      1 TF**3))
        K(3)=EXP(-0.6676+0.02974*TF-0.0001625*(TF**2)+0.00000048*(
      1 TF**3))
        K(4)=EXP(-1.84353+0.02857*TF-0.00006977*(TF**2))
        K(5)=EXP(-3.336254+0.0425575*TF-0.0001772*(TF**2)+0.00000035*(
      1 TF**3))
        K(6)=EXP(-4.30225+0.0401*TF-0.000091*(TF**2))
        GF=PMV/100.
        LF=1.0-GF
        SUMYF=0.0
        DO 3 I=1,NOC
        YF(I)=(XF(I)*(LF/GF+1.0))/(1.0+(LF/(GF*K(I))))
        SUMYF=YF(I)+SUMYF
3       CONTINUE
        ERR=0.01
        DELSUM=1.0-SUMYF
        IF(ABS(DELSUM).LE.ERR)GOTO5
        WRITE(5,4)
        WRITE(24,4)
4       FORMAT(' THE ESTIMATED TEMP.IS NOT CORRECT')
        GOTO1
5       DO 6 I=1,NOC
        ALFA(I)=K(I)/K(HK)
6       CONTINUE
C CHECKING THE CORRECTNESS OF CHOSEN KEYS.
        XDLK=1.0-XBLK
        IMAX=LK-1
        DO 7 I=1,IMAX
        RA1=((ALFA(I)-1.0)*XDLK*XF(LK))/((ALFA(LK)-1.0)*XF(LK))
        RA2=((ALFA(LK)-ALFA(I))*XDHK*XF(HK))/((ALFA(LK)-1.0)*XF(HK))
        RATIO(I)=RA1+RA2
        IF(RATIO(I).LT.-0.01)GOTO7
        IF(RATIO(I).GT.1.01)GOTO7
        WRITE(5,916)
        WRITE(24,916)
        GOTO500
7       CONTINUE
        JMAX=HK+1
        DO 8 J=JMAX,NOC
        RA3=((ALFA(J)-1.0)*XDLK*XF(LK))/((ALFA(LK)-1.0)*XF(LK))
        RA4=((ALFA(LK)-ALFA(J))*XDHK*XF(HK))/((ALFA(LK)-1.0)*XF(HK))
        RATIO(J)=RA3+RA4
        IF(RATIO(J).LT.-0.01)GOTO8
        IF(RATIO(J).GT.1.01)GOTO8
        WRITE(5,916)
        WRITE(24,916)
        GOTO500
8       CONTINUE
C       CARRY OUT NEWTON-RAPHSON ITERATION
        KMAX=20
        DELTA=1.E-5
        DO100 KK=1,KMAX
        CALL HG(S(1),S(2),C2)
        FUNC(1)=XD(HK)-XDHK
        FUNC(2)=XB(LK)-XBLK
```

```
      IF(ABS(FUNC(1)).LT..0001.AND.ABS(FUNC(2)).LT..0001)GOTO200
C
C     ESTIMATE THE FOUR PARTIAL DERAVATIVES.
C
      DO 9 I=1,2
9     G(I)=FUNC(I)
      DO 20 I=1,2
      S(I)=S(I)+DELTA
      CALL HG(S(1),S(2),C2)
      FUNC(1)=XD(HK)-XDHK
      FUNC(2)=XB(LK)-XBLK
      DO 10 J=1,2
10    DG(J,I)=(FUNC(J)-G(J))/DELTA
20    S(I)=S(I)-DELTA
C
C     UPDATE DFLK AND BFHK
C
      DM=DG(1,1)*DG(2,2)-DG(1,2)*DG(2,1)
      DELS1=(G(2)*DG(1,2)-G(1)*DG(2,2))/DM
      DELS2=(G(1)*DG(2,1)-G(2)*DG(1,1))/DM
      S(1)=S(1)+DELS1
      S(2)=S(2)+DELS2
      IF(S(1).GT.1.) S(1)=.9999
      IF(S(2).GT.1.) S(2)=.9999
100   CONTINUE
      WRITE(24,914)
      GOTO500
C
C     PRINT DISTRIBUTION OF COMPONENTS
C
200   WRITE(24,908)
      WRITE(24,909)KK,S(1),S(2)
      WRITE(24,910)(I,D(I),XD(I),B(I),XB(I),I=1,NOC)
      WRITE(24,955)SUMD,SUMB
      WRITE(24,904)
      WRITE(24,905)((I,XF(I),ALFA(I)),I=1,NOC)
C
C     PRINT NMIN BY FENSKE'S EQ..
C     IN GEDDES EQ.
C
      WRITE(24,911)NMIN
C
C     CALCULATE RMIN BY UNDERWOOD'S EQ.
C
      CALL UWD(Q,PHI,RMIN)
      WRITE(24,912)PHI,RMIN
C
C     FIND NO.OF T.P.AT SPECIFIED R BY GILLILAND'S CORRELATIONS.
C
      R=RRM*RMIN
      CALL GLLD(R,RMIN,N,NMIN)
      WRITE(24,913)R,N
C
C     OUTPUT FORMAT
C
900   FORMAT(//10X,' **** INPUT ****')
901   FORMAT(//5X,' TOTAL NO.OF COMPONENTS=',I5)
902   FORMAT(5X,' LIGHT KEY IS COMPONENT NO.',I5/
     1 5X,' HEAVY KEY IS COMPONENT NO.',I5)
903   FORMAT(5X,' FEED THERMAL CONDITION Q=',F7.1)
920   FORMAT(5X,' THE OPERATING REFLUX RATIO IS',F6.2,' TIMES RMIN')
```

```
904   FORMAT(/5X,' THE FEED COMPOSITION AND THE RELATIVE'
     1 ' VOLATILITIES ARE'//3X,' I',6X,' XF(I)',7X,' ALFA(I)')
905   FORMAT(I5,2F15.8)
906   FORMAT(/5X,' THE SPECIFIED MOLE FRACTION OF THE KEYS'
     1 ' IN THE DISTILLATE AND IN THE BOTTOMS ARE'//
     2 10X,' XD(HK)=',F10.4,5X,' XB(LK)=',F10.4)
907   FORMAT(/5X,' THE INITIAL GUESSED VALUE OF THE'/
     1 ' DISTRIBUTIONS ARE'//10X,' DFLK=',F10.4,5X,' BFHK=',F10.4)
908   FORMAT(//10X,' **** OUTPUT ****')
909   FORMAT(//5X,' AFTER',I5,' ITERATIONS THE ACCEPTED VALUES'
     1 ' OF THE DISTRIBUTIONS ARE'//
     2 10X,' DFLK=',F10.4,5X,' BFHK=',F10.4)
910   FORMAT(/3X,' I',6X,' D(I)',11X,' XD(I)',10X,' B(I)'
     1 9X,' XB(I)'/(I5,4E15.5))
911   FORMAT(/5X,' MINIMUM NUMBER OF PLATES=',F7.2)
912   FORMAT(/5X,' PHI=',F10.6,5X,' RMIN=',F7.3)
913   FORMAT(/5X,' AT R=',F7.3,5X,' NO.OF T.P =',F7.3)
914   FORMAT(//5X,' KMAX EXCEEDED')
915   FORMAT(' THE ESTIMATED AV.COLUMN TEMPERATURE IS ',F5.2)
916   FORMAT(' THE CHOSEN KEYS ARE NOT CORRECT')
955   FORMAT(2X,' TOTAL',E13.5,15X,E15.5)
500   STOP
      END
C
C
C
C
      SUBROUTINE HG(DFLK,BFHK,C2)
      INTEGER LK,HK
      COMMON/BLOCK1/XF(15),XD(15),ALFA(15)
      COMMON/BLOCK2/FD,SUMB,SUMD,D(15),B(15),F(15),XB(15)
      COMMON NOC,LK,HK
C
C     ESTIMATE DISTRIBUTION OF COMPONENTS IN THE DISTILLATE
C     AND THE BOTTOMS BY HENGSTEBECK-GEDDES METHOD.
C
      DO 10 I=1,NOC
10    F(I)=FD*XF(I)
      D(LK)=DFLK*F(LK)
      B(LK)=F(LK)-D(LK)
      D(HK)=(1.-BFHK)*F(HK)
      B(HK)=F(HK)-D(HK)
      C1=ALOG(D(HK)/B(HK))
      C2=ALOG(D(LK)/D(HK)*B(HK)/B(LK))/ALOG(ALFA(LK))
      DO 20 I=1,NOC
      IF(I.EQ.LK)GOTO20
      IF(I.EQ.HK)GOTO20
      B(I)=F(I)/(1.+EXP(C1+C2*ALOG(ALFA(I))))
      D(I)=F(I)-B(I)
20    CONTINUE
C
C
C
C
C     CALCUATE THE MOLE FRACTION
C
      SUMD=0.0
      SUMB=0.0
      DO 30 I=1,NOC
      SUMD=SUMD+D(I)
30    SUMB=SUMB+B(I)
```

```
      DO 40 I=1,NOC
      XD(I)=D(I)/SUMD
40    XB(I)=B(I)/SUMB
      RETURN
      END
C
C
C
C
      SUBROUTINE UWD(Q,PHI,RMIN)
C
C
C     THIS SUBROUTINE CALCULATES RMIN BY THE UNDERWOOD'S EQ.
C     THE VALUE OF PHI LYING BETWEEN THE ALFA'S OF THE KEYS
C     IS OBTAINED BY THE BISECTION METHOD.
C     PHILL=LOWER LIMIT OF PHI'
C     PHIUL=UPPER LIMIT OH PHI.
C
      REAL NMIN,N
      INTEGER LK,HK
      COMMON/BLOCK1/XF(15),XD(15),ALFA(15)
      COMMON NOC,LK,HK
      PHILL=ALFA(HK)
      PHIUL=ALFA(HK-1)
      DO 10 I=1,20
      PHI=0.5*(PHILL+PHIUL)
      FPHI=Q-1.
      DO 20 J=1,NOC
20    FPHI=FPHI+ALFA(J)*XF(J)/(ALFA(J)-PHI)
      IF(FPHI) 30,50,40
30    PHILL=PHI
      GOTO10
40    PHIUL=PHI
10    CONTINUE
50    RMIN=-1.
      DO 60 I=1,NOC
60    RMIN=RMIN+ALFA(I)*XD(I)/(ALFA(I)-PHI)
      RETURN
      END
C
C
C
C
      SUBROUTINE GLLD(R,RMIN,N,NMIN)
      REAL N,NMIN
      X=(R-RMIN)/(R+1.)
      Y=1.-EXP((1.+54.4*X)*(X-1.)/((11.+117.2*X)*SQRT(X)))
      N=(Y+NMIN)/(1.-Y)
      RETURN
      END
```

VITA

Qamar Haris Manzoor was born in Karachi, Pakistan, on January 8, 1960. He attended elementary school in that city and was graduated from Cantt Public School in Karachi with First Class in July, 1974. After going through a two year Junior College he entered the N.E.D. University of Engineering and Technology in Karachi, in December 1976. In December 1981 he was awarded a Bachelor of Engineering degree in Chemical Engineering.

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