INFORMATION TO USERS

This reproduction was made from a copy of a document sent to us for microfilming. While the most advanced technology has been used to photograph and reproduce this document, the quality of the reproduction is heavily dependent upon the quality of the material submitted.

The following explanation of techniques is provided to help clarify markings or notations which may appear on this reproduction.

1. The sign or "target" for pages apparently lacking from the document photographed is "Missing Page(s)". If it was possible to obtain the missing page(s) or section, they are spliced into the film along with adjacent pages. This may have necessitated cutting through an image and duplicating adjacent pages to assure complete continuity.
2. When an image on the film is obliterated with a round black mark, it is an indication of either blurred copy because of movement during exposure, duplicate copy, or copyrighted materials that should not have been filmed. For blurred pages, a good image of the page can be found in the adjacent frame. If copyrighted materials were deleted, a target note will appear listing the pages in the adjacent frame.
3. When a map, drawing or chart, etc., is part of the material being photographed, a definite method of "sectioning" the material has been followed. It is customary to begin filming at the upper left hand corner of a large sheet and to continue from left to right in equal sections with small overlaps. If necessary, sectioning is continued again—beginning below the first row and continuing on until complete.
4. For illustrations that cannot be satisfactorily reproduced by xerographic means, photographic prints can be purchased at additional cost and inserted into your xerographic copy. These prints are available upon request from the Dissertations Customer Services Department.
5. Some pages in any document may have indistinct print. In all cases the best available copy has been filmed.

University
Microfilms
International

300 N. Zeeb Road
Ann Arbor, MI 48106

Reproduced with permission of the copyright owner. Further reproduction prohibited without permission.

8527465

Chawla, Harpreet Singh

AN INDUSTRIAL ETHANOL AZEOTROPIC DISTILLATION PROCESS: MODELING, ANALYSIS, AND SIMULATION

New Jersey Institute of Technology D.ENG.SC. 1985

University
Microfilms
International 300 N. Zeeb Road, Ann Arbor, MI 48106

PLEASE NOTE:

In all cases this material has been filmed in the best possible way from the available copy. Problems encountered with this document have been identified here with a check mark ✓.

1. Glossy photographs or pages _____
2. Colored illustrations, paper or print _____
3. Photographs with dark background _____
4. Illustrations are poor copy _____
5. Pages with black marks, not original copy _____
6. Print shows through as there is text on both sides of page _____
7. Indistinct, broken or small print on several pages _____
8. Print exceeds margin requirements _____
9. Tightly bound copy with print lost in spine _____
10. Computer printout pages with indistinct print ✓
11. Page(s) _____ lacking when material received, and not available from school or author.
12. Page(s) _____ seem to be missing in numbering only as text follows.
13. Two pages numbered _____. Text follows.
14. Curling and wrinkled pages _____
15. Dissertation contains pages with print at a slant, filmed as received ✓
16. Other _____

University
Microfilms
International

AN INDUSTRIAL ETHANOL AZEOTROPIC DISTILLATION PROCESS: MODELING, ANALYSIS, AND SIMULATION

by

Harpreet Singh Chawla

Dissertation submitted to the Faculty of the Graduate School
of the New Jersey Institute of Technology in partial
fulfillment of the requirements for the degree of
Doctor of Engineering Science
1985

APPROVAL SHEET

Title of Dissertation: An Industrial Ethanol Azeotropic Distillation Process: Modeling, Analysis, and Simulation

Name of Candidate: Harpreet Singh Chawla
Doctor of Engineering Science, 1985

Dissertation and Abstract Approved:

-- ----------
Edward C. Roche, Jr.
Professor
Department of Chemical
Engineering & Chemistry
Date

-- ----------
Dennis L. Blackmore
Date

-- ----------
John E. McCormick
Date

-- ----------
Dana E. Knox
Date

-- ----------
Charles M. Tsai
Date

VITA

Name: Harpreet Singh Chawla

Degree and date to be conferred: D. Eng. Sc., Oct. 1985

Secondary Education: Holy Cross Higher Secondary School, 1974

Collegiate Institutions Attended	Dates	Degree	Date of Degree
Govt. College of Eng. & Technology	7/74-6/79	B.E.ChE	June 79
Indian Institute of Technology	8/79-6/81	M.Tech ChE	June 81
New Jersey Institute of Technology	9/81-7/85	D.Eng.Sc.	Oct. 85

Major: Chemical Engineering

Publications: Chawla, H.S. and Hussain, S.Z., "Kinetics of Esterification of Maleic Anhydride with Ethanol Catalized by Sulfuric Acid", Indian J. of Tech., vol. 20, Jan 1982, pp. 22-28.

Chawla, H.S., "Studies in Esterification of Maleic Anhydride with Ethanol", M.Tech. Thesis, Indian Institute of Technology, Bombay, 1981.

Positions Held:

1981-1985 Graduate/Teaching Assistant
Department of Chemical Engineering and Chemistry
New Jersey Institute of Technology
Newark NJ 07102

ABSTRACT

Title of Dissertation: An Industrial Ethanol Azeotropic
Distillation Process: Modeling,
Analysis, and Simulation

Harpreet Singh Chawla, Doctor of Engineering Science, 1985

Dissertation directed by:

Edward C. Roche, Jr., Professor of Chemical Engineering

A steady state process simulator with extensive capabilities was developed for the simulation of process plants involving non-ideal multicomponent systems. A comprehensive stand alone program was developed to represent process systems encountering three phases. A computer program was also developed to handle simultaneous regression of vapor-liquid and liquid-liquid equilibria data to estimate the liquid phase activity coefficients via a global set of parameters for the ethanol azeotropic distillation process, using benzene as the entrainer.

An industrial ethanol azeotropic distillation process has been simulated using the developed process simulator (PROSIM). A study of the azeotropic column's aqueous ethanol feed composition reveals 82.9 mole % (ethanol) as the optimum concentration. The complete process plant as well as the individual process units were found to operate under a very narrow range of operating conditions. A sensitivity study on the process plant was conducted with respect to the ethanol product specifications and benzene stripping column

pressure.

In an extensive study on the azeotropic column, the optimum entrainer to binary feed ratio and the dry ethanol product rate have been established for aqueous ethanol feed concentration ranging from 70 to 89.4 mole % (ethanol). A multiple solution phenomena was investigated for the azeotropic column, and it was found to require a very stiff material balance to obtain the desired product split.

A global set of modified UNIQUAC interaction parameters has been determined using the regression program. This single set of parameters, obtained by simultaneous regression of binary isobaric vapor-liquid equilibria data and a single liquid-liquid tie line, has been established on the basis of its performance in the key units of the ethanol azeotropic distillation process.

Finally, twelve potential entrainers have been evaluated for the ethanol dehydration process using the UNIFAC activity coefficient equation. A set of suitable entrainers has also been prepared, based on extensive analysis using the model of the azeotropic distillation column to demonstrate production of marketable ethanol.

DEDICATION

Dedicated to my late grand parents,
Mrs. and Mr. Karam Singh Chawla.

ACKNOWLEDGEMENTS

The author wishes to acknowledge with deep gratitute and extend his profound sense of respect to his faculty advisor, Prof. Edward C. Roche, Jr. for his precise guidance and co-operation. The author is grateful to Dr. Dana Knox of Chemical Engineering Department for his critical suggestions and providing micro computer facility for text processing.

The author wishes to express his sincere thanks to the authorities of the New Jersey Institute of Technology for the computing facility and the financial support, which enabled him to participate in this doctoral dissertation. The author is very much indebted to his family for their co-operation and encouragement throughout the course ofthis work.

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

LIST OF COMPUTER PROGRAMS

CHAPTER 1

INTRODUCTION

This dissertation embodied the process modeling, detailed process analysis, and the steady state simulation of the industrial ethanol azeotropic distillation process. A new process simulator (PROSIM) has been developed based on the executive of the CHESS program. This simulation program was used to perform the simulation and optimization studies associated with the extensive analysis of the ethanol recovery process.

The improved Chemical Engineering Simulation System (Andreyuk, 1983) was not capable of completely simulating the alcohol dehydration process. The new process simulator is equipped with the new and advanced control blocks, the rigorous distillation/ absorption model reported by Tsai (1982), and an enhanced three phase flash model based on methods by Roche (1977).

A detailed analysis of the major segments of ethanol dehydration process plant and the development of the flow-scheme is also presented. The impact of various aqueous ethanol feed compositions to the azeotropic column, the ethanol product specifications, and the benzene stripping column pressure on the integrated process has been evaluated.

The estimation of a global set of thermodynamic interaction parameters (activity equation) has been incorporated in this dissertation. The modified UNIQUAC (Anderson, 1980) equation was chosen for global thermodynamic representation of ethanol-water-benzene process plant involving non-ideal vapor-liquid and liquid-liquid operations. A Marquardt non linear regression program was extensively enhanced for the simultaneous regression of both multicomponent vapor-liquid and liquid-liquid data. An in depth evaluation of potential entrainers for ethanol dehydration azeotropic column was also included in this work.

The analysis of twelve potential entrainers in the ethanol azeotropic column using the UNIFAC (Fredenslund, 1975) group contribution model for the prediction of activity coefficients was studied. A few of the entrainers (benzene, n-pentane,and diethyl ether) have been previously evaluated by Black (1980).

The concept of representing ternary liquid-liquid equilibria using parameters obtained from simultaneous regression of binary vapor-liquid and ternary liquid-liquid data was introduced by Prausnitz (1980). A rigorous approach to estimate a global set of parameters for the complete process representation has been demonstrated, and presented. This analysis is supported by screening and selection of various vapor-liquid and liquid-liquid equilibria minimization objective functions, proper root selection criteria, and assessment of the estimated set of parameters.

This dissertation incorporates a detailed study of the optimum entrainer to feed rate ratio, dry ethanol product rate, and multiplicity of solutions for a wide range of ethanol-water feed compositions to the azeotropic column. A graphical relationship between the above stated process variables is also included in this chapter.

Finally, the overall conclusions of this research and the recommendations for further studies are presented.

CHAPTER 2

PROCESS SIMULATION PROGRAM AND SUPPORTING MODELS

The research work incorporated in this dissertation can be broadly classified into the following major areas:

A. Steady state simulation of the integrated alcohol-water-entrainer (for example ethanol-water-benzene) process plant.

B. Detailed analysis of each of the process units in the ethanol process plant and optimization of various process variables.

C. Search of a single set of thermodynamic interaction parameters, for the modified UNIQUAC equation, which can be used to represent VLE and LLE for the same system.

D. Evaluation of the azeotropic distillation column performance with various potential entrainers. An Entrainer is defined as a foreign component used to break the alcohol-water azeotrope and make the dry alcohol production process feasible.

Each of the areas stated above demands computer programs with advanced and rigorous computational methods. Global thermodynamic parameter search (to obtain activity co-efficient equation parameters) requires regression software which can analyse simultaneously various combinations of experimental vapor-liquid and liquid-liquid equilibrium data. The details of the expanded program are presented in

Chapter 4. A general purpose stand alone flash algorithm, discussed in Section 2.2, can be used for any of the thirteen available options. In addition to simple dew point and bubble point calculations, it can also simulate isothermal and adiabatic flash operation for three phase systems (two liquid and a vapor phase).

A rigorous algorithm to simulate absorption and distillation columns for highly non-ideal systems in included in Section 2.3. Section 2.4 discusses a process simulation program developed as part of this research work, which has all of the available features incorporated in the flash and distillation programs. The process simulator uses the CHESS (Chemical Engineering Simulation System) executive, and has various new control blocks and advanced modules. The simulator can simulate the much difficult and non-ideal processes like production of dry alcohol via azeotropic distillation.

Above all, a common thermodynamic library has been enhanced by incorporating models for liquid phase activity coefficients, heats of mixing, and vapor phase fugacity coefficient estimation.

2.1 Enhancement in Thermodynamics Library (THERMO1)

Thermodynamic modules are the building blocks of process simulation program. For non-electrolytic non-ideal systems, a two equation approach was adopted in the research work. Therefore additional modules have been incorporated for

A. the estimation of component activity coefficients and heats of mixing,

B. the prediction of component activity coefficients in a multicomponent mixture, and

C. the estimation of second Virial coefficients for a mixture of components in the vapor phase proposed by Hayden et al. (1975).

The subsequent sections include UNIQUAC and UNIFAC equations corresponding to the liquid phase non-ideal computations. The detailed version of the modified UNIQUAC, NRTL, and, UNIFAC equations are covered in Appendix A. A complete set of available UNIFAC group interaction parameters along with constants r and q are compiled in the form of a database. Gmehling et al. (1982) have published the revised group interaction parameters including the new ones which make altogether 41 primary and 77 secondary groups.

2.1.1 Modified UNIQUAC for Activity Coefficient

UNIQUAC (UNIversal QUAsi Chemical) equation was first published by Abrams et al. (1975). A modified version was later proposed by Anderson et al. (1978). Anderson introduced an additional area parameter, q', for the pure components. Except for water and a few alcohols, there is no difference between q and q'. The activity coefficient for a component in a multicomponent mixture is given by

$$\ln \gamma_i = \ln \frac{\phi_i}{x_i} + (\frac{Z}{2}) q \ln \frac{\theta_i}{\phi_i} + l_i - \frac{\phi_i}{x_i} \sum_j x_j l_j - q'_i \ln (\sum_j \theta'_j \tau_{ji}) +$$

$$q'_i - q'_i \sum_j \frac{\theta'_j \tau_{ij}}{\sum_k \theta'_k \tau_{kj}} \qquad (2.1)$$

Where

$$\tau_{ji} = \exp (- \frac{a_{ji} + b_{ji}/T}{T}) \qquad (2.1A)$$

Definition of variables, constants, and parameters is provided in Appendix A.1.2.

2.1.2 Modified UNIQUAC for Heats of Mixing

The general relationship between excess heats of mixing and activity coefficient of component i in the mixture is given by

$$h^E = -RT^2 \sum x_i (\frac{\partial \ln \gamma_i}{\partial T})_{P,x} \qquad (2.2)$$

The implementation of activity coefficient equation in Eq. 2.3 yields the following equation

$$h^E = R \sum_i [\frac{q'_i x_i}{\sum_j \theta'_j \tau_{ji}} \sum_j \theta'_j \tau_{ji} (a_{ji} + 2b_{ji}/T)] \qquad (2.3)$$

Where

$$\tau_{ji} = \exp (- \frac{a_{ji} + b_{ji}/T}{T}) \qquad (2.1A)$$

2.1.3 UNIFAC for Activity Coefficient

UNIFAC (UNIquac Functional Group Activity Coefficients) was first proposed by Fredenslund et al. (1975). This model is based on functional groups rather than molecules but is essentially based on the UNIQUAC equation. The activity coefficient of a component in a mixture can be predicted by the following equations

$$\ln \gamma_i = \ln \gamma_i^C + \ln \gamma_i^R \tag{2.4}$$

where the superscripts C and R refer to the combinatorial and residual parts of the activity coefficient respectively.

The combinatorial part of the activity coefficient is represented by

$$\ln \gamma_i^C = \ln \frac{\phi_i}{x_i} + \left(\frac{Z}{2}\right) q \ln \frac{\theta_i}{\phi_i} + l_i - \frac{\phi_i}{x_i} \sum_j x_j l_j \tag{2.5}$$

The residual part of the activity coefficient is computed as follows

$$\ln \gamma_i^R = \sum_k v_{ki} (\ln \Gamma_k - \ln \Gamma_{k,i}) \tag{2.6}$$

The activity coefficient Γ_k is computed as follows

$$\ln \Gamma_k = Q_k \left[1 - \ln \left(\sum_m \beta_m \xi_{mk}\right) - \sum_m \left(\frac{\beta_m \xi_{km}}{\sum_n \beta_m \xi_{km}}\right)\right] \tag{2.7}$$

The activity coefficient $\ln \Gamma_{k,i}$ is computed as follows

$$\ln \Gamma_{k,i} = Q_k \left[1 - \ln \left(\sum_m \beta_{mi} \xi_{mk}\right) - \sum_m \left(\frac{\beta_{mi} \xi_{km}}{\sum_n \beta_{ni} \xi_{nm}}\right)\right] \tag{2.8}$$

Details of each of the terms is summarized in Appendix A.1.3

2.2 General Purpose Flash Program (FLASH2)

A generalized flash algorithm consisting of multiple computation features has been developed based on models suggested by Leach (1977), Roche (1977), and Prausnitz et al. (1980). This stand alone software, FLASH2, has the following capabilities:

A. Thirteen computational options are:

   a. Dew point temperature

   b. Bubble point temperature (1 or 2 liquid phases)

   c. All vapor enthalpy with prior dew point

   d. All liquid enthalpy with prior bubble point (1 or 2 liquid phases)

   e. All vapor enthalpy

   f. All liquid enthalpy (1 or 2 liquid phases)

   g. Isothermal flash (1 or 2 liquid)

   h. Isothermal flash ... no dew/bubble point (1 or 2 liquid phases)

   i. Adiabatic flash (1 or 2 liquid phases)

   j. Adiabatic flash ... no dew/bubble point (1 or 2 liquid phases)

   k. Dew point pressure

   l. Bubble point pressure (1 or 2 liquid phases)

   m. Liquid-liquid separation below bubble point

B. In case of three phase equilibria calculations, ability to switch thermodynamic interaction parameters for the same or different activity coefficient equations is available to represent vapor-liquid and liquid-liquid equilibria

C. Self initialization technique to characterize two liquid phases for liquid-liquid equilibria has also been incorporated.

D. Program can handle supercritical, condensable, normal, and nonvolatile non-electrolytic components using the two equation approach to represent vapor and liquid phase properties separately.

E. The software is completely compatible with thermodynamics library (THERMO1), regression supporting program (FOFX2) covered in section Section 4.2, and the steady state chemical engineering process simulation program (PROSIM) discussed in Section 2.4.

F. In liquid-liquid equilibria calculations, four different objective functions are included for convergence criteria. These functions are based on component activities, component mole fractions in both the liquid phases, and combination of components activities and mole fractions.

Basic equations for the major modules are given below.

Dew Point Temperature

Dew point temperature is established using the following relationship:

$$F = \sum_{i} (y_i/K_i) - 1.0 = 0.0 \qquad (2.9)$$

The secant method is used to solve the Equation 2.9 and Wegstein's algorithm is used for better estimates of liquid phase compositions.

Bubble Point Temperature (Two Liquid Phase)

Two design equations given by Equations 2.10 and 2.11 are solved simultaneously using the Newton-Raphson method to compute bubble point temperature.

$$F_1 = \sum (x_{1,i} - x_{2,i}) = \sum \frac{z_i(1 - (\gamma_{1,i}/\gamma_{2,i})}{R + (1-R)} = 0 \qquad (2.10)$$

$$F_2 = \sum (x_{1,i} - y_i) = \sum \frac{z_i(1 - K_{1,i})}{R + (1-R)} = 0 \qquad (2.11)$$

Where $R = L_1/(L_1+L_2)$, liquid phase distribution factor, whose value range between 0 and 1.0. The extreme values of R, 0 or 1.0, lead to single liquid phase system with the existence of 'liquid 2' or 'liquid 1', respectively. The better estimates of x's are obtained using Wegstein's algorithm.

Liquid Liquid Equilibria Below Bubble Point

The two liquid phase algorithm is based on the computation of phase compositions of two phases and liquid phase distribution factor at isothermal conditions. In the decoupling solution method the inner loop solves for R, defined earlier, using Equation 2.10 and the outer loop must satisfy one of the convergence criterions stated below.

A. $|(x_{1,i}\gamma_{1,i} - x_{2,i}\gamma_{2,i})|/(x_{2,i}\gamma_{2,i}) <= 1.0E-5$ (2.12)

B. $|(x_{j,i}^{(k)} - x_{j,i}^{(k-1)})|/x_{j,i}^{(k)} <= 1.0E-5$ (2.13)

C. $\sum |(x_{1,i}\gamma_{1,i} - x_{2,i}\gamma_{2,i})| <= 1.0E-3$ (2.14)

D. Both Eqs. 2.12 and 2.13

Where i denotes component, j denotes phase, and k denotes the iteration counter.

Isothermal Three Phase Flash

In three phase calculations (consisting of two liquid and a vapor phase) all three phases are in thermodynamic equilibrium with one another. Thus, the equations resulting from mass balance and equilibrium relationships are mentioned below:

$$F_1 = \sum (x_{1,i} - y_i) = \sum \frac{z_i(1 - K_{1,i})}{W_i} = 0 \qquad (2.15)$$

$$F_2 = \sum (x_{1,i} - x_{2,i}) = \sum \frac{z_i(1 - (K_{1,i}/K_{2,i}))}{W_i} = 0 \qquad (2.16)$$

Where $W_i = R(1 - U) + (1 - R)(1 - U)(K_{1,i}/K_{2,i}) + UK_{1,i}$ (2.17)

$x_{1,i} = z_i/W_i$ (2.18)

$x_{2,i} = (z_i/W_i)(K_{1,i}/K_{2,i})$ (2.19)

$y_i = (z_i/W_i)(K_{1,i})$ (2.20)

$$U = V/F \tag{2.21}$$

V, F, and z_i are defined as moles of vapor, moles of feed, and mole fraction of component i in the feed respectively. Other variables have the same definition as described before. The system can be in one, two, or three phase region depending upon the values of both U and R. When U is 0or 1.0, the system consists of only liquid phase(s) or only vapor phase respectively. The extreme value of R, of 0 or 1.0, simulates the single liquid phase system. The algorithm also uses Wegstein's method for convergence acceleration of phase compositions.

Adiabatic Three Phase Flash

Adiabatic flash operation is simulated using decoupling technique to solve a set of equations assuming initially a three phase system. This method involves repetitive isothermal flash calculations at estimated temperature using Secant method based on discrepancy in calculated and specified enthalpy of the system. The equations associated with adiabatic flash calculations, in addition to Eqns. 2.15 and 2.16, are given below:

$$H_F = UH_V + (1 - U) R H_{L1} + (1 - U) H_{L2} \tag{2.22}$$

where $$H_V = \sum h_{v,i}y_i + h_d \tag{2.23}$$

$$H_{L1} = \sum h_{L,i}x_{1,i} + h_1^{mix} \tag{2.24}$$

$$H_{L2} = \sum h_{L,i}x_{2,i} + h_2^{mix} \tag{2.25}$$

where $h_{V,i}$ = ideal gas enthalpy per mole of component i

$h_{L,i}$ = enthalpy per mole of pure liquid i

h_d = enthalpy departure from ideal vapor enthalpy

h^{mix} = heat of mixing

Equations 2.22 to 2.25 are based on one mole of feed.

2.3 General Purpose Absorption/Distillation Column Model (ABDIS)

The general purpose vapor-liquid equilibrium stage unit operations model is designed to demonstrate the following capabilities:

A. Modes of column operation
  a) Absorber (end feed column)
  b) Stripper (end feed column)
  c) Distillation column (reflux ratio specified)
  d) Distillation column (boilup ratio specified)
  e) Reboiled Absorber (boilup ratio specified)
  f) Refluxed Stripper (reflux ratio specified)

B. Multiple feeds (up to a maximum of 10)

C. Vapor and Liquid Sidestreams (up to a maximum of 10)

D. Multicomponent highly non-ideal system (up to a maximum of 10 components)

E. Multiple stages (up to a maximum of 100 stages)

F. Multiple stage heat exchangers (up to a maximum of 10)

G. Incorporation of Murphree efficiencies

H. Vapor, subcooled liquid, or vapor/liquid distillate product

2.3.1 Equations Associated to the Column

The solution strategy is based on the algorithm developed by Naphthali-Sandholm (1971) which can accommodate the non-ideal systems chosen for this research. This model is supported by thermodynamic library discussed earlier in Section 2.1 and the detailed phase equilibria calculations method is reported elsewhere (Tsai, 1982). Figure 2.1 shows the n th stage configuration and nomenclature. For a N stage column, reboiler as stage one, the generalized discrepancy functions associated with stage n are given below:

Component Material Balance

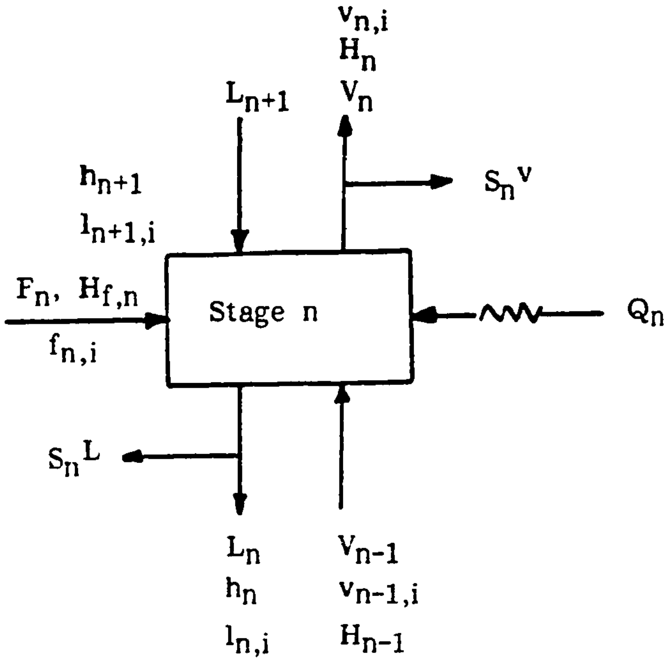
$$F_{1(n,i)} = (1 + \frac{S_n^L}{L_n}) l_{n,i} + (1 + \frac{S_n^V}{V_n}) v_{n,i} + v_{n-1,i} - l_{n+1,i} - f_{n,i} = 0 \quad (2.26)$$

Equilibrium Relationship coupled with the Murphree stage efficiency, η_n

$$F_{2(n,i)} = \eta_n \frac{K_{n,i} V_n}{L_n} l_{n,i} - v_{n,i} + (1 - \eta_n) \frac{V_n}{V_{n-1}} = 0 \quad (2.27)$$

Where the Murphree stage efficiency is defined by

$$\eta_n = \frac{y_{n,i} - y_{n-1,i}}{K_{n,i} x_{n-1,i} - y_{n-1,i}} \quad (2.28)$$



Subscript n = stage, n = 1, 2, ... N

i = component, i = 1, 2, ... c

H = vapor phase enthalpy

h = liquid phase enthalpy

H_f = feed enthalpy

V = total vapor flow

v = component vapor flow

L = total liquid flow

l = component liquid flow

F = total feed

f = component feed

S^L = liquid sidestream

S^V = vapor sidestream

Q_n = external heat exchanger

Figure 2.1 Stage Configuration

and the equilibrium constant is defined by

$$K_{n,i} = \left(\frac{y_i}{x}\right)_n = \left(\frac{\gamma_i f_i^o}{\phi_i P}\right)_n \qquad (2.29)$$

Energy Balance

$$F_{3(n)} = \left(1 + \frac{S_n^L}{L_n}\right)h_n + \left(1 + \frac{S_n^V}{V_n}\right)H_n - H_{n-1} - h_{n+1} -$$

$$h_n^F - Q_n + h_{n+1}^{mix} = 0 \qquad (2.30)$$

The enthalpy calculations associated with Eq. 2.30 are calculated as follows:

Liquid Enthalpy

$$h_n = l_i \int_{T_{ref}}^{T} C_{PL}(T)dT + h_n^{mix} \qquad (2.31)$$

where, $C_{PL}(T)$ = the component specific heat capacity which is a polynomial function of temperature

T_{ref} = the reference temperature, normal boiling point

h_n^{mix} = the heat of mixing

Vapor Enthalpy

$$H_v = v_i\{\lambda_i + \int_{T_{ref}}^{T} C_{Pv}(T)dT + \Delta H\} \qquad (2.32)$$

where, $C_{Pv}(T)$ = the component specific heat capacity which is a polynomial function of temperature

λ_{ref} = the component heat of vaporization

ΔH = the enthalpy correction due to pressure

2.3.2 Solution Algorithm

The componential vapor flow ($v_{n,i}$), componential liquid flow ($l_{n,i}$), and temperature (T_n) on each stage are treated as independent variables to represent the column conditions. Whereas the discrepancy functions, $\bar{F}_n$, are the quantitative measure of the failure of the independent variables. The subscripts n and i denote the stage and system component respectively. The Naphthali-Sandholm method proposed grouping of equations and variables according to stage, in which matrix of partial derivatives, needed in the Newton-Raphson algorithm, form a tridiagnonal sparse matrix. The functions and variables in the form of vector are given below:

$$\bar{F}(\bar{x}) = \begin{vmatrix} \bar{F}_1 \\ \bar{F}_2 \\ \bar{F}_3 \end{vmatrix} = 0 \qquad \bar{x} = \begin{vmatrix} \bar{l} \\ \bar{v} \\ \bar{T} \end{vmatrix} \qquad (2.33 \ \& \ 2.34)$$

where the vector $\bar{l}$, $\bar{v}$, and $\bar{T}$ contains all the elements $l_{n,i}$, $v_{n,i}$, and T_i respectively. Simultaneous solution of all the variables involve Newton-Raphson iterative procedure to estimate the new set of independent variables, $\bar{x}^{m+1}$.

$$\overline{\Delta x}^{\,m+1} = -\left(\frac{\overline{\overline{dF}}}{dx}\right)^{-1} \bar{F}_m \quad \text{and} \quad \bar{x}^{m+1} = \bar{x}^{m} + \overline{\Delta x}^{\,m+1} \qquad \begin{matrix}(2.35)\\(2.36)\end{matrix}$$

A flowchart describing the overall executive program and the affiliated major subprograms is given in the Appendix B.

2.4 Process Simulator (PROSIM)

PROSIM has been developed as part of the research work. It is driven by an executive program from Chemical Engineering Simulation System (CHESS). CHESS is based on the sequential modular approach to solve for one process unit after another in a predefined sequence of blocks/nodes. This method requires known input streams and process conditions in order to establish unknown conditions in the output streams. PROSIM includes new and improved modules, new control blocks, and an enhanced thermodynamics package which altogether increases the capabilities to simulate highly non-ideal and complex processes like azeotropic distillation process. The system description of each of the new and improved blocks is discussed ahead.

ADBF - General Purpose Three Phase Flash Package

The ADBF package is supported by routines which can simulate isothermal and adiabatic two and three phase flash, liquid-liquid separation, bubble and dew point temperature and pressure. Following routines are part of ADBF: ANYONE, DEWT, BUBT, BUBT2, DEWP, BUBP, FLSH2, FLSH1, AFLSH2, TWOLIQ, INTLIZ, KCALC2, and the thermodynamic subprogram library.

The package provides 13 different modes as options, which are summarized in the Equipment Parameters List (Appendix B.2). The basic design equations are described in section 2.2. The algorithm is capable of handling supercritical, condensable, normal, and nonvolatile components. All the computational modes are self initializing. Choice of four objective functions for liquid-liquid equilibria calculations provide flexibility to the user. These objective functions are based on phase compositions, activity coefficients and componential activities. Additional features discussed in section 2.3 have also been incorporated in ADBF.

ACTL- Azeotropic Column Control Block, Variable Distillate Rate

The ACTL block is designed to control the performance of ternary azeotropic distillation column. The column, up to a maximum of four feed streams and no side stream may be operated by varying the split to achieve the desired bottoms product specification. In the research problem, of ethanol-water-benzene system the bottoms specifications of 99+ mole % ethanol, 1.E-4 mole % water, and less than 1 mole % benzene may be set as the desired goal. The computational algorithm estimates new values of the distillate rate and distillation calculations via DIST are performed in order to meet the objective.

The new estimate of the distillate rate is made after the analysis of bottoms product composition. Two unsatisfactory but computationally feasible solutions may arise and therefore the following steps are taken:

A. If alcohol is below specification and water is above specification the Secant method is used for obtaining a new estimate of distillate rate with calculated water composition in bottoms less specification as the objective function.

B. If alcohol is below specification and benzene is above specification then a step change in the predetermined direction is made in the distillate rate.

BCTL - Benzene Stripping Column Control Block, Variable Distillate Rate - I

BCTL is a control block which may be used to update the distillate rate of a predefined distillation column. Information on distillate type, component code, and reference stream numbers is required to determine the bottoms rate based on component balance. The distillate rate is thereafter computed for the conventional column, assuming no side streams. The information componential flow rate is retrieved from the stream matrix (SEXTSV) corresponding to i th component and j th process stream. Retrieval of data is limited to a maximum of four components and four streams.

BZTL - Benzene Stripping Column Control Block, Variable Distillate Rate - II

The function of BCTL block is to control the performance of the benzene stripping column or a similar distillation column. It is supported by the rigorous distillation block DIST and data retrieval technique discussed in systems description of BCTL. The data retrieval method is used for the initial estimate of the split. The desired bottoms component rate and component code are read through DATA statements because of the limitation of 25 Equipment Parameters for a block.

A new estimate of the distillate rate is made by using the secant method, with flowrate of first component as the objective function. Maximum number of data retrieval streams is three.

CNTL - Stream Rate Control Block - I

The function of CNTL block is to update the flow of the specified component in a stream. It may be used to update the make-up process stream during the iterative process of the flowsheet calculations. First input stream to the block is used for information retrieval where as the second input stream is used for updating the values.

The updating methods available are:

A. Manipulation of the componential flow based on the difference in the flow rates of the two input streams, and

B. Manipulation of the componential flow based on the flow ratio of the first input stream over the second input stream.

Minimum and maximum permissible ratios and maximum permissible flow rate of the target stream may be provided through the equipment parameter list. The product stream is established via an isothermal flash.

DCTL - Control Block, Feed-Forward Control of the Split - I

The DCTL block dynamically simulates the feed-forward control of the split in a distillation column based on the composite feed composition and rate and assumed distillate and bottoms product compositions.

DIST - Rigorous Distillation Package

DIST is a rigorous distillation package which is supported by DIST1, DIST2, MATRIX, CORECT, TESTCL, routines and the thermodynamic subprogram library. The following distillation options are available in the package:

A. Distillation column with reflux ratio specified

B. Distillation column with boilup ratio specified

C. Self refluxing distillation column

D. Self reboiling distillation column

The computational algorithm is based on Naphthali and Sandholm (1971) method.

In brief, the solution methodology incorporates stagewise grouping of linearized set of mass balance, heat balance, and equilibrium equations. The block-tridiagonal matrix structure is solved by Thomas algorithm, whereas overall computational strategy is based on Newton-Raphson method. Distribution coefficient is treated as the function of temperature, liquid and vapor phase compositions. The algorithm also takes into account the Murphree plate efficiencies in a rigorous manner.

DSPT - Control Block, Feed-Forward Control of the Split - II

The function of DSPT block is similar to that of DCTL block, but the methods for the calculation of conventional column split are different. The DSPT block allows to read the feed multipliers, whose values range from 0 to 1, pertaining to each of the components up to a maximum of ten. The multipliers for for each of the components and the composite feed entering the distillation column compute the the gross distillate and bottoms stream rates. A unique DSPT block can control distillate rate of a prespecified distillation block.

ECTL - Azeotropic Column Control Block, Variable Entrainer Rate

The in depth analysis of the azeotropic column requires the estimation of optimum entrainer rate for a given process. Therefore, the ECTL block was designed to estimate the suitable entrainer flow rate (first feed) without changing its composition, which in effect can generate a bottoms product of given specification. This Block is modeled to study the effect of entrainer to second feed rate ratio on the azeotropic column's operation. Multiplicity of column solutions, discussed in Chapter 5, demand a sophisticated computational control of the column and stability in the sequence modular flowsheet calculations.

The new estimate of entrainer rate is made after the analysis of the bottoms product composition. Two unsatisfactory, but computationally feasible, solutions may arise and thus the following steps are taken:

A. If alcohol is too wet then the secant method is used to estimate the new entrainer rate with calculated water composition in bottoms less specification as the objective function.

B. If alcohol is below specification and entrainer is above specification then a step change in the predetermined direction is made in the entrainer rate.

RCTL - Stream Rate Control Block - II

RCTL block's function is to update a stream's componential rate. The stream used for the manipulation of rate is an input stream to the block. A maximum of four components may be selected for rate adjustment based on mass balance established by data retrieved from up to four different process streams. A typical example of such a block is to material balance a process by incorporating a make-up stream.

SBOX - Dummy Separation Block

This block can replace a conventional distillation column and can be incorporated for preliminary flowsheet simulation purposes. The present version takes into account an overhead vapor product and a bottoms product as the output streams, with one feed to the column, which are established by dew and bubble point calculations respectively. Distillate and bottoms conditions are passed through equipment parameter matrix, summarized in Appendix

B.4. Data retrieval technique is similar to that described in system description of RCTL block, which in effect is used for computing bottoms rate and distillate rate. SBOX may be most useful for the columns whose separation is constrained. For example, ternary azeotrope formation in the overhead product of benzene stripping column in the ethanol-water-benzene azeotropic distillation process.

SMIX - Special Mixer-Splitter Block

SMIX is a special mixer-splitter block. If one or more input streams after mixing form two liquid phases at the output stream conditions, then this block may be used. Two output streams are in equilibrium with each other and leave at the same temperature and pressure. This block can replace, for example, a mixer, condenser, and decanter in case two liquid phases are formed after mixing and cooling of one or more streams. Heat added or removed is stored in one of the EQPAR matrix locations, which can be fetched if required. Process equipment parameters specification are summarized in Appendix B.2.

The source code may be modified in future for three output streams leaving separately in equilibrium.

CHAPTER 3

STUDY OF VARIOUS ENTRAINERS FOR THE AZEOTROPIC DISTILLATION PROCESS

Ethanol and water form an azeotrope which requires techniques like azeotropic distillation for the recovery of water free alcohol. Introduction of an entrainer into the system materially increases the relative volatility of water and thus permits the recovery of the ethanol as an effective high boiler. The detriment is that the entrainer must be recovered to produce an economic process.

3.1 Selection of Potential Entrainers

Holland (1981) proposed a selection criteria based upon the polarity of the entrainer with respect to the polarity of alcohol and water. Berg (1969) has reported more exhaustive criteria based upon systems forming hydrogen bonds and systems not forming hydrogen bonds. The most important single cause for the formation of the alcohol-water azeotrope is hydrogen bonds. Berg includes the following methods for entrainer selection to separate a minimum azeotrope:

A. The entrainer forms a minimum binary azeotrope with one component, which is sufficiently lower in boiling point than the original azeotrope.

B. The entrainer forms a ternary minimum boiling azeotrope which is sufficiently lower than any binary azeotrope, and in which the ratio of the original components is different from their ratio in the binary azeotrope.

The criteria (suggested by Berg) for solubility of one component into another is internal pressure and hydrogen bonding dependent phenomena, and has little relation to polarity of compounds. To ascertain the alcohol dehydration and process flexibility the following criteria was adopted in the investigation of potential entrainers:

A. Entrainer with boiling point about or below that of alcohol to be separated.

B. Relatively non-polar component in nature, for example benzene and cyclohexane.

C. Form a large positive deviation from Raoult's Law to give a minimum azeotrope with alcohol or water in the mixture.

D. Be soluble in the alcohol-water mixture at the azeotropic distillation temperature range.

E. Be easily separated from water and alcohol.

F. Be stable at the azeotropic distillation temperature.

G. Be nonreactive with the components and the column materials.

Some of the entrainers mentioned Table 3.1 have been reported by Black (1980). The set of entrainers selected based upon above stated criteria are listed in Table 3.1.

3.2 Why UNIFAC was used for Activity Coefficient Data

The representation of ternary vapor-liquid equilibria

Table 3.1

List of Potential Entrainers

Serial No.	Entrainer
1	Benzene
2	Cyclohexane
3	N-pentane
4	Cyclopentane
5	Methyl Cyclopentane
6	Isopentane
7	N-Hexane
8	2-Methyl Pentane
9	1-Hexene
10	Diethyl Ether
11	2,2-Dimethyl Pentane
12	2,2,3-Trimethyl Butane

(VLE) data in the azeotropic distillation column requires very accurate prediction of activity coefficients. The NRTL (Renon, 1969) and modified UNIQUAC (Anderson, 1978) activity coefficient models can be used for the ethanol-water-entrainer systems provided the interaction parameters or experimental data is available at or near the operating conditions. Experimental ternary VLE data is available only for the ethanol-water-benzene and ethanol-water-di ethyl ether systems. The prediction of ternary VLE with parameters obtained from binary data is recommended only if all the binary pairs are miscible.

All the ternary systems considered in Table 3.1 have one immiscible pair, that is water and the entrainer. Since the ternary VLE experimental data is unavailable for most of the systems to be studied and considering the other facts stated above, the UNIFAC (Fredenslund, 1977) group contribution model was selected for the prediction of activity coefficients. The data bank consisting of group area and volume constants for 77 secondary groups and VLE interaction parameters for 41 primary groups is shown in Appendix (A.3).

Thus, this research work includes the qualitative analysis of the azeotropic distillation column using various entrainers as represented by UNIFAC activity coefficient model to evaluate their relative performance.

3.3 Performance of Entrainers in the Azeotropic Column

Benzene, cyclohexane, n-pentane and diethyl ether have been reported as potential entrainers by Black (1980), Keister (1982), Prokopakis (1980), Tsai (1982), Venkatesh (1983) and . The capability of UNIFAC was established for the systems whose binary or ternary data were available. The ternary data is preferred over the binary data because of the presence of one immiscible pair per ethanol-water-entrainer system. The published (Gmehling, 1977) NRTL VLE parameters for ethanol-water-benzene and ethanol-water-diethyl ether obtained from ternary data are reported in Table 3.2. Also the NRTL VLE and LLE parameters for certain alcohol-entrainer and water-entrainer pairs are summarized in Tables 3.3 and 3.4.

Direct comparison of ethanol-water-benzene and ethanol-water-diethyl ether systems is made using the NRTL and the UNIFAC equations. The azeotropic distillation column temperature (T) and liquid phase composition (x) profiles for these systems are reported in Appendices C.1.3 and C.10.3 respectively. In the case of benzene in the azeotropic column, UNIFAC predicts column profiles similar to that of NRTL, except for five stages near the reboiler. UNIFAC thus simulates the production of dry ethanol with approximately 8.3 mole % benzene. when diethyl ether is used, the T and x profiles from UNIFAC match those from NRTL, but only qualitatively. Contrary to comments made by Black (1980), the performance of diethyl ether was poor. Black has not reported the results of ethanol-water-diethyl ether system using UNIFAC equation for the prediction of activity coefficients.

Table 3.2

Binary VLE NRTL Interaction Parameters

from Ternary VLE Data

System: (1) Ethanol - (2) Water - (3) Entrainer

Reference: Gmehling (1977)

(3)	P mm Hg	Interaction Parameters in cal/g mole		
Benzene	760	A_{12} = -86.763	A_{21} = 1289.908	α_{12} = 0.270
		A_{13} = 282.332	A_{31} = 1096.899	α_{13} = 0.295
		A_{23} = 3820.954	A_{32} = 2213.355	α_{23} = 0.267
Diethyl -Ether	3862.9	A_{12} = 175.652	A_{21} = 1932.235	α_{12} = 0.295
		A_{13} = 633.869	A_{31} = -18.524	α_{13} = 0.275
		A_{23} = 2022.547	A_{32} = 390.447	α_{23} = 0.283

Table 3.3

Binary VLE NRTL Interaction Parameters

from Binary VLE Data

System: (1) Ethanol - (2) Water - (3) Entrainer

Reference: Gmehling (1977)

(3)	T deg C	P mm Hg	Interaction Parameters cal/g mole A_{13}	 A_{31}	 α_{13}	Data Ref.
Cyclohexane		760	761.7739	1393.7993	0.4376	Yuan (1963)
n-Pentane	20		412.7546	1183.3812	0.2886	Ishii (1935)
Methyl Cyclopentane		760	644.0719	1564.8490	0.4320	Sinor (1960)
n-Hexane		760	603.0883	1179.2617	0.2887	Kudrayavtseva (1963)

Table 3.4

Binary LLE NRTL Interaction Parameters

from Binary LLE Data

System: (1) Ethanol - (2) Water - (3) Entrainer

Reference: Sorensen (1979)

(3)	T deg C	Interaction Parameters cal/g mole A_{13}	A_{31}	α_{13}
Cyclohexane	25	5644.6696	3589.5155	0.200
n-Pentane	25	5759.1208	3766.5572	0.200
Methyl Cyclopentane	25	5798.8608	4345.4580	0.200
n-Hexane	40	6769.9077	3302.3940	0.200

The pressure (high pressure for some of the systems) and hydrogen bonding between water and ethanol causes the non-ideality in the vapor phase. Therefore, the calculation of equilibrium coefficient incorporates the vapor phase fugacities. The vapor phase fugacity was estimated using the Virial equation of state, with the second virial coefficient B for the mixture evaluated using the Hayden and O'Connell (Hayden et al., 1975) method.

The system behavior with cyclohexane as the entrainer is presented in Appendix C.2.3. The liquid phase compositions, for the ethanol-water-cyclohexane, predicted by UNIFAC and NRTL match to a great degree but the temperature profile is not comparable. It should be noted that the NRTL parameters for the ethanol-water-cyclohexane system were obtained using binary data. The results for n-pentane, methyl cyclopentane and n-hexane with NRTL were found to be in the non-convergence region. This may be attributed to the fact that:

A. The binary data for ethanol-n-pentane, water-n-pentane, water-methyl cyclopentane and water-n-hexane were not in the domain of process conditions of the column, or

B. The prediction of ternary VLE with only binary data may be inappropriate for the systems under consideration, or

C. The process conditions, for example ethanol to entrainer ratio chosen were inadequate for the production of dry ethanol as the bottoms product.

The effect of number of stages in the column on the bottoms product composition for system with benzene is shown in the Table 3.5. Both NRTL and UNIFAC predict the buildup of the water concentration in the bottoms product as the number of stages is reduced in the column. Depletion of water, at the ppm (parts per million) level, in ethyl alcohol product demand a significant number of stages in the stripping section. It should be noted that increase in the number of stages from 20 to 40 (for example), in Table 3.5, improves only the water level but does not affect the benzene concentration. To obtain the computational stability the boilup ratio and pressure level in the column had to be adjusted. The comparison of performance of various entrainers is reported in the Table 3.6, which also shows different column pressure and boilup ratio for the different systems. The cases with cyclopentane, isopentane and 2,2-di methyl pentane did not converge.

The effect of process variables, like pressure and boilup ratio, on the column separation is investigated and reported in Tables C.1.2 to C.12.2 for all the entrainers listed in Table 3.1. It is observed that the effect of column pressure and boilup ratio on the bottoms composition was significant in the systems with benzene, cyclohexane, methyl cyclopentane, 1-hexene and 2,2,3-trimethyl butane. The solution with n-pentane and diethyl ether cases, shown in Appendices C.3 and C.10, was in the unacceptable region, that is in the stripping section only depletion of entrainer was predicted, instead of depletion of both water and

Table 3.5

Comparison of the Effect of Column Stages on Separation Using NRTL and UNIFAC Models

System: Ethanol - Water - Benzene

Models: UNIFAC, NRTL for liquid phase and ideal vapor

Bottoms Product Composition in mole %

No. of Stages	NRTL			UNIFAC		
	EtOH	Wtr	Entnr	EtOH	Wtr	Entnr
50	98.4074	2.4214E-8	1.5926	91.6666	3.2900E-6	8.3350
45	98.4074	3.3175E-7	1.5926	91.6666	3.6300E-9	8.3340
* 40	98.4075	3.2486E-6	1.5925	91.6666	3.8430E-9	8.3340
35	98.4074	3.2188E-5	1.5926	91.6660	1.0460E-10	8.3340
30	98.4072	3.1857E-5	1.5928	91.6650	6.9590E-9	8.3350
25	98.4048	3.1485E-3	1.5920	91.6650	4.3700E-7	8.3350
20	98.2433	0.0304	1.7267	91.6640	2.7110E-5	8.3360
15	98.1628	0.2932	1.5440	91.6640	1.6820E-3	8.3340
10	96.3264	2.5008	1.1728	91.5870	0.1036	8.3100

Note : * means the Base case

entrainer, which is not in agreement with the study done by Black (1980). All the systems studied had regions of computational instability. Appendix C consists of column results and input to the ABDIS program for all the entrainers considered for study.

3.4 Assessment of UNIFAC and Potential Entrainers

The comparison of performance of twelve entrainers is summarized in the Table 3.6. Based on the VLE prediction by UNIFAC, a qualitative analysis is made for the selection of the entrainer for the ethanol-water azeotropic distillation process. Three cases (4D, 4F, and 4K), shown in the Table 3.6 corresponding to cyclopentane, isopentane, and 2,2-dimethyl cyclopentane as entrainers, failed to converge for a very wide range of pressures and boilup ratios. The entrainers under consideration exert a wide range of vapor pressures therfore the system pressures are different for the different systems. Thus a constant set of operating conditions like entrainer rate and composition, and distillate or bottoms rate may not be suitable for all the systems. This part of the research was conducted at the earlier stages and optimum conditions were unavailable for each of the systems under consideration.

UNIFAC as the tool for predicting VLE of the highly non-ideal systems involving water and entrainer concentrations at the ppm (parts per million) or ppb (parts per billion) levels in the stripping section of the column is suitable for the following studied systems:

Table 3.6

Comparison of Performance of Various Entrainers in The Azeotropic Distillation Column

Models : UNIFAC and Virial (Hayden & O'connell) vapor

Case No.	Entrainer	Top Stage Pressure (psia)	Boilup Ratio	Bottoms Product Composition		
				Ethanol	Water	Entrainer
4A13	Benzene	12.0	5.113	99.4347	3.6523E-9	0.5653
4B14	Cyclo-C6	12.0	7.100	99.0900	1.0111E-9	0.9100
4C23	N-Pentane	30.0	6.015	67.8646	32.1354	4.38E-14
4D*	Cyclo-C5			-	-	-
4E10	Methyl Cyclo-C5	36.0	6.750	99.4025	6.9560E-11	0.5975
4F*	Isopentane			-	-	-
4G11	N-Hexane	50.0	9.624	99.5394	9.7283E-9	0.4606
4H25	2-Methyl Pentane	124.0	5.714	99.7446	7.7106E-10	0.2554
4I11	1-Hexene	71.0	6.015	99.3832	3.9961E-11	0.6168
4J1	Diethyl - Ether	135.0	6.015	68.7874	31.2126	5.16E-18
4K*	2,2-Di - methyl-C5			-	-	-
4L19	2,2,3-Tri- methyl-C4	10.0	9.150	99.0554	1.600E-12	0.9446

Note : All the compositions are in mole % .

* means the unconverged cases

A. Ethanol-water-benzene

B. Ethanol-water-cyclohexane

C. Ethanol-water-methyl cyclopentane

D. Ethanol-water-n-hexane

E. Ethanol-water-2-methyl pentane

F. Ethanol-water-1-hexene

G. Ethanol-water-2,2,3-trimethyl butane

CHAPTER 4

GLOBAL THERMODYNAMIC INTERACTION PARAMETERS ESTIMATION

The concept of representing vapor-liquid (VLE) and liquid-liquid equilibria (LLE) for a system using one set of parameters was introduced by Prausnitz (1980). An in depth analysis of this subject was conducted, as applicable to an ethanol-water-benzene system. A single set of parameters may be defined as global when they can represent simultaneous both the binary/ternary VLE and the ternary LLE in the temperature and pressure range of interest. The assessment of estimated parameters is done on the basis of its performance in the process environment, the expanded definition is presented in the Section 4.1. A two equation approach to represent vapor and liquid phase non-ideality demands a suitable equation, like UNIQUAC, NRTL or LEMF (Marina and Tassios, 1973), to predict liquid phase activity coefficients. NRTL is three parameter equation and LEMF is essentially a two parameter NRTL equation with α equals to a constant, -1. The modified UNIQUAC equation

$$\ln \gamma_i = \ln \frac{\phi_i}{x_i} + \left(\frac{Z}{2}\right) q \ln \frac{\theta_i}{\phi_i} + l_i - \frac{\phi_i}{x_i} \sum_j x_j l_j - q'_i \ln \left(\sum_j \theta'_j \tau_{ji}\right) + q'_i - q'_i \sum_j \frac{\theta'_j \tau_{ij}}{\sum_k \theta'_k \tau_{kj}} \qquad (2.1)$$

where

$$\tau_{ji} = \exp\left(- \frac{a_{ji} + b_{ji}/T}{T}\right) \qquad (2.2)$$

was selected for the study because of the fact that it has two temperature independent parameters per binary embedded in the variable τ and its reported performance is as good as or better than that of the NRTL for both, VLE and LLE. The research objective was to estimate temperature independent parameters (a_{ji}) in Equation 2.2 stated above with the temperature parameter (b_{ji}) equal to 0. The Ethanol-water-benzene system was undertaken for the study because of three reasons:

A. This system involves the existence of VLE and LLE in the alcohol drying process plant.

B. The system experimental data (VLE and LLE) is available for the temperature and pressure range of interest.

C. This system is also chosen for an in depth analysis of the process variables presented in Chapters 5 and 6.

A global set of temperature independent parameters was obtained based on the strategy discussed in the following Section and is reported in the Section 4.7.

4.1 Research Problem Definition

The global thermodynamic interaction parameters for the modified UNIQUAC model is defined as a set of parameters which can predict isobaric binary and ternary VLE, and isothermal ternary LLE. This global representation is to be used in the distillation columns and the two liquid phase decanter of the ethanol-water-benzene azeotropic separation process plant as shown in the Fig. 6.6. The major advantages of obtaining such a set are:

A. Investigation of the capability of a global set of parameters to simulate vapor-liquid-liquid equilibrium operations in processes like three phase distillation.

B. Assessment of the UNIQUAC model with respect to the level of its sophistication and flexibility.

Prausnitz et al. (1980) has presented results of a few systems demonstrating the performance of a set of parameters estimated from simultaneous regression of binary VLE data and one or more LLE tie lines. For the ethanol-water-benzene process a set of parameters may be called global if it can simulate the column profiles of the key process units like, alcohol concentrator, azeotropic distillation tower, and benzene recovery column(s) at low pressures, and the two liquid phase compositions in the decanter.

The nonlinear regression analysis requires a comprehensive program which should be capable of handling isothermal multicomponent VLE data, isobaric multicomponent VLE data, and isothermal multicomponent LLE data, either independently or in combination. The following subsections discuss:

- o The selection of the main algorithm and the salient features of the developed software.
- o Various objective functions for the regression of

the VLE, LLE and VLE+LLE data.

- VLE and LLE data regression results and the associated objective functions

A simple technique for the selection of a unique set of roots has also been suggested. In addition, an approach to the global parameter set has been discussed along with its performance in the key process steps.

4.2 Nonlinear Regression Program and its Limitations

The nonlinear regression program consists of two major sections. The first section of the code was the least-squares minimization algorithm proposed by Marquardt (1964). The algorithm is essentially a maximum neighborhood method which, in effect, performs an optimum interpolation between the Taylor series method and the gradient method. The function to be minimized

$$\emptyset = \sum_{j=1}^{m} [Y_j - Z_j]^2 \qquad (4.1)$$

is used to compute the parameters, where Z is the predicted value and Y is the experimental or the target value of the dependent variable at the j-th data point. The use of either total pressure, temperature, vapor phase composition, activity coefficient or activity coefficient of a component at infinite dilution as a dependent variable for the regression of isothermal or isobaric multicomponent VLE data have been reported in the literature. In this research work the various VLE objective functions used to compute Z_j are discussed in Section 4.3.

The limitation of a single dependent variable in Eq. 4.1 becomes more severe in the case of multicomponent LLE data regression, where the function could be based upon multiple estimated variables. Various LLE objective functions are discussed in Section 4.3.

The second section of the program deals with the user subroutine FOFX. The original capability of the program was limited to the regression of isothermal multicomponent VLE data. As part of this research work the second section was extended to serve the purpose of global parameters estimation.

4.2.1 Salient Features of the Enhanced Program

The revised version of the program includes the following diversified capabilities:

A. Multicomponent data regression of
    a. Isothermal VLE data
    b. Isobaric VLE data
    c. Isothermal LLE data of the systems in which only one of the pairs is partially miscible (Type I system)
    d. Isothermal VLE data and LLE data
    e. Isobaric VLE data and LLE data together

B. Self initialization of the two liquid phase calculations, including the selection of dominating components in both the phases.

C. In Equation 2.2, a_{ji} and b_{ji} are temperature independent and temperature dependent parameters respectively. The option exists for the evaluation of $a_{ji}(b_{ji}=0)$, or a_{ji} and b_{ji}.

D. Various objective functions to compute Z_j in the Equation 4.1 for the VLE data regression are incorporated. A selected list of such functions is presented in Table 4.1, with an exhaustive list given in Appendix D.2.

E. Objective functions to estimate Z_j in the Eq. 4.1 for the LLE data regression. A selected list of functions is presented in Table 4.2, with a complete list given in Appendix D.3. The weights (weight variables) associated with the tie lines are dynamically computed based on the relative error in the compositions.

F. Compatibility with the general purpose flash program (FLASH2), absorption/distillation program (ABDIS) (Tsai, 1982), and the improved process simulator (PROSIM) based upon CHESS (Motard et al., 1972).

4.3 Objective Functions

The development of an objective function for the minimization of errors is of utmost importance. The structure of such a function is based on one dependent variable (Z_j) in the overall minimization function, represented by the Equation 4.1. The following subsections discuss separately the VLE and LLE objective functions.

4.3.1 Vapor-Liquid Equilibria Objective Functions

The area of VLE data regression has been extensively covered in the literature references. Isothermal data regression incorporates computation of bubble point pressure (P) and corresponding vapor phase component mole fractions (y_i). Isobaric data involves the calculation of bubble point temperature (T) and y_i's. In a study by Silverman and Tassios (1984), objective functions based on the total system pressure (P), and a combination of y_i's and P's have been found to perform better than those based upon activity coefficients, activity coefficients at infinite dilution, Gibbs free energy, or just y_i's. The VLE objective functions selected for the study are listed in Table 4.1. A complete list of functions is presented in Appendix D.2.

It should be noted that most of the objective functions take into account the absolute or relative difference of experimental and estimated dependent variable values. Therefore the target is to make the computed dependent variable in the minimization equation as close to zero as possible. The value 1.0E-4 is used, instead of 0.0, so as to avoid overflow problems in the calculation process.

4.3.2 Liquid-Liquid Equilibria Weighted Objective Functions

Sorensen et al. (1979) have investigated functions in terms of activities and in terms of mole fractions. In addition, LLE objective functions can also be structured based on distribution coefficients, and on a suitable combination of component activities, mole fractions, and

Table 4.1

Selected Objective Functions for VLE Data Regression

VLE Func (VLEFN) #	VLE Objective Function
7	$Z_j = \frac{1}{n}\sum_{i=1}^{n} \lvert y_{ei} - y_{ci}\rvert$
8	$Z_j = \frac{1}{n}\sum_{i=1}^{n} \frac{\lvert y_{ei} - y_{ci}\rvert}{y_{ei}}$
9	$Z_j = \frac{1}{n}\sum_{i=1}^{n} \lvert \text{Ln } y_{ei} - \text{Ln } y_{ci}\rvert$
10	$Z_j = \frac{1}{n}\sum_{i=1}^{n} \lvert y_{ei} - y_{ci}\rvert + \frac{\lvert P_e - P_c\rvert}{P_e}$
11	$Z_j = \frac{1}{n}\sum_{i=1}^{n} \frac{\lvert y_{ei} - y_{ci}\rvert}{y_{ei}} + \frac{\lvert P_e - P_c\rvert}{P_e}$
12	$Z_j = \frac{1}{n}\sum_{i=1}^{n} \lvert \text{Ln } y_{ei} - \text{Ln } y_{ci}\rvert + \lvert \text{Ln } P_e - \text{Ln } P_c\rvert$
13	$Z_j = \lvert P_e - P_c\rvert$
15	$Z_j = \frac{\lvert P_e - P_c\rvert}{P_e}$
17	$Z_j = \lvert T_e - T_c\rvert$
19	$Z_j = \frac{\lvert T_e - T_c\rvert}{T_e}$
20	$Z_j = \lvert \text{Ln } (T_c / T_e) \rvert$

Table 4.1 (Contd.)

Selected Objective Functions for VLE Data Regression

VLE Func (VLEFN) #	VLE Objective Functions
21	$Z_j = \lvert T_e - T_c \rvert + \frac{1}{n} \sum_{i=1}^{n} \lvert y_{ei} - y_{ci} \rvert$
22	$Z_j = \frac{\lvert T_e - T_c \rvert}{T_e} + \frac{1}{n} \sum_{i=1}^{n} \lvert y_{ei} - y_{ci} \rvert$

Note: The objective functions for the regression of vapor-liquid equilibria are computed for the j th data point and n number of components. Z_j, e, and c are defined as estimated dependent variable in the minimization Equation 4.1, experimental, and calculated values respectively. T and y_i are bubble point temperature and vapor phase component mole fraction respectively.

distribution coefficients. The functions based upon isoactivity criterion have a severe drawback in that its minimization does not guarantee the minimization of errors in the experimental and calculated mole fractions. In this research work, investigation was done with functions based on component mole fractions and on the distribution coefficient of the solute. In a ternary system, for example, solute is a distributed component in both the liquid phases. The distribution coefficient is the ratio of activity coefficient of a component in the heavy phase and that in the light phase. The selected LLE objective functions are reported in Table 4.2, with a complete list in Appendix D.2. For the ethanol-water-benzene LLE system, ethanol and benzene are defined as solute and solvent respectively. Benzene rich and water rich phases are defined as extract and raffinate phases respectively.

Care was taken to set value of Y_j = 1.0E-8 in Equation 4.1, as mentioned earlier to avoid computational difficulties. In the weighted objective functions the variable w_i, in expressions listed in Appendix D.3, is defined as weight or (weight variable). The dynamic computation of weights, as suggested by Sorensen, on the basis of the error in the experimental and calculated mole fractions has been incorporated. Therefore manipulation of weights is done by reading a constant 'W'. For example, W = 100 would magnify the Z_j, calculated dependent variable for the Eq. 4.1, values by hundred times for LLE data points. This feature introduces great flexibility in parameter estimation from

Table 4.2

Selected Objective Functions for LLE Data Regression

LLEFN #	LLE Objective Functions
5	$Z_j = \frac{1}{2n} \sum_{i=1}^{n} w_i^{I} \lvert x_{ei}^{I} - x_{ci}^{I} \rvert + w_i^{II} \lvert x_{ei}^{II} - x_{ci}^{II} \rvert$
6	$Z_j = \frac{1}{2n} \sum_{i=1}^{n} w_i^{I} \lvert \mathrm{Ln}\, x_{ei}^{I} - \mathrm{Ln}\, x_{ci}^{I} \rvert + w_i^{II} \lvert \mathrm{Ln}\, x_{ei}^{II} - \mathrm{Ln}\, x_{ci}^{II} \rvert$
7	$Z_j = \frac{1}{2n} \sum_{i=1}^{n} w_i^{I} \frac{\lvert x_{ei}^{I} - x_{ci}^{I} \rvert}{x_{ei}^{I}} + w_i^{II} \frac{\lvert x_{ei}^{II} - x_{ci}^{II} \rvert}{x_{ei}^{II}}$
8	$Z_j = \frac{1}{2n} \sum_{i=1}^{n} w_i^{I} \frac{\lvert x_{ei}^{I} - x_{ci}^{I} \rvert}{x_{ei}^{I} + x_{ci}^{I}} + w_i^{II} \frac{\lvert x_{ei}^{II} - x_{ci}^{II} \rvert}{x_{ei}^{II} + x_{ci}^{II}}$
9	$Z_j = \frac{1}{2n} \sum_{i=1}^{n} w_i^{I} \frac{\lvert x_{ei}^{I} - x_{ci}^{I} \rvert}{x_{ei}^{I}} + w_i^{II} \frac{\lvert x_{ei}^{II} - x_{ci}^{II} \rvert}{x_{ei}^{II}} + \sum_{\substack{i=1 \\ i \neq Ie, Ir}}^{n} \frac{\lvert \beta_{ei} - \beta_{ci} \rvert}{\beta_{ei}}$
10	$Z_j = \frac{1}{2n} \sum_{i=1}^{n} w_i^{I} \lvert \mathrm{Ln}\, x_{ei}^{I} - \mathrm{Ln}\, x_{ci}^{I} \rvert + w_i^{II} \lvert \mathrm{Ln}\, x_{ei}^{II} - \mathrm{Ln}\, x_{ci}^{II} \rvert + \frac{1}{2(n-2)} \sum_{\substack{i=1 \\ i \neq Ie, Ir}}^{n} \lvert \mathrm{Ln}\, \beta_{ei} - \mathrm{Ln}\, \beta_{ci} \rvert$

Table 4.2 (Contd.)

Selected Objective Functions for LLE Data Regression

LLEFN #	LLE Objective Functions
11	$Z_j = \frac{1}{2n} \sum_{i=1}^{n} w_i^{I} \frac{\lvert x_{ei}^{I} - x_{ci}^{I} \rvert}{x_{ei}^{I} + x_{ci}^{I}} + w_i^{II} \frac{\lvert x_{ei}^{II} - x_{ci}^{II} \rvert}{x_{ei}^{II} + x_{ci}^{II}} + \frac{1}{2(n-2)} \sum_{\substack{i=1 \\ i \neq Ie, Ir}}^{n} \frac{\lvert \beta_{ei} - \beta_{ci} \rvert}{\beta_{ei} + \beta_{ci}}$

For all of the objective functions (w_i) weights are computed using W as a constant in the following equations

$$w_i^{I} = \left| 1.0 + W \frac{\lvert x_{ei}^{I} - x_{ci}^{I} \rvert}{x_{ei}^{I}} \right| \text{ and}$$

$$w_i^{II} = \left| 1.0 + W \frac{\lvert x_{ei}^{II} - x_{ci}^{II} \rvert}{x_{ei}^{II}} \right|$$

Note: The objective functions for the regression of liquid-liquid equilibria are computed for the j th data point and n number of components. Subscripts e and c are defined for experimental and calculated values respectively. β_i and x_i are defined as the distribution factor (activity coefficients ratio) and liquid phase mole fraction respectively.

the simultaneous regression of VLE and LLE data.

4.4 Binary Vapor-Liquid and Liquid-Liquid Equilibrium Data Regression

In order to meet the research objective of global parameter estimation for the ethanol-water-benzene azeotropic process analysis of the systems listed in the Table 4.3 were studied, where n denotes the number of data points. The major experimental data source was Gmehling et al. (1977) and Sorensen et al. (1979) of the DECHEMA series. In systems 6, 7 and 8 a single data point was chosen by averaging the constant temperature points reported by various contributors. This strategy would average out the errors encountered in recording the experimental data.

Ethanol and water are highly polar in nature, possess a high degree of association, and form hydrogen bonds. Therefore Virial equation of state was used to represent the vapor phase non-ideality. The second virial coefficients for the mixture were estimated using the Hayden and O'Connell method (1975). This method incorporates critical temperature, critical pressure, dipole moment, mean radius of gyration, and the association parameter to account for weak physical forces and chemical forces.

The modified UNIQUAC (Anderson, 1978) equation (Eq. 2.1) was used to estimate the liquid phase activity coefficients. The model consists of two temperature independent parameters per binary and is discussed at length in Appendix A.

Table 4.3

Equilibrium Datasets for Regression Analysis

#	Binary Systems	Type	Condition	n	Reference	Case Series
1.	Ethanol-Water	VLE	760 mm Hg	34	Reider (1949)	04
2.	Ethanol-Water	VLE	40 °C	13	Mertl (1949)	08
3.	Ethanol-Benzene	VLE	750 mm Hg	9	Tyrer (1949)	06
4.	Ethanol-Benzene	VLE	40 °C	11	Udovenko (1962)	09
5.	Water-Benzene	LLE	25 °C	1	Polak (1962)	22
6.	Water-Benzene	LLE	25 °C	1	Sorensen (1979)	23
7.	Water-Benzene	LLE	35 °C	1	Sorensen (1979)	24
8.	Water-Benzene	LLE	70 °C	1	Sorensen (1979)	25

4.4.1 Selection of the Objective Functions

The purpose of this part of research was to evaluate different functions for the minimization of the errors between experimental and calculated values of the dependent variables for isothermal and isobaric systems. Preliminary screening was done to isolate the selection of suitable VLE objective function(s) for further regression analysis. A list of objective functions, included for this study, are summarized in the Table 4.1. An acronym, VLEFN, would be used later for vapor-liquid equilibria objective functions.

Vapor-Liquid Systems

Seven different functions were investigated for the isobaric VLE systems and it was observed that functions based upon T's (VLEFN # 17,19, and 20) predict better T and y_i values as compared to those based upon only y_i's (VLEFN # 7, 8, and 9). For the ethanol-water system at 760 mm Hg, VLEFN # 21 (Case 04G in Table 4.4) predicts mean deviation in T and y_i of the order of 0.13 ^oC and 0.88 mole % respectively. Mean deviations in T and y_i are 0.1 ^oC and 0.58 mole %, respectively, for the ethanol-benzene system at 760 mm Hg using VLEFN # 21 (Case 06G in Table 4.5).

Cases 04G and 06G, in Tables 4.4 and 4.5 respectively, show that function involving both T's and y_i's (VLEFN # 21) predict somewhat better results as compared to those predicted using other objective functions. A complete set of estimated parameter and corresponding predicted results for isobaric ethanol-water and ethanol-benzene systems are reported in Appendices E.1.1 and E.1.3. Thus, further

Table 4.4

Evaluation of VLE Objective Function from Regression Results of Isobaric Ethanol-Water (VLE) System

System: (1) Ethanol - (2) Water   Condition: P = 760 mm Hg

Gamma Model: Modified UNIQUAC   Phi Model: Virial EOS

Reference: Reider, R.M.,et al. (1949)   No. of data points = 34

Case No.	VLEFN #	$T_{exp}-T_{cal}$ in deg C		$Y_{1exp}-Y_{1cal}$ in mole %		Inf. Dilution Activity Coeff	
		Mean	Max	Mean	Max	(1)	(2)
04A	7	0.38	0.93	0.534	2.726	5.128	2.329
04B	8	0.25	0.81	0.623	2.630	5.169	2.405
04C	9	0.22	0.77	0.655	2.591	5.188	2.422
04D	17	0.15	0.45	0.897	2.509	5.436	2.465
04E	19	0.15	0.43	0.902	2.547	5.454	2.462
04F	20	0.15	0.43	0.903	2.545	5.453	2.462
04G	21	0.13	0.56	0.883	2.362	5.299	2.508

Table 4.5

Evaluation of VLE Objective Function from Regression Results of Isobaric Ethanol-Benzene (VLE) System

System: (1) Ethanol - (2) Benzene   Condition: P = 750 mm Hg

Gamma Model: Modified UNIQUAC   Phi Model: Virial EOS

Data reference: Tyrer D., (1912)   No. of data points = 9

Case No.	VLEFN #	$T_{exp}-T_{cal}$ in deg C		$Y_{1exp}-Y_{1cal}$ in mole %		Inf. Dilution Activity Coeff	
		Mean	Max	Mean	Max	(1)	(2)
06A	7	0.33	0.68	0.624	1.869	9.198	4.562
06B	8	0.44	0.75	0.749	1.490	9.061	4.562
06C	9	0.46	0.76	0.769	1.438	9.049	4.581
06D	17	0.11	0.26	0.668	2.491	8.143	4.235
06E	19	0.12	0.26	0.685	2.458	8.048	4.249
06F	20	0.12	0.26	0.685	2.457	8.050	4.249
06G	21	0.10	0.36	0.579	2.672	8.809	4.159

research on isobaric VLE systems was performed using function # 21 shown in Table 4.1.

A similar analysis was made for the isothermal ethanol-water and ethanol-benzene systems. In addition to functions based on only y_i's (VLEFN # 7, 8, and 9), functions based on P and y_i's (VLEFN # 10, 11, and 12) and functions based on only P's (VLEFN # 13, 15, and 16) were incorporated for the evaluation, and are therefore included in the Table 4.2. The evaluation of the above nine different VLE objective functions for the ethanol-water and the ethanol-benzene systems at 40 ^oC was done on the basis of predicted pressure and component vapor mole fractions, and infinite dilution activity coefficients. The selected results are summarized in Tables 4.6 and 4.7, and show that all the chosen functions predict good P, y_i, and γ_i^∞ values for all the components, but the objective function(s) (VLEFN # 9,and 10) having combination of P's and y_i's yield better fits in terms of both pressure and vapor phase compositions.

Liquid-Liquid Equilibria Systems

Seven different objective functions (LLEFN # 5, 6, 8, 10, and 11) were considered for LLE data analysis. The chosen functions consist of the x_i's of phases I and II, and the combination of x_i's and distribution coefficient of solute(s). The work reported by Soares (1983) suggests an improvement in predictions near the plait point for functions using phase compositions combined with distribution coefficient(s). The criteria for evaluation was based

Table 4.6

Evaluation of VLE Objective Function from Regression Results of Isothermal Ethanol-Water (VLE) System

System: (1) Ethanol - (2) Water Condition: T = 40 C

Gamma Model: Modified UNIQUAC Phi Model: Virial EOS

Data reference: Mertl, I., et al. (1972) No. of data points = 13

Case No.	VLEFN #	$P_{exp}-P_{cal}$ in mm Hg		$Y_{1exp}-Y_{1cal}$ in mole %		Inf. Dilution Activity Coeff	
		Mean	Max	Mean	Max	(1)	(2)
08A*	7	1.89	8.60	0.529	1.331	5.276	2.520
08B*	8	1.67	8.69	0.561	1.244	5.239	2.613
08C	9	1.66	8.72	0.564	1.239	5.243	2.615
08D*	10	1.85	7.93	0.577	1.561	5.004	2.726
08E	11	1.74	8.35	0.541	1.289	5.140	2.644
08F*	12	1.72	8.32	0.560	1.433	5.108	2.695
08G*	13	1.74	8.24	0.559	1.412	5.092	2.688
08H*	15	2.09	7.25	0.673	1.805	4.833	2.783

Note: '*' means unconverged cases, values shown were obtained after 99 iterations

Table 4.7

Evaluation of VLE Objective Function from Regression Results of Isothermal Ethanol-Benzene (VLE) System

System: (1) Ethanol - (2) Benzene   Condition: T = 40 C

Gamma Model: Modified UNIQUAC   Phi Model: Virial EOS

Reference: Udovenko, V.V.,et al. (1952)   No. of data points = 11

Case No.	VLEFN #	$P_{exp}-P_{cal}$ in mm Hg		$Y_{1exp}-Y_{1cal}$ in mole %		Inf. Dilution Activity Coeff	
		Mean	Max	Mean	Max	(1)	(2)
09A	7	1.55	3.25	0.358	0.819	15.371	4.973
09B	8	2.34	4.70	0.394	1.065	15.218	5.115
09C	9	2.46	4.90	0.406	1.128	15.194	5.136
09D	10	0.88	2.02	0.404	2.020	14.817	4.863
09E*	11	1.28	2.94	0.371	0.854	15.031	4.948
09F	12	1.37	3.15	0.376	0.825	15.002	4.969
09G	13	0.84	1.88	0.436	1.066	15.092	4.798
09H	15	0.83	1.89	0.442	1.075	15.028	4.792
09I	16	0.83	1.89	0.441	1.073	15.020	4.793

Note: '*' shows unconverged case after 99 iterations on the mean percentage relative difference of experimental and calculated component mole fractions in each of the two liquid phases. Results with the benzene-water system at 25°C are summarized in the Table 4.8. However the results of estimated and assessed parameters for benzene-water LLE system at 25, 35, and 75°C are reported in Appendix E.2.

The Series 22 cases shown in the Table 4.8, for the water-benzene system, show that function consisting of the difference in mole fractions (LLEFN # 5) correlates poorly. LLEFN # 8 from the group of functions based on only x_i's (LLEFN # 6, 7, and 8) was observed to yield superior results. From the group of functions (LLEFN # 9, 10, and 11) based on x_i's and the distribution coefficients, function 11 predicted better results. Therefore, two of the objective functions, LLEFN # 8 and 11, were selected for the further study. Function # 11 was expected to be more suitable for the multicomponent system, in which the distribution coefficient of only the solute (ethanol) was considered along with the x_i's. The region of ternary liquid-liquid phase separation in the decanter, Fig. 6.6, exists near to the plait point.

4.4.2 Regression Results, Including Discussion of Proper Root Selection

Marquardt's algorithm has the tendency to yield a local minima instead of a global minima. Therefore, the final estimated parameters are extremly sensitive to the initial estimate of the parameter values. This was clearly

Table4.8

Evaluation of LLE Objective Function from Regression Results of Benzene-Water (LLE) System at 25 C

System: (1) Benzene - (2) Water Condition: T = 25 C

Gamma Model: Modified UNIQUAC

Data reference: Polak, J. (1973) No. of data points = 1

Case No.	LLEFN #	Phase Rich in (1) Mean % Rel. X Diff.*		Phase Rich in (2) Mean % Rel. X Diff.*	
		(1)	(2)	(1)	(2)
22V	5	0.1890E-1	8.3530E+0	2.7090E+0	0.1120E-2
22BB	6	0.2390E-3	0.1053E+0	0.1422E+0	0.5960E-4
22CC	7	0.0000E+0	0.1750E-3	0.4472E+0	0.1850E-3
22Y	8	0.1255E-3	0.5621E-1	0.1337E+0	0.5963E-4
22M	9	4.9980E+1	0.2207E+5	1.0000E+2	1.0000E+2
22T	10	0.1595E-2	0.7025E+0	0.7315E+0	0.3000E-3
22Z	11	0.3920E-2	1.7350E+0	1.1290E+0	0.4711E-3

* $(X_{iexp}-X_{ical})/X_{iexp}*100$

demonstrated by starting the regressions with initial parameter values ranging from -3000 to 3000 $^{\circ}K$ in the normal x-y plane of reference. The parameter values ranging of -3000 to 3000 are the extreme possible values for a wide variety of systems. Evaluation of estimated parameters was done on the basis of their capability to correlate the experimental VLE/LLE data.

Selected results compiled in the Tables 4.9 and 4.10 for the ethanol-water (VLE) and the benzene-water (LLE) systems show different final values for the binary interaction parameters. A wide range of final parameter values may also be observed in all of the binary data regression cases reported in Tables E.1.1 to E.2.4. One way to eliminate the erroneous roots is to compare the estimated VLE or LLE results with that of the experimental data. In all of the binary systems (ethanol-water, ethanol-benzene and benzene-water) studied, the initial parameter values near unity have been found as the most reliable place to initiate the Marquardt non-linear regression algorithm.

The binary VLE results shown in the Tables 4.9-4.10 and in Appendices E.1 thru E.2 were evaluated using pressure or temperature, vapor phase compositions and infinite dilution activity coefficients. The LLE results were evaluated using component values in both the liquid phases. Hence, the parameter values can be safely located in the global minima region based on its capability to produce the targeted profile(s).

Table 4.9

Multiple Roots Illustration with Isobaric Ethanol-Water (VLE) System

System: (1) Ethanol - (2) Water	Condition: P = 760 mm Hg
Gamma Model: Modified UNIQUAC	Phi Model: Virial EOS
Data reference: Reider, R.M.,et al. (1949)	No. of data points = 34

Case No.	VLE -FN #	Interaction Parameters, ^{o}K Initial		Final		ΔT ^{o}C	Δy_1 mol %	γ^{∞}	
		A_{12}	A_{21}	A_{12}	A_{21}	Mean	Mean	(1)	(2)
04G	21	1	1	-50.48	342.07	0.13	0.883	5.299	2.508
04H	21	500	500	-54.12	347.85	0.13	0.879	6.580	2.490
04I	21	-500	500	-55.88	349.86	0.13	0.865	5.319	2.490
04J	21	500	-500	-55.43	349.03	0.13	0.864	5.315	2.491
04K	21	-500	-500	-50.82	342.21	0.13	0.877	5.295	2.506
04L	21	3000	3000	-361.09	9963.07	3.00	6.987	-	1.515
04M	21	-3000	3000	-361.09	9100.83	3.00	6.987	-	1.515
04N	21	3000	-3000	8070.10	-206.88	1.48	3.648	3.625	-
04O	21	-3000	-3000	-57.02	351.70	0.14	0.864	5.326	2.487

Note: '-' shows very high calculated values

Table 4.10

Multiple Roots Illustration with Benzene-Water (LLE) System at 25°C

System: (1) Benzene - (2) Water Condition: T = 25 C

Gamma Model: Modified UNIQUAC LLEFN # 8

Data reference: Sorensen, et al. (1979) No. of data points = 1

Case No.	Interaction Parameter, °K Initial		Final		Phase Rich in 1 Mean % X Diff.*		Phase Rich in 2 Mean % X Diff.*	
	A_{12}	A_{21}	A_{12}	A_{21}	(1)	(2)	(1)	(2)
23A	1	1	392.17	424.59	6.27E+0	2.08E+3	1.27E+0	0.51E-3
23B	100	100	1332.69	354.44	0.42E-2	1.40E+0	1.48E+0	0.60E-3
23C	200	200	1335.51	354.21	0.69E-2	2.30E+0	1.65E+0	0.66E-3
23D	200	-200	1216.70	5192.00	0.41E-2	1.35E+0	1.00E+2	0.40E-1
23E	-200	-200	-145.93	-286.40	4.93E+1	0.16E+5	0.12E+6	4.92E+1
23F	300	300	1325.14	355.17	0.31E-2	1.04E+0	0.95E+0	0.38E-3
23G	500	500	221.37	482.87	1.10E+1	3.64E+3	0.39E-2	0.00E+0
23H	-500	500	-287.84	1150.50	5.00E+1	0.12E+5	1.34E+0	0.54E-3
23I	500	200	1327.85	356.37	0.78E-4	0.25E-4	0.55E-1	0.29E-4
23J	1000	1000	1326.61	356.80	0.10E-2	0.34E+0	0.40E+0	0.16E-3
23K	1000	200	1326.94	356.69	0.72E-3	0.24E+0	0.31E+0	0.13E-3
23L	3000	3000	1217.13	9032.94	0.36E-2	1.20E+0	1.00E+2	0.41E-1

* $(X_{iexp}-X_{ical})/X_{iexp}*100$

4.5 Multicomponent VLE and LLE data Regression Results

Regression analysis of multicomponent experimental data was grouped into three categories:

A. Ternary ethanol-water-benzene VLE system (Case Series 03)

B. Combination of ethanol-water and ethanol-benzene binaries with ternary VLE data (Case Series 70-74)

C. Ethanol-water-benzene LLE system (Case Series 21).

Results from each of these Case Series are tabulated in the Tables 4.11 - 4.13.

Category A

Each of the three VLE cases, 03A, 03B, and 03C, were initiated with parameter values obtained from the regression of the respective binaries that are reported in the Table 4.11. It should be noted that benzene-water binary is a partially miscible system. Case 03C (Table 4.11) produced the best results in terms of vapor phase compositions, mean deviations of 0.33 C in T, 1.2 mole % in y_1 (ethanol), and 2.6 mole % in y_2 (water) were recorded.

The regression of ternary VLE data starting with the results obtained from the respective binary regression would be the safest and the best move to avoid local minimas. The prediction of ternary VLE at 760 mm Hg using with parameters (Case 03X) obtained from only binaries was poor in terms of both T and y_i's.

Category B

Significant improvement was recorded in the cases with

Table 4.11

Regression Results of Ethanol-Water-Benzene (VLE) System

System: (1) EtOH - (2) Water (3) Bz Condition: P = 760 mmHg

Gamma Model: Modified UNIQUAC Phi Model: Virial EOS

Data Reference: Hands, C.H.G., et al. (1945)

Data set: Ethanol-Water-Benzene (VLE, 760 mmHg)

Case #	Mean β (Max) T and Y's		
	dev** in T deg C	dev** in mole% Y1	Y2
03A*	0.28 (0.91)	2.101 (7.140)	3.324 (6.054)
03B#	0.29 (0.83)	1.953 (6.790)	3.296 (6.001)
03C+	0.33 (0.83)	1.242 (3.601)	2.597 (5.234)
03X+	4.65 (11.58)	7.007 (14.127)	5.370 (5.234)

Initial Binary Interaction Parameters in deg K

*	1.0	1.0	1.0	1.0	1.0	1.0
#	-57.02	351.70	-151.47	961.51	1.0	1.0
+	-57.02	351.70	-151.47	961.51	375.24	892.72

** dev in T = $(T_{exp}-T_{cal})$ and dev in Y_i = $(Y_{iexp}-Y_{ical})*100$

combined regression of binary and ternary data and the results are presented in Table 4.12. The best results were obtained when complete datasets of two miscible binaries (ethanol-water, ethanol-benzene) and a partial set of ternary dataset were regressed together. Case 74A shown in Table 4.12 has no more than 0.14 °C mean deviation in temperature and 0.87 mole % mean deviation in vapor phase mole fraction for binary as well as ternary VLE system. It was observed in section 4.4 that the UNIQUAC activity coefficient model is more sensitive to initial initialization in LLE data regression than in VLE data regression. The strategy, of initiating the computation from the parameter values obtained from respective binaries, discussed earlier was found to be unsatisfactory in the ternary liquid-liquid data regression.

Category C

Cases falling in the category of LLE experimental data regression are reported in Table 4.13. Case 21A, with starting values of unity, did not converge and Case 21C with starting values from respective binaries lead to a poor correlation. Out of three correlation cases, Case 21B yielded the best results with overall mean difference in experiment and calculated composition of 0.6638 mole % and with mean difference of solute distribution ratio of 0.0502. The detailed results corresponding to multicomponent regression analysis are reported in Appendix E.3 and E.4.

Table 4.12

Regression Results of Combinations of Isobaric Binary and Ternary VLE System

System: (1) EtOH - (2) Water - (3) Bz Condition: P=760 mm Hg

Gamma Model: Modified UNIQUAC Phi Model: Virial EOS

Data Sets and References:

(a) EtOH-Water, Reider, R.M., et al. (1949)

(b) EtOH-Bz, Tyrer, D., (1912)

(c) EtOH-Wtr-Bz, Hands, C.H.G., et al. (1945)

Case #	Mean & (Max) Abs (Te-Tc) deg C			Mean Abs. diff. in mole % Y_1			Y_2	Data Sets used in the Regression
	System			System			System	
	(a)	(b)	(c)	(a)	(b)	(c)	(c)	
70A	0.14	0.45	0.55	0.920	1.391	1.620	1.881	a + b + c
71A	-	0.48	0.33	-	2.316	1.218	2.596	b + c
72A	-	0.12	0.49	-	0.594	1.818	2.300	b(x4) + c
73A	0.14	0.12	0.62	0.931	0.586	1.819	1.820	a + b(x4)
74A	0.14	0.12	0.14	0.874	0.572	0.274	0.610	a + b + c (partial)

Note: '-' means system not included in the regression

Table 4.13

Regression Results of Ethanol-Water-Benzene (LLE) System

System: (1) EtOH - (2) Water - (3) Bz Condition: T = 35 C

Gamma Model: Modified UNIQUAC

Data set: Ethanol-Water-Benzene (LLE, 35 C)

Data Reference: Moracheskii, A.G., et. al. (1958)

Case #	Diff.+ of compositions in mole %, Mean							Mean diff of d. ratio
	Phase Rich in (3)			Phase Rich in (2)			over-	
	(1)	(2)	(3)	(1)	(2)	(3)	all	(1)
21B	0.693	0.634	0.519	0.707	0.983	0.449	0.664	0.050
21C	1.755	3.605	4.718	1.047	2.295	1.248	2.445	0.090

Case #	Initial Binary Interaction Parameters in deg K					
	A_{12}	A_{21}	A_{13}	A_{31}	A_{23}	A_{32}
21A*	1.0	1.0	1.0	1.0	1.0	1.0
21B	1.0	1.0	1.0	1.0	375.24	892.72
21C	-19.16	272.65	-121.87	1017.74	375.24	892.72

* unconverged case

\+ Difference = $(X_{iexp}-X_{ical})/X_{iexp}*100$

4.6 Global Thermodynamic Parameters Estimation

With the VLE and LLE data regression procedure established, simultaneous regression of VLE and LLE data was initiated. Various cases and variables are explained in Table 4.14. Each of the series has one or more cases, depending on the value of weight constant 'W'. Each of the cases listed in Table 4.14 has preselected VLE and LLE objective functions, two or more different data sets, and inclusion on either only one tie line or all the tie lines in the ternary ethanol-water-benzene liquid-liquid equilibria experimental datasets. In the 'one-tie-line' cases, the third tie line from the plait point in the data reported by Morachevskii (1958) was included in the regression. This was decided based on the approximately known operating region of the decanter shown in Fig. 6.6.

4.6.1 Results of Simultaneous VLE and LLE data Regression

Fifty one different cases have been extensively investigated and reported in Appendix E.5. For each of the cases estimated parameters have been evaluated based on its prediction of binary VLE, ternary VLE, and ternary LLE. The results can broadly divided into four Groups as shown in the Table 4.14.

Group I

Results of Group I, obtained from isobaric binary VLE and ternary LLE data, are summarized in Tables E.5.1A to E.5.1C (Appendix E.5). In 'one-tie-line' cases, 40A and 40B, increase in weight constant (W) improves the ternary VLE

Table 4.14

Simultaneous VLE and LLE Data Regression Cases and Variables

Case series	# of cases	Data sets used for regression	# of tie lines	VLEFN	LLEFN	Variable
Group I						
40	2	a + b + g	1	21	8	W
41	5	a + b + g	All	21	8	W
42	3	a + b + g	1	21	11	W
43	5	a + b + g	All	21	11	W
Group II						
46	4	c + d + g	1	9	8	W
47	4	c + d + g	All	9	8	W
48	4	c + d + g	1	9	11	W
49	4	c + d + g	All	9	11	W
Group III						
50	3	c + d + g	1	10	8	W
51	3	c + d + g	All	10	8	W
52	4	c + d + g	1	10	11	W
53	4	c + d + g	All	10	11	W

Table 4.14 (Contd)

Simultaneous VLE and LLE Data Regression Cases and Variables

Case series	# of cases	Data sets used for regression	# of tie lines	VLEFN	LLEFN	Variable
Group IV						
60	3	a + b + f + g	All	21	11	W
61	1	e + f	All	21	11	W
63	1	a + b + e + f	All	21	11	W
66	1	f + g	All	21	11	W

Total 51 cases

Where

a.	ethanol-water,	VLE, P=760 mm Hg	Ref.:	Reider	(1949)
b.	ethanol-bz,	VLE, P=760 mm Hg	Ref.:	Tyrer	(1912)
c.	ethanol-water,	VLE, T=40 C	Ref.:	Mertl	(1972)
d.	ethanol-bz,	VLE, T=40 C	Ref.:	Udovenko	(1952)
e.	water-benzene,	LLE, T=35 C	Ref.:	Sorensen	(1979)
f.	etoh-wtr-bz,	VLE, P=760 mm Hg	Ref.:	Hands	(1945)
g.	etoh-wtr-bz,	LLE, T=35 C	Ref.:	Morachevskii	(1958)

prediction but increases deviations in the liquid phase compositions in the ternary LLE prediction. In the other 'one-tie-line' cases, 42A, 42B, and 42C, (with LLEFN # 11) the increase in weight constant (W) from 0 to 100 improves VLE and LLE fits. Increase in weight constant above that is not desirable. Regression of all the tie lines instead of one improves the LLE predictions, but introduce large errors in VLE, specially for ternary systems. Cases 41D and 41E show significant improvement in the overall mean difference in experimental and calculated compositions and solute distribution ratio. Cases 43C and 43F show that a weight value (W) of the order of 80-100 yield better results.

Group II

In Group II isobaric binary VLE at 760 mm Hg is replaced with isothermal binary VLE data at 40 C, which in fact introduced large errors in prediction of isobaric ternary VLE in 'one tie line' cases 46A to 46D. Temperature extrapolation has much greater impact on the prediction of liquid-liquid equilibria as compared to that on the prediction of vapor-liquid equilibria. Based on the temperature in the distillate drum (Fig. 6.1) of 35 ^{0}C, recommended by Tsai (1982), the isothermal VLE data available around this temperature was taken into account.

Increase in the weight constant in these cases improves the LLE fit in the region away from plait point. Changing in the LLEFN # 8 to # 11, case series 48, does not improve VLE and LLE fits. Regression of all the tie lines, significantly improves the LLE prediction. Cases 47D and 49B show overall mean deviation of about 1 mole % in x's and mean deviation of 0.05 in solute distribution coefficient. Increase in weight from 0 to 45 significantly improves LLE fit for cases (47 series) with LLEFN # 8. The estimated parameters, mean and maximum deviations in P's and y's for VLE systems, and mean and max deviations in x's and distribution ratio of solute (ethanol) for the cases 46 to 49 are reported in Table E.5.3.

Group III

The cases (46-49) in Group II, possess large deviations in binary as well as ternary VLE predictions, hence VLEFN # 9 was replaced with VLEFN # 10 in the Group III category. Group III category incorporates cases 51 thru 53, which are reported with complete details in Appendix E.5. An improvement in binary VLE fit is observed in the Group III cases as compared to the Group II cases but ternary VLE prediction is similar in both the Groups II and III. Inclusion of 'all-the-tie-lines' in the regression analysis introduce large errors in the VLE fit. Cases 51C and 53D show very good LLE results but poor VLE prediction.

The results with isobaric VLE data regression is better than that of isothermal VLE data, in simultaneous VLE and LLE data regression. The developed regression software, discussed in Section 4.2, is not capable of simultaneous regression of isothermal and isobaric VLE data.

Group IV

Further study, falling in Group IV category, was continued with combination of different data sets consisting of isobaric binary and ternary VLE as well as isothermal binary and ternary LLE experimental data. The resulting Cases 60 thru 66 are reported in Table E.4. Inclusion of isothermal ternary VLE with isothermal binary VLE and ternary LLE improve the parameters significantly for binary and ternary VLE prediction, but at the cost of LLE correlation.

Cases 60A to 60D also show that increase in weight constant (W) improves LLE fit at the cost of VLE fit. Regression of only ternary VLE data with binary LLE data (Case 61A) or ternary LLE (Case 66A) data yield absolutely unacceptable LLE results though ternary VLE fit was very good. On the other hand binary and ternary VLE data with binary LLE data (Case 63A), give mean temperature deviation of 0.52 ^{o}C for ternary VLE and deviation in y_i's of the order of 1 mole %, while overall mean deviation in LLE x_i's was 5.25 mole %. This shows that different combinations of binary and ternary, VLE and LLE, data (Group IV) could produce the parameters which are unsatisfactory for ternary LLE predictions. The best case in this Group IV is Case 63A.

The evaluation of the parameters was being made on the basis of comparison with experimental data reported in the literature, shown in Table 4.3. The final set of parameters may be global only if that set can represent temperature and composition profiles in the azeotropic tower, and the phase compositions in the distillate drum. This is important because the available complete set of ternary VLE data covers a wider range of temperature and liquid phase compositions than that existing in the real operating column. Thus the following section presents the performance of parameters in the real process environment and concluding remarks on the thermodynamic analysis of VLE and LLE data for the specific system of ethanol-water-benzene.

4.7 Conclusions Based on Separation Performance in the Key Process Operations

The testing of parameters in the two key process units, the azeotropic distillation column and the two liquid phase decanter, would qualify the set(s) to be used in the complete process plant. The parameters obtained only from ternary VLE data regression (Case series 03) fail in the distillation column. This may be attributed to the fact that column operating range is part of the experimental data published by Hands et al. (1945). The estimated distillate rate, overhead vapor, and bottoms composition in the azeotropic tower for the converged cases are reported the Table 4.15.

The estimated liquid phase split and two liquid phase compositions in the liquid-liquid phase decanter for all the converged cases, are summarized in the Table 4.16. Table 4.17 is part of Table 4.16 in which the overall mean difference in phase compositions and the phase distribution factor are listed. It should be noted that the results of this section were obtained only after establishing the process equipment operating conditions discussed extensively

Table 4.15

Performance of Azeotropic Column with Various Sets of Modified UNIQUAC Parameters

Major fixed conditions

Stream	Rate lbmole/hr	Composition in mole % Ethanol	Water	Benzene
Entrainer(E)	279.5856	28.104	11.771	60.125
Feed (F)	115.1506	82.820	17.180	0.0

Case #	Dist Rate (D)	% Diff of D *	Distillate Comp.			Bottoms Composition		
			EtOH	Wtr	Bz	EtOH	Wtr	Bz
03X	315.75	1.61	30.251	16.688	53.061	99.292	0.31E-10	0.708
21B	298.67	3.88	38.221	5.947	55.833	66.200	36.316	1.484
21C	310.00	0.24	29.009	16.998	53.993	99.146	0.43E-07	0.854
21X	318.38	2.46	30.872	16.550	52.578	99.082	0.90E-14	0.918
40A	313.41	0.86	29.810	16.813	53.378	99.007	0.15E-12	0.994
40B	317.75	2.26	30.478	16.585	52.937	99.996	0.65E-03	0.003
41A	314.35	1.16	30.017	16.762	53.221	99.005	0.97E-14	0.995
41D	317.88	2.30	25.842	18.547	55.611	99.589	0.59E-07	0.411
42A	313.10	0.76	29.681	16.830	53.489	99.233	0.96E-12	0.767
42D	313.10	0.76	29.700	16.830	53.470	99.160	0.42E-12	0.840
43B	310.62	0.04	29.175	16.964	53.862	99.054	0.13E-13	0.946

Table 4.15 (Contd)

Performance of Azeotropic Column with Various Sets of Modified UNIQUAC Parameters

Major fixed conditions

Stream	Rate	Composition in mole %		
	lbmole/hr	Ethanol	Water	Benzene
Entrainer(E)	279.5856	28.104	11.771	60.125
Feed (F)	115.1506	82.820	17.180	0.0

Case #	Dist Rate (D)	% Diff of D *	Distillate Comp.			Bottoms Composition		
			EtOH	Wtr	Bz	EtOH	Wtr	Bz
43C	310.15	0.19	29.066	16.989	53.945	99.068	0.17E-11	0.932
43D	301.80	2.88	26.891	17.452	55.658	99.946	0.94E-08	0.054
43E	310.46	0.09	29.130	16.972	53.898	99.090	0.40E-14	0.911
43F	307.15	1.16	28.393	17.155	54.452	99.030	0.27E-12	0.970
47A	310.46	0.09	29.139	16.972	53.889	99.058	0.31E-13	0.942
49A	306.18	1.47	28.169	17.210	54.621	99.026	0.15E-10	0.974
50C	311.55	0.26	29.379	16.913	53.707	99.071	0.30E-12	0.929
53A	313.25	0.81	29.755	16.821	53.424	99.084	0.80E-09	0.916
53B	310.00	0.24	28.986	16.998	54.016	99.232	0.40E-13	0.768

Note: * is the absolute difference of distillate rates as compared to that predicted by the NRTL equation.

Table 4.16

Performance of Two Liquid Phase Decanter at 35 ^{o}C with Various Sets of Modified UNIQUAC Parameters-I

Major fixed conditions

Feed Composition in mole %			Temperature
Ethanol	Water	Benzene	deg C
29.00	17.00	54.00	35

Case #	Fracl (λ)	% Diff in λ *	Benzene Phase			Water Phase		
			EtOH	Wtr	Bz	EtOH	Wtr	Bz
NRTL	0.8811	0.0	28.104	11.771	60.125	35.785	55.626	8.589
03X	0.8396	4.71	28.666	7.330	64.004	30.749	67.617	1.635
21C	0.8456	4.03	28.451	8.031	63.519	32.017	66.114	1.870
21X	0.7519	14.66	24.076	5.494	70.430	43.907	51.858	4.235
40A	0.8252	6.34	27.904	7.366	64.731	34.195	62.432	3.373
40B	0.8155	7.44	27.346	7.422	65.232	36.313	59.356	4.333
41A	0.8124	7.80	27.634	6.633	65.733	34.897	61.888	3.215
42A	0.8305	5.74	27.925	7.821	64.253	34.250	61.948	3.802
42D	0.8257	6.29	27.879	7.507	64.614	34.311	61.972	3.717
43B	0.8199	7.85	27.810	6.330	65.860	34.130	63.073	2.797
43C	0.7947	9.81	26.817	6.173	67.010	37.451	58.912	3.636
43D	0.8410	4.55	28.465	7.777	63.765	31.834	65.794	2.372

Table4.16 (Contd)

Performance of Two Liquid Phase Decanter at 35 °C with Various Sets of Modified UNIQUAC Parameters -I

Major fixed conditions

Feed Composition in mole %			Temperature
Ethanol	Water	Benzene	deg C
29.00	17.00	54.00	35

Case #	Fracl % (λ)	Diff in λ *	Benzene Phase EtOH	Wtr	Bz	Water Phase EtOH	Wtr	Bz
43E	0.8147	7.54	27.912	6.424	65.664	33.790	63.492	2.718
43F	0.8166	7.32	27.806	6.726	65.469	34.330	62.796	2.875
47A	0.8050	8.64	27.297	6.686	66.018	36.041	59.591	4.368
49A	0.8200	6.93	27.600	7.205	65.195	35.401	61.567	3.032
50C	0.8126	7.77	27.175	7.023	65.802	36.910	60.232	2.858
53A	0.8244	6.44	27.989	6.944	65.068	33.751	64.198	2.051
53B	0.8175	7.26	28.094	6.334	65.572	33.047	64.626	2.327

Note: * is the absolute difference of the distillate rates as compared to that predicted by the NRTL equation.

Table 4.17

Performance of Two Liquid Decanter with Various Sets of Modified UNIQUAC Parameters -II

NRTL parameters (Sorensen, 1979) as the basis of comparison

Parameters from case #	Absolute difference in λ	Overall mean diff. in phase comp. in mole %
03X	0.0415	5.4772
21C	0.0354	4.7427
21X	0.1292	6.1423
40A	0.0559	3.8038
40B	0.0665	3.1213
41A	0.0687	3.9567
41D	0.3287	20.6315
42A	0.0505	3.4835
42D	0.0554	3.6117
43B	0.0692	4.3940
43C	0.0863	3.9458
43D	0.0401	4.7218
43E	0.0664	4.4683
43F	0.0644	4.1710
47A	0.0761	3.3712

Table 4.17 (Contd)

Performance of Two Liquid Decanter with Various Sets of Modified UNIQUAC Parameters-II

NRTL parameters (Sorensen, 1979) as the basis of comparison

Parameters from case #	Absolute difference in λ	Overall mean diff. in phase comp. in mole %
49A	0.0611	3.6703
50C	0.0685	3.8027
53A	0.0567	4.5048
53B	0.0640	4.8157

Where λ = moles of light phase/total moles in both phases in Chapters 5 and 6.

The Cases 03X and 21X show that parameters obtained from only binary data predict good column composition profiles. The column profiles of each of the case are compared with that estimated by NRTL parameters obtained from ternary VLE data reported by Gmehling et al. (1977). The two basic requirements of column profile are, existence of overhead vapor composition, after condensation to 35 °C, in the two liquid phase region, and at the same time high purity alcohol (ethanol) with parts per million of water and small amount of benzene as the bottoms product. The Cases 03X and 21X give large error in the prediction of tie line compositions.

The performance of some of the parameters obtained from the simultaneous regression of binary VLE data and ternary LLE data show acceptable results in both process operations. Table 4.18 shows all the successful cases in the azeotropic column, and the two liquid phase decanter. The cut-off overall mean difference in phase compositions in the two liquid phase decanter was considered to be 4.0 mole %. The best results are observed in Case 40B, which has overall mean difference in composition of 3.12 mole % as compared to that with NRTL parameters. This may be attributed to the fact that only one tie line near to the drum operating conditions was regressed. The best case (40B) in both the process units, showed improvement by 43.01 % (case 03X), 34.19 % (case 21C), and 49.18 % (case 21X) in terms of

Table 4.18

List of Acceptable Parameters for Azeotropic Distillation Column and Decanter

Case Series #	Acceptable Cases for		
	Column	Decanter	Column&Decanter
03	03X	-	-
21	21C,21X	-	-
40	40A,40B	40A,40B	40A,40B
41	41A,41D	41A	41A
42	42A,42D	42A,42D	42A,42D
43	43B,43C,43D 43E,43F	43C	43C
46	-	-	-
47	47A	47A	47A
48	-	-	-
49	49A	49A	49A
50	50C	50C	50C
51	-	-	-
52	-	-	-
53	53A,53B	-	-

overall mean difference in composition. Hence the global set of modified UNIQUAC parameters (deg K) for (1) ethanol - (2) water - (3) benzene azeotropic distillation process is the following:

$A_{12} = -46.98$ $A_{21} = 336.04$ $A_{13} = -133.65$ $A_{31} = 890.55$

$A_{23} = 187.00$ $A_{32} = 1249.35$

CHAPTER 5

STUDY OF PROCESS VARIABLES IN AZEOTROPIC DISTILLATION COLUMN

The ethanol-water-benzene azeotropic distillation column operates under very restricted conditions. The desirable bottoms product is very high purity alcohol with no more than a few parts per million (ppm) of water and minimal amount of entrainer. Benzene was selected as a potential entrainer for the detailed study of each of the process units as well as for process plant simulation because of availability of ternary VLE and LLE experimental data. A detailed research study of ethanol dehydration with various entrainers was presented in Chapter 2.

The overhead vapor product has two major constraints: firstly, the ternary azeotropic composition, and secondly the overhead vapor after condensation (at $95^{o}F$) must form two liquid phases. The phase separation phenomena in the decanter drives water out of the system and makes the azeotropic distillation process eligible for water removal from alcohol feeds that have been concentrated. This raw alcohol-water feed from biomass processes contains about 3.2 mole % (7.79 wt. %) alcohol, and is concentrated near the azeotropic composition.

The major process variables which have an impact on the azeotropic column are:

a. Ethanol-water feed concentration

b. Entrainer composition

c. Entrainer to feed rate ratio

d. Entrainer entry location

e. Feed entry location

f. Vapor distillate or bottoms product rate

g. Column pressure

Tsai (1982) has reported N (top stage) and N-3 as the suitable entrainer and feed entry locations for an N stage column. In the subsequent subsections the effect of ethanol-water feed concentration, entrainer rate, and vapor distillate rate have been studied in detail. The investigation was carried out in an atmospheric column. The effect of operating pressure was not incorporated in this research work.

5.1 Effect of Distillate Rate and Multiplicity of Solutions

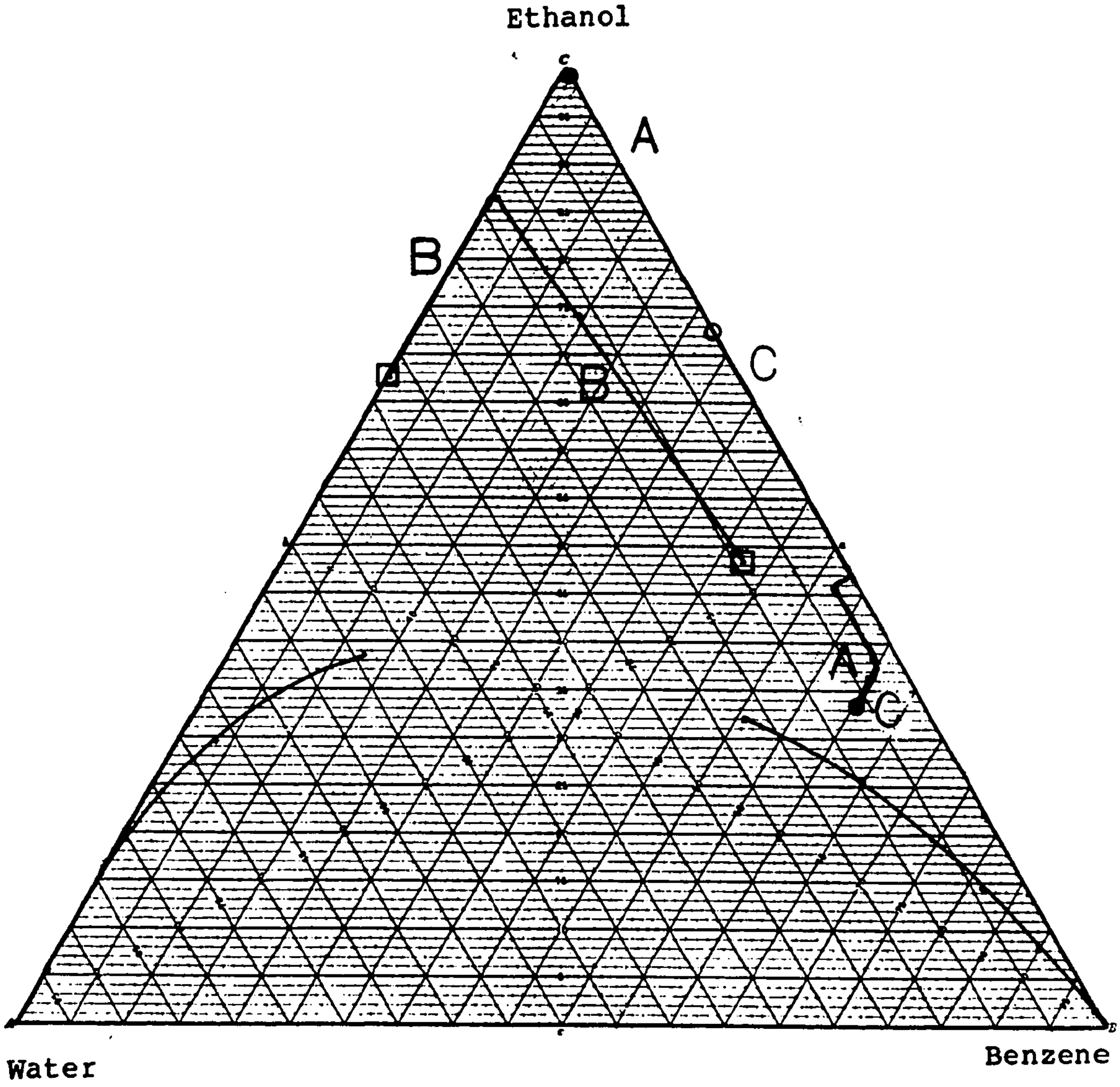
Since there are no side streams in the azeotropic column, an increase in the distillate rate results in a corresponding decrease the bottoms product rate. System description of the ACTL block, introduced in PROSIM, has been previously discussed (Chapter 2.4). PROSIM (PROcess SIMulator) is an improved version of Chemical Engineering Simulation System (CHESS). The necessity of such a control block arose from the fact of multiplicity of solutions. Distillation calculations are repeated by the ACTL block until the column profile is in the desired region and the bottoms product specifications are met.

The solutions fall in the region A, B or C as shown in the Fig. 5.1. The profile A leads to the correct solution consisting of traces of water and small amount of entrainer in the ethanol product. The profile B dumps lots of water in the product, and profile C shows large quantity of entrainer in the dry alcohol. The computational procedure, discussed in the system description of ACTL, forces the distillation column into the desired operational region.

The results presented in Table 5.1 are for an 85 mole % ethanol feed, and entrainer to feed ratio of 6.6098. On one hand, high distillate rate (distillate to total feed ratio of 0.9336) predicts too wet an ethanol product as bottoms, and places the overhead vapor composition outside of the two liquid phase envelope. On the other hand, low distillate rate produces alcohol product with large amounts of entrainer as an impurity. It is evident from the investigation that only a small range of distillate or bottoms rates are permitted for the column operation in the proper region.

5.2 Effect of Entrainer Rate on the Azeotropic Column

The entrainer feed stream enters at the top stage of the main column. The entrainer feed rate and composition has significant impact on the column performance. A study of the effect of entrainer rate on the column temperature and concentration profiles was conducted. The entrainer rate was changed in each run by maintaining constant ethanol-water feed conditions and bottoms rate. A new block, ECTL, introduced in the simulator treats the entrainer rate as an



Curve A: Dry and pure ethanol as bottoms (correct solution)
Curve B: Wet ethanol as bottoms (incorrect solution)
Curve C: Dry ethanol with excess benzene (incorrect solution)
Curves A, B & C are liquid phase composition profiles of the azeotropic distillation column.

Fig. 5.1 Multiple Solutions in the Azeotropic Column

Table 5.1

Effect of Vapor Distillate Rate on Azeotropic Column

Major fixed conditions

Stream	Rate lbmole/hr	Composition in mole %		
		Ethanol	Water	Benzene
Entrainer(E)	698.9380	28.104	11.771	60.125
Feed(F)	115.1506	85.0	15.0	0.0

Entrainer/Feed Rate Ratio = 698.938/115.1506 = 6.0698

Cas #	Dist Rate	$\frac{D}{E+F}$ Ratio	Distillate Comp.			Bottoms Composition		
			EtOH	Wtr	Bz	EtOH	Wtr	Bz
2C1	760.0	0.9336	35.196	13.494	51.309	66.178	33.822	0.0
2C2	684.0	0.8402	28.230	17.668	54.102	84.710	0.259E-5	15.290
2C3	694.3	0.8528	28.504	17.407	54.089	87.958	0.167E-5	12.042
2C4	704.7	0.8656	28.786	17.150	54.064	91.799	0.114E-5	8.201
2C5	708.2	0.8699	28.873	17.065	54.063	93.315	0.104E-5	6.685
2C6	711.7	0.8743	28.958	16.980	54.062	94.949	0.976E-6	5.051
2C7	715.3	0.8786	29.038	16.895	54.067	96.748	0.978E-6	3.252
2C8	718.9	0.8830	29.125	16.811	54.064	98.635	0.113E-5	1.365

Note: All the rates and compositions are in lbmoles/hr and mole % respectively.

D is the column vapor product rate

independent manipulative variable. The system description of the ECTL block is presented in the Section 2.4. Results compiled in Table 5.2 show that low bottoms rates as well as high entrainer rates are favorable for the production of dry ethanol within specifications, but overhead vapor composition tend to go towards the phase boundary. High bottoms rates and low entrainer rates tend to predict distillate compositions within the two liquid phase envelope, but at the cost of bottoms specifications. Excess entrainer (benzene) in the alcohol product requires a unidirectional decrease in the entrainer feed rate until the bottoms specifications are met.

Hence, the entrainer to feed rate ratio of approximately 2.8 and an associated bottoms rate of 79.0 lbmoles/hr make the column operate in the proper region for the 80 mole % ethanol feed and constant entrainer composition. Case 3C2, in Table 5.2 using a 60 stage column, demonstrates the requirement of additional theoretical stages for the production of drier alcohol in the case of binary feed compositions nearer to the azeotrope. Tables 5.3 and 5.4 summarize the overhead vapor and bottoms composition for 83 and 85 mole % ethanol feeds respectively. These results also illustrate the requirement of additional separation stages discussed earlier. Further investigation was conducted with a tall column with 80 stages because it can handle large range of aqueous alcohol feed compositions. The study shows that the sensitivity of the entrainer requirement is more in the case of fresh feed with higher ethanol concentration.

Table 5.2

Effect of Entrainer/Feed Rate Ratio on Azeotropic Column - I

Major fixed conditions

Stream	Rate	Composition in mole %		
	lbmole/hr	Ethanol	Water	Benzene
Entrainer(E)		28.104	11.771	60.125
Feed(F)	115.1506	80.0	20.0	0.0

#	Btms Rate	$\frac{E}{F}$ Ratio	Distillate Comp.			Bottoms Composition		
			EtOH	Wtr	Bz	EtOH	Wtr	Bz
3C1	78.0	2.8452	29.295	16.886	53.859	99.331	0.103E-3	0.669
3C2	79.0	2.8000	29.135	17.007	53.858	99.070	0.130E-5	0.930
3C3	80.0	2.6855	28.886	17.257	53.857	99.434	0.319E-3	0.565
3C4	82.0	2.5348	28.510	17.656	53.835	99.372	0.103E-2	0.627
3C5	85.0	2.3447	27.902	18.259	53.839	99.120	0.109E-1	0.869

Note: All the rates and compositions are in lbmoles/hr and mole % respectively.

means the Case number

No. of stages = 60 in case # 3C2

No. of stages = 40 in all other cases

Table 5.3

Effect of Entrainer/Feed Rate Ratio on Azeotropic Column - II

Major fixed conditions

Stream	Rate lbmole/hr	Composition in mole % Ethanol	 Water	 Benzene
Entrainer(E)		28.104	11.771	60.125
Feed(F)	115.1506	83.0	17.0	0.0

#	Btms Rate	$\frac{E}{F}$ Ratio	Distillate Comp.			Bottoms Composition		
			EtOH	Wtr	Bz	EtOH	Wtr	Bz
6C1	84.5	2.3750	29.149	16.993	53.858	99.152	0.1022	0.746
6C2	84.0	2.4359	29.265	16.876	53.859	99.049	0.304E-6	0.951
6C3	80.0	2.4605	29.311	16.830	53.859	98.839	0.137E-6	1.161

Note: All the rates and compositions are in lbmoles/hr and mole % respectively.

means the Case number

No. of stages = 80 in case # 6C1

No. of stages = 90 in all other cases

Table 5.4

Effect of Entrainer/Feed Rate Ratio on Azeotropic Column - III

Major fixed conditions

Stream	Rate lbmole/hr	Composition in mole % Ethanol	Water	Benzene
Entrainer(E)		28.104	11.771	60.125
Feed(F)	115.1506	85.0	15.0	0.0

#	Btms Rate	$\frac{E}{F}$ Ratio	Distillate Comp.			Bottoms Composition		
			EtOH	Wtr	Bz	EtOH	Wtr	Bz
4C1	88.5	2.1711	29.696	16.453	53.873	97.157	1.4040	1.439
4C2	85.0	2.3554	29.798	16.325	53.877	99.174	0.811E-4	0.826
4C3	80.0	2.7531	30.582	15.501	53.917	99.091	0.540E-7	0.909

Note: All the rates and compositions are in lbmoles/hr and mole % respectively.

\# means the Case number

No. of stages = 70

Since the process plant is very sensitive with respect to the two liquid phase composition and amount of the streams leaving the distillate drum, the lower ethanol feed concentration value should provide better control.

5.3 Effect of Feed Concentration on the Azeotropic column

Alcohol-water feed to the azeotropic column is essentially the overhead product of the ethanol concentrator. The upper limit of ethanol concentration in the gross feed to the recovery plant is the azeotropic composition. At 760 mm Hg pressure ethanol-water azeotrope is formed at 89.43 mole % or 95.2 wt. % (Weast, 1975) ethanol. The azeotropic composition can be attained using the batch distillation process, whereas the continuous distillation require a large number of stages. Therefore study of an azeotropic column was conducted with the feed concentrations ranging from 70 to 89.4 mole % alcohol.

Calculations were performed by fixing the bottoms rate and specifications, as well as the feed rate and entrainer stream composition. It was observed that higher feed concentrations require lesser amounts of entrainer to perform the operation, the entrainer to feed ratio decreases with an increase in alcohol content in the feed. Also, the overhead and bottoms product specifications can be met by setting a suitable entrainer to feed rate ratio and a distillate or bottoms rate. The relationship between entrainer to aqueous feed rate ratio versus mole % of

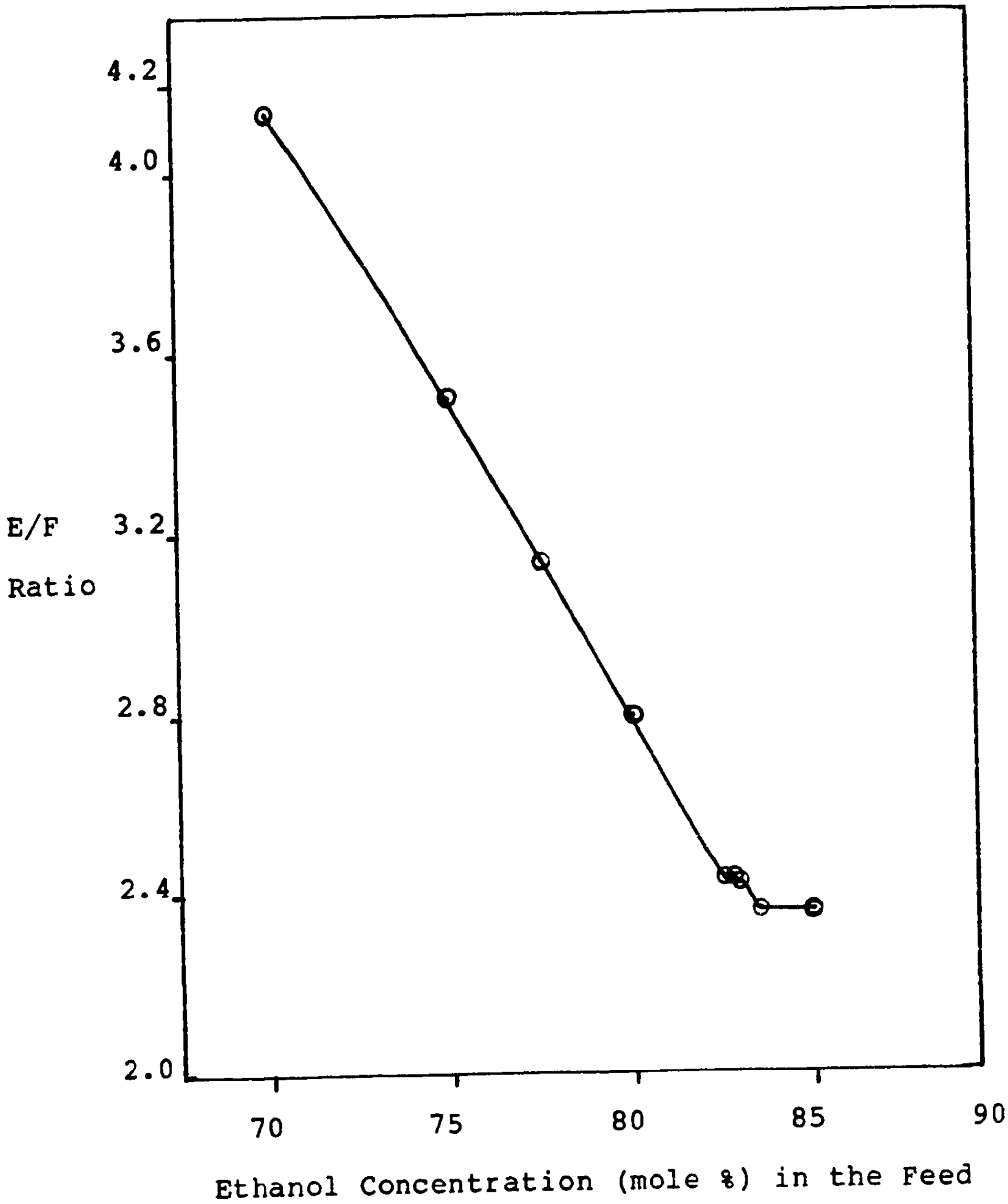


Fig. 5.2 Entrainer/Feed Rate Ratio Vs EtOH in the Feed to the Azeotropic Column

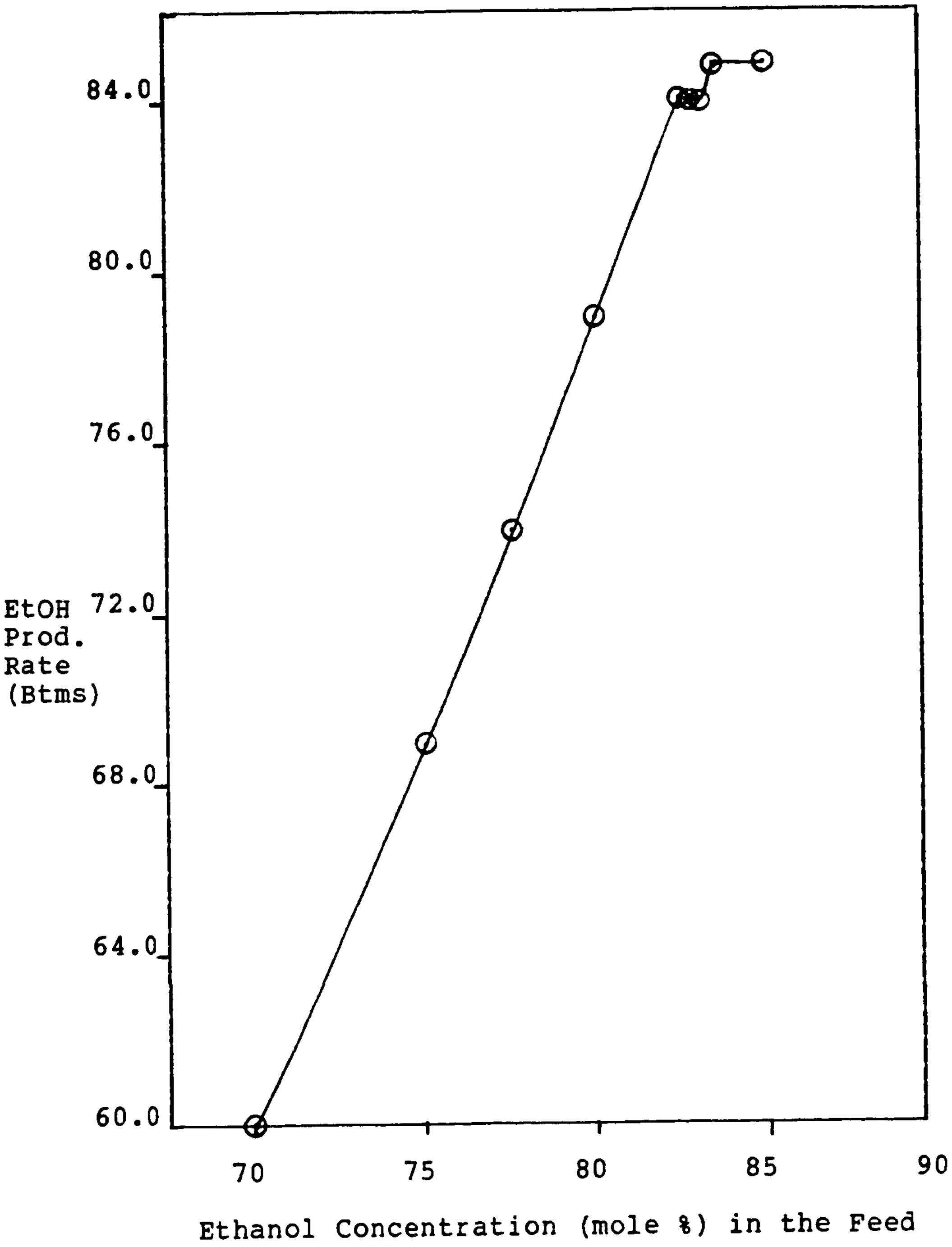


Fig. 5.3 Ethanol Product (Bottoms) Rate Vs EtOH in the Feed to the Azeotropic Column

ethanol in the feed is shown in Fig. 5.2. Fig 5.3 presents the relationship between ethanol product (bottoms) rate versus ethanol concentration in the azeotropic column binary feed.

Figure 5.3 illustrates an approximately linear relationship between bottoms rate versus ethanol concentration up to 82.5 mole %. Above that concentration the curve flattens out showing limitation on the production rate of dry alcohol. This analysis would directly provide the best initial values for the simulation of individual process unit as well as the complete process plant. A very similar behavior, but in the opposite direction, is observed with entrainer to feed rate ratio (Fig. 5.2). Also, the ratio becomes approximately constant above feed concentration of 82.5 mole %.

The overhead vapor, from the azeotropic column, composition corresponding to the cases with alcohol concentration in the feed below 82.5 % is approximately 29 (ethanol) - 17 (water) - 54 (benzene) mole %. If the feed concentration is very near to the azeotrope then the overhead vapor composition falls nearer to the two liquid phase boundary. In addition, azeotropic alcohol-water feed composition leads distillate composition in the single liquid phase region and predicts too wet bottoms product. For a constant feed composition, bottoms product rates other than shown in Table 5.5 do not converge.

5.4 Conclusions

The azeotropic distillation column can be operated in

Table 5.5

Effect of Feed Concentration on Azeotropic Column

Major fixed conditions

Stream	Rate	Composition in mole %		
	lbmole/hr	Ethanol	Water	Benzene
Entrainer(E)		28.104	11.771	60.125
Feed(F)	115.1506			0.0

#	Etoh comp in F	Btms Rate	$\frac{E}{F}$ Ratio	Distillate Comp.			Bottoms Comp.	
				EtOH	Wtr	Bz	EtOH	Wtr
5C1	70.00	60.0	4.1286	29.084	17.084	53.858	99.846	0.034E-9
5C2	75.00	69.0	3.5000	29.171	16.971	53.859	99.421	0.167E-8
5C3	77.50	74.0	3.1387	29.138	17.004	53.858	99.343	0.375E-7
5C4	80.00	79.0	2.8000	29.135	17.007	53.858	99.070	0.130E-5
5C5	82.50	84.1	2.4316	29.070	17.073	53.857	99.037	0.781E-5
5C6	82.75	84.0	2.4413	29.183	16.958	53.859	99.002	0.338E-5
5C7	82.82	84.0	2.4280	29.184	16.957	53.859	99.116	0.516E-5
5C8	83.00	84.0	2.4359	29.265	16.876	53.859	99.049	0.304E-6
5C9	83.50	84.9	2.3750	29.288	16.853	53.859	99.023	0.551E-4
5CA	85.00	84.8	2.3700	29.831	16.290	53.879	99.162	0.595E-5
5CB	89.40	99.0	1.4963	31.137	14.911	53.952	93.626	4.4330

Note: All the rates and compositions are in lbmoles/hr and mole % respectively.

means the Case number

the desired region by manipulating the column material balance. The column's working region is very narrow and sensitive to minor variations in the process variables like, bottoms product rate, entrainer to aqueous alcohol feed rate ratio, and the amount of alcohol in the alcohol-water feed. The operating flexibility of the entrainer and the distillate rates decrease with an increase in percentage of alcohol in the feed.

The entrainer to feed rate ratio increases from 2.37 to 4.13 if the ethanol concentration in the feed is lowered from 85 mole % to 70 mole %. Very high alcohol concentrations near to the azeotrope makes the continuous ethanol concentrator uneconomical, but makes azeotropic column rather economical in operation from entrainer load point of view. On the other hand alcohol concentration as low as 70 mole % has an opposite affect. Sensitivity of feed concentration on the complete process plant, shown in Fig. 6.6, is discussed in detail in the subsequent chapter.

The relationship between entrainer to feed rate ratio and bottoms rate versus mole % ethanol in the feed provides useful control setting information for the design and simulation. The drastic change in the slope of the curves, shown in Figs. 5.2 and 5.3, has an impact on the process configuration and is discussed further in the next chapter.

CHAPTER 6

STEADY STATE SIMULATION OF INTEGRATED ETHANOL DEHYDRATION PROCESS PLANT

Azeotropic distillation is a proven process for the production of industrial and fuel grade ethanol. The modeling and simulation of this process requires a process simulator of extensive capabilities. The process simulator (PROSIM) developed as part of this research is discussed in Chapter 2.4. PROSIM incorporates rigorous computational techniques, advanced models and parameters to represent process units, and special control blocks to achieve viable solutions from the flowscheme. This research problem requires an ethanol concentrator, azeotropic distillation column, two liquid phase decanter, and an entrainer and alcohol recovery section which introduces one or two additional columns in the process.

After concentrating the ethanol feed to a composition near the binary ethanol-water azeotrope, an additional column (azeotropic column) is required for the production of water free alcohol. The azeotropic tower consists of two feeds, an alcohol-water feed and an entrainer rich feed. Various entrainers and their predicted performances have been investigated and reported in Chapter 3. The overhead vapor product from the azeotropic column forms two liquid phases, after condensation, the light phase is organic rich and the heavy phase is aqueous rich. This phenomena of liquid-liquid separation introduces the following two facts:

A. The decanter forces water out of the system and enhances bulk recovery of the entrainer, which is recycled.

B. The liquid-liquid separation process requires an appropriate equation and its parameters for phase equilibria representation.

The light (entrainer rich) phase is recycled to the top of the azeotropic column. Recovery of the balance of the entrainer and the ethanol from the aqueous phase leaving the distillate drum gives rise to an additional recovery and recycle scheme.

Various flow schemes with two, three, or four distillation columns are reported in the literature. The schemes differ mainly in the recovery and recycle of the entrainer and the ethanol.

- A flowscheme, reported by Venkatesh (1982) is shown in Fig. 6.1, recycles the heavy aqueous phase from the decanter to the ethanol concentrator.
- Keister (1980) and Prokopakis (1983) have simulated the ethanol-water-benzene process scheme as shown in Fig. 6.2. The process consists of a stripping column with the liquid distillate directed to the decanter, and the bottoms mixed with the fresh feed to the ethanol concentrator. Keister simulated this process using ASPEN PLUS (Aspen Tech, 1982)
- The process scheme shown in Fig. 6.3 withdraws water as the bottoms product from the stripper following decanter drum. This scheme has been reported by

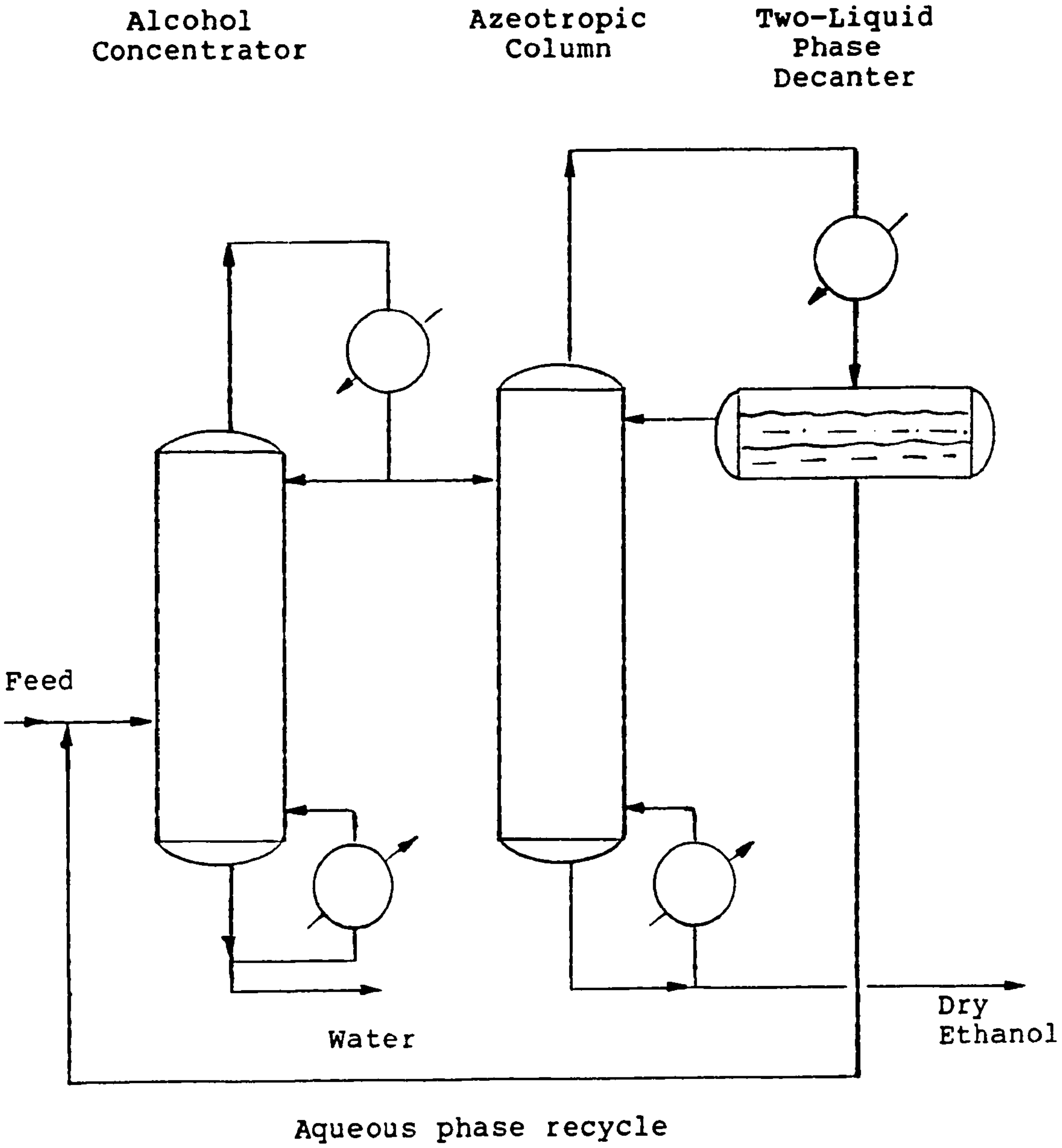


Fig. 6.1 Alcohol Azeotropic Distillation Process Flowscheme - I (Venkatesh, 1982)

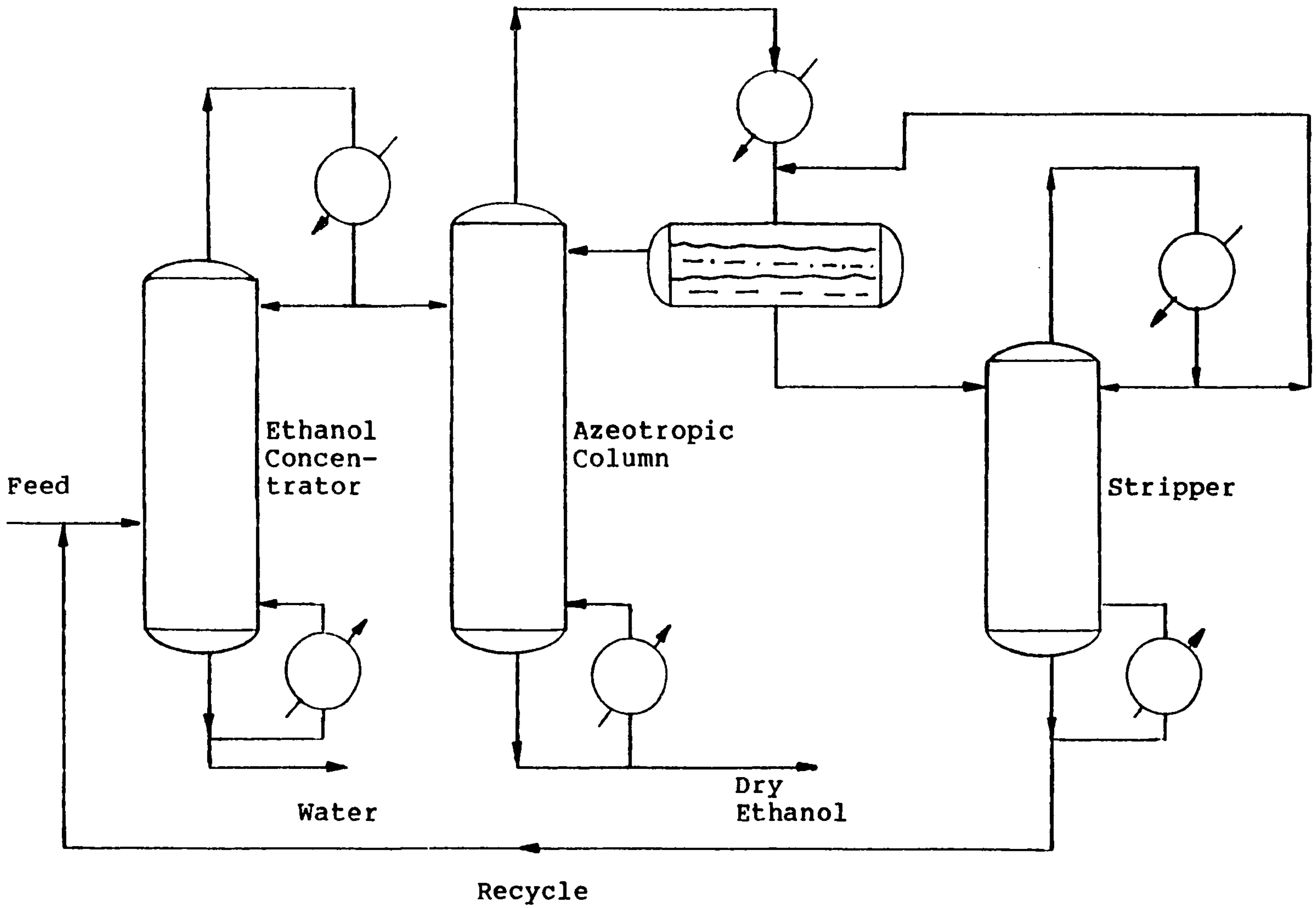


Fig. 6.2 Alcohol Azeotropic Distillation Process Flowscheme - II (Keister, 1982 and Prokopakis, 1983)

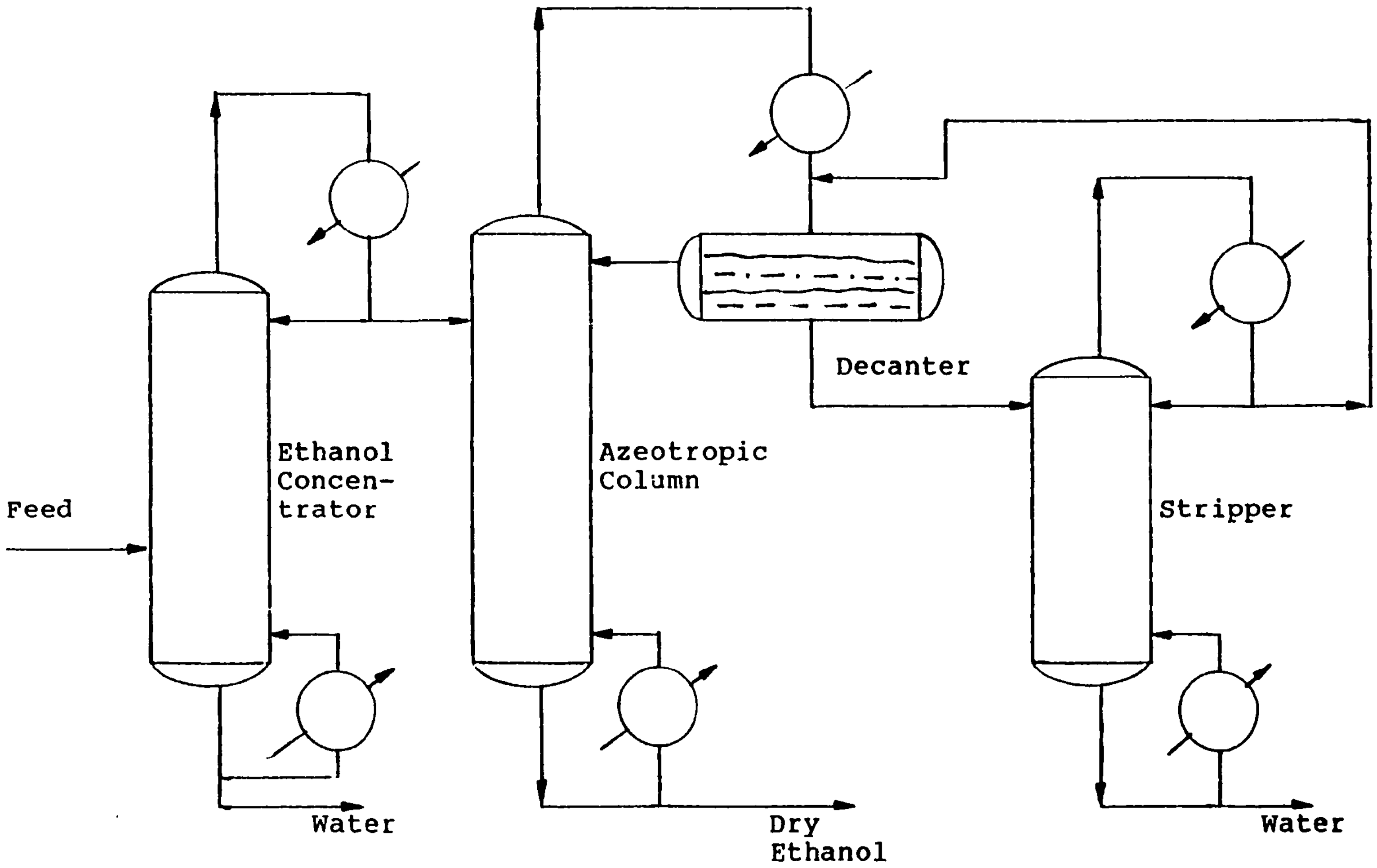


Fig. 6.3 Alcohol Azeotropic Distillation Process Flowscheme - III (Black, 1980 and Prokopakis, 1983)

Black (1980) for the ethanol-water-pentane system and by Prokopakis (1983) for the ethanol-water-benzene system. Black simulated the flow configuration with PROCESS (Simulation Sciences, Inc.).

- A three column configuration presented by Venkatesh (1982) for an optimization study is shown in Fig. 6.4. This scheme differs from the one presented by Black and Prokopakis (Fig. 6.3) in two ways. First the overhead vapor from the azeotropic tower is condensed in two heat exchangers, and the partially condensed stream is mixed with light organic phase from the two liquid phase decanter. Secondly, the liquid distillate from the entrainer stripping column is added to the light phase from decanter.
- Fig 6.5 presents the four column arrangement suggested by Tsai (1982). In this scheme, make-up benzene is added to the vapor overhead from the benzene stripper and then is added to the light organic phase as the upper feed (reflux) to the azeotropic tower. An additional column purges the water from the system. The final column's liquid distillate (with negligible benzene) is mixed with the feed to the azeotropic column. Ethanol in the aqueous phase from the two liquid phase decanter is thus completely recovered via two columns.

6.1 Analysis of Major Segments in the Flowscheme

Modeling of individual process units:

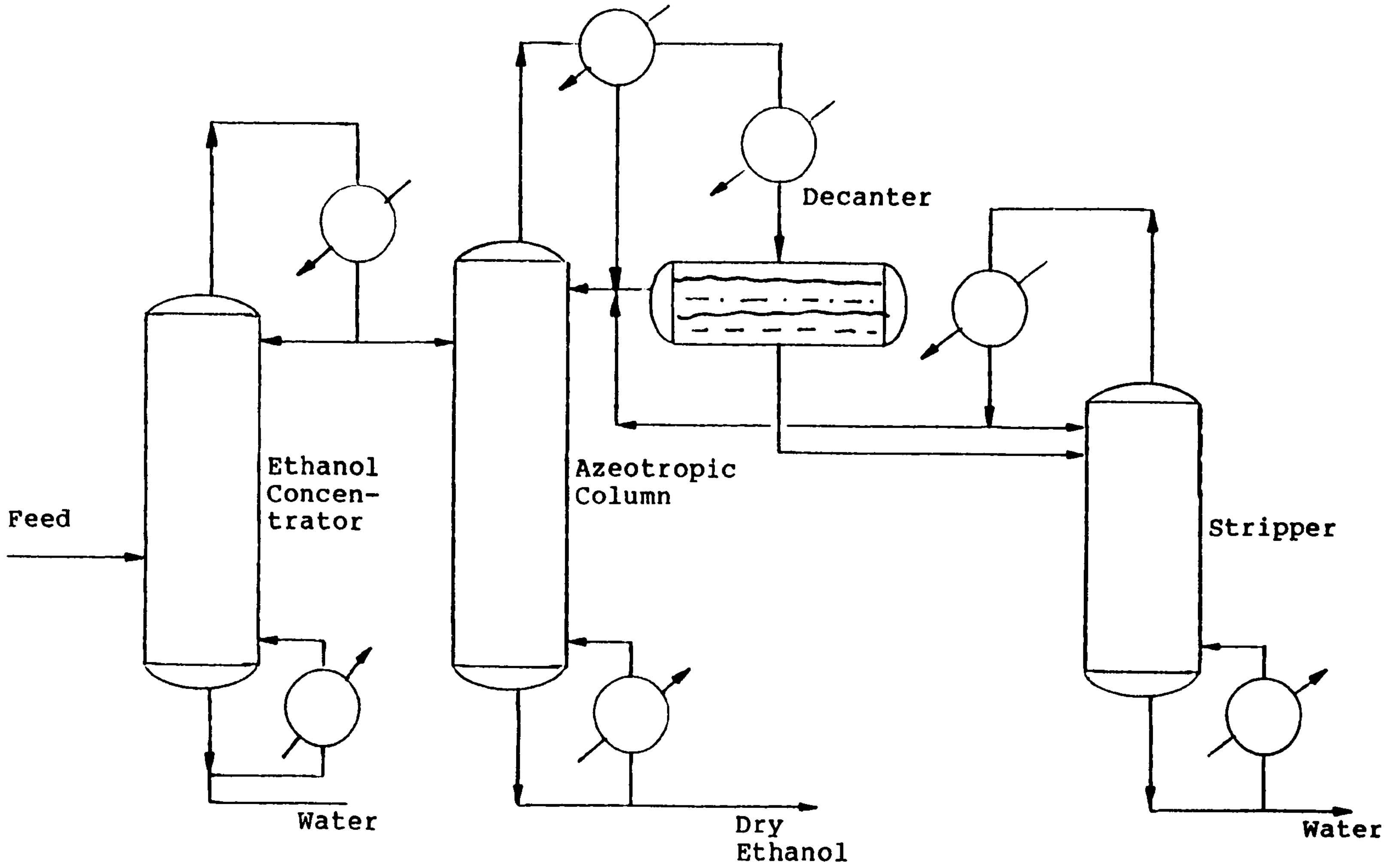


Fig. 6.4 Alcohol Azeotropic Distillation Process Flowscheme - IV (Venkatesh, 1982)

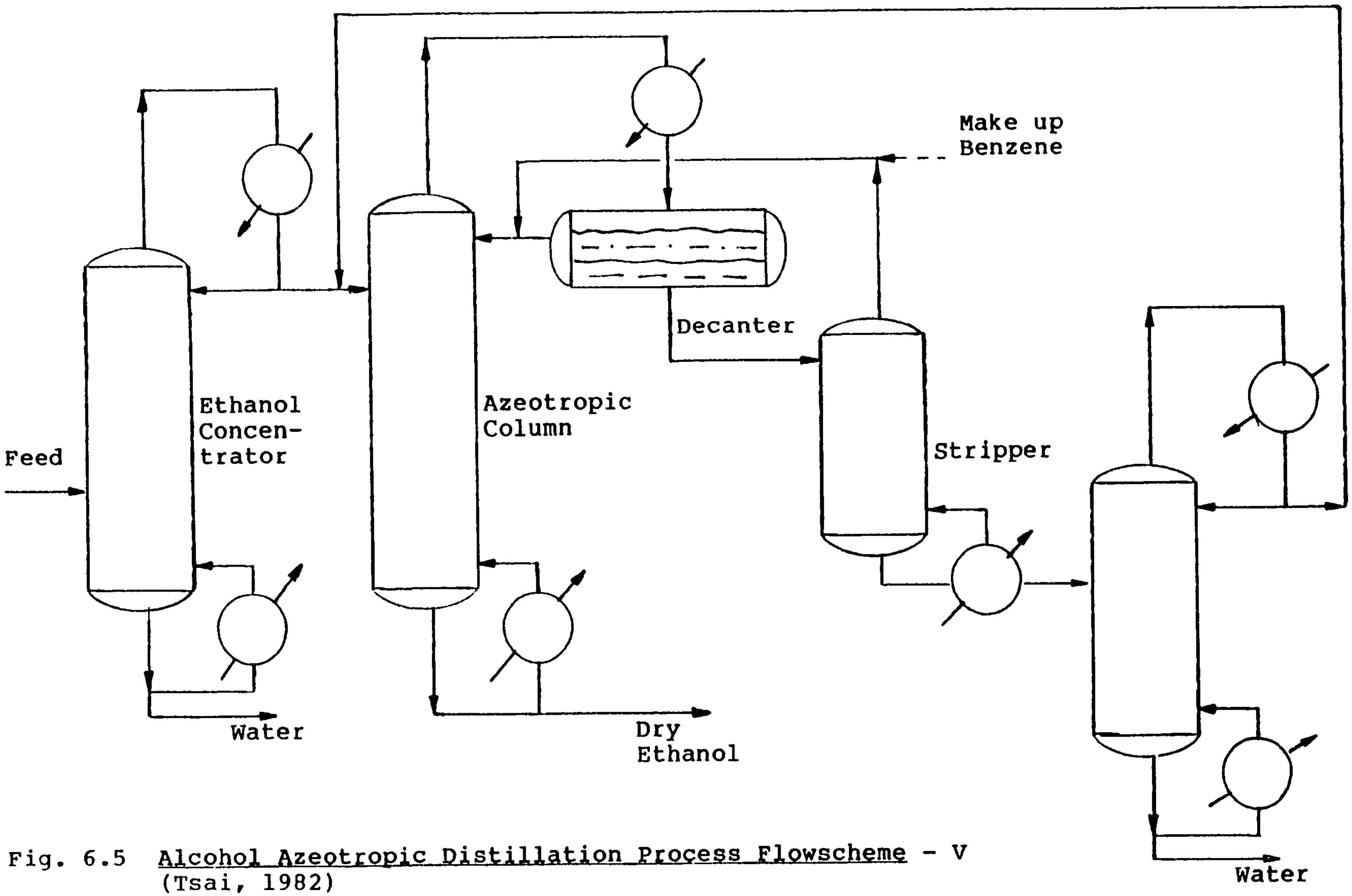


Fig. 6.5 Alcohol Azeotropic Distillation Process Flowscheme - V
(Tsai, 1982)

1) Ethanol concentrator,
2) Azeotropic distillation tower,
3) Two liquid phase decanter, and
4) Downstream stripping/recovery column(s),

is the building block of the complete process. An in depth analysis has been performed for the ethanol-water-benzene system. The developed flowscheme, which is similar to Fig. 6.2, is presented in Fig. 6.6.

6.1.1 Gross Water Removal

If the ethanol concentrator is incorporated in the flowscheme then the bulk quantity of water is removed as the bottoms. In the process of concentrating a very dilute aqueous ethanol (approximately 3.2 mole % or 7.79 wt. %) the result is a concentrated ethanol solution (approximately 82.8 mole %) near the ethanol-water azeotrope. The two feed binary column is a straight forward design as compared to the other columns in the process.

6.1.2 Azeotropic Column and Two Liquid Phase Decanter

The operation of the azeotropic column is very restricted, in the sense that for certain ethanol-water feed rate and concentration, the entrainer stream and bottoms rate are constrained so that one achieves the desired dry ethanol product as bottoms and the column overhead composition lies in the two liquid phase envelope. Two points B and D in Fig. 6.7 represent bottoms and distillate compositions. A detailed study of this tower has been presented in Chapter 5.

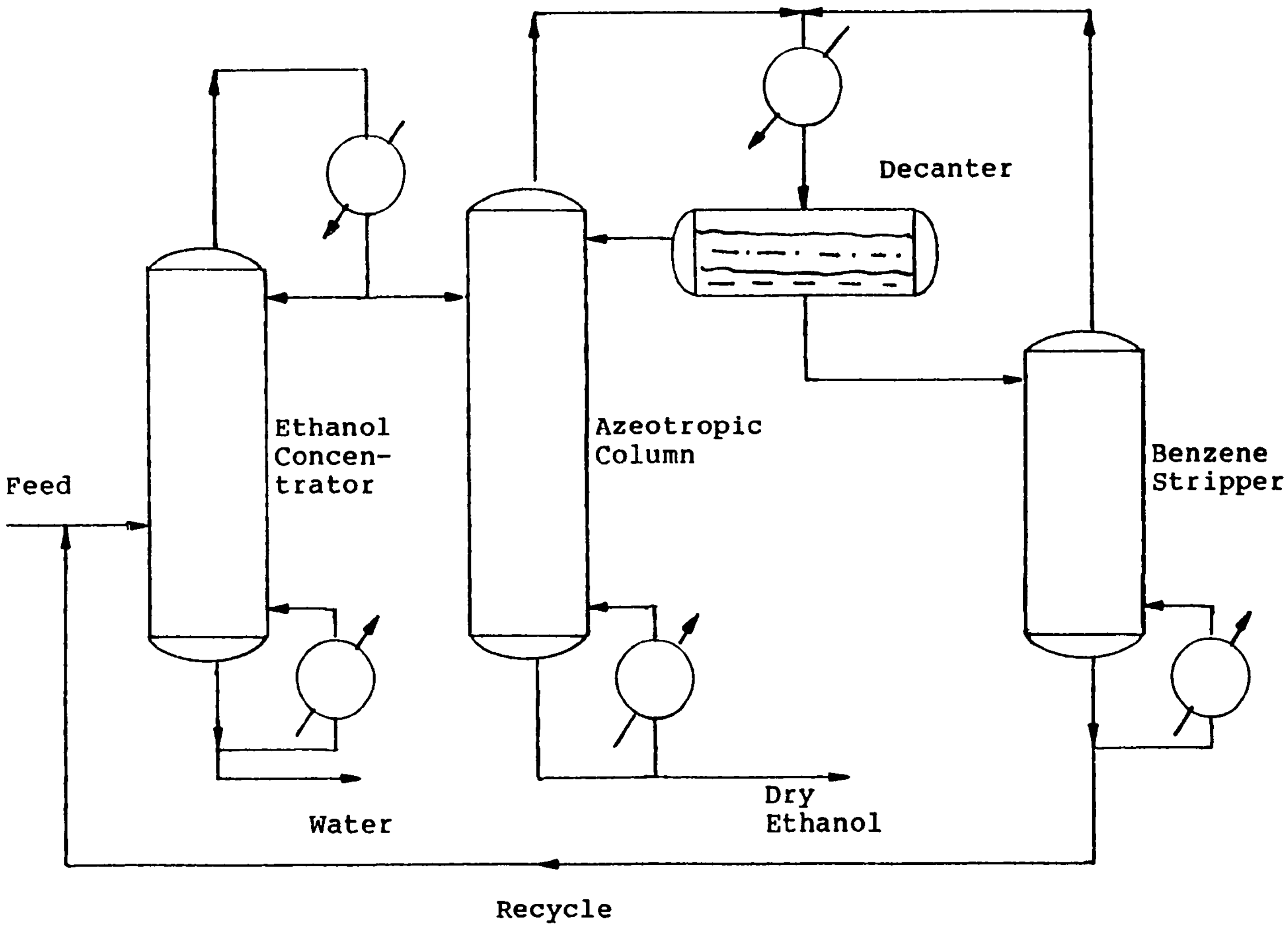
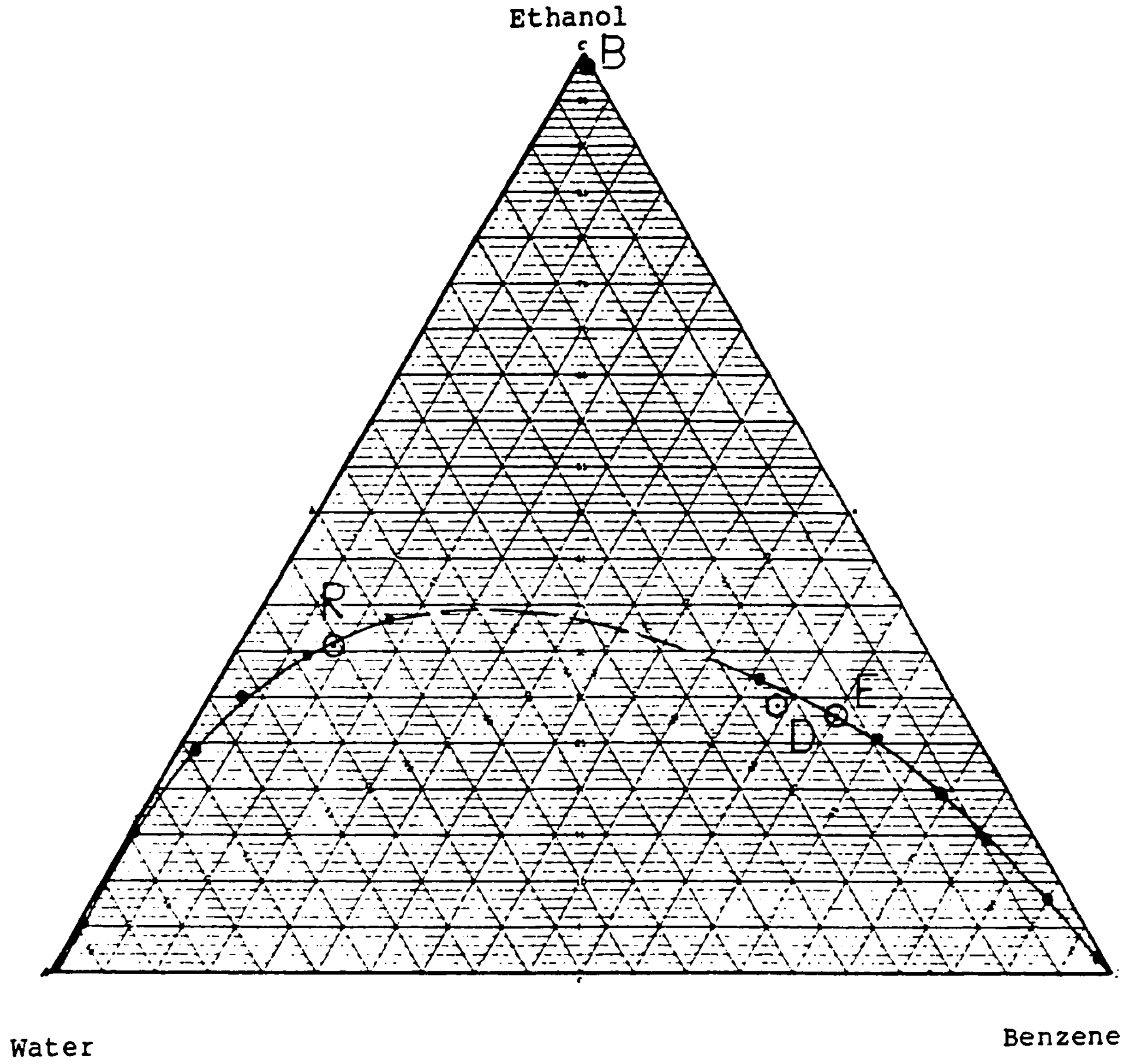


Fig. 6.6 Proposed Ethanol Azeotropic Distillation Process Flowscheme (Research Problem)



D - Vapor Distillate
E - Light Phase from the Decanter

B - Bottoms Product
R - Heavy Phase from the Decanter

Fig. 6.7 Representation of Output Streams from the Azeotropic Column and the Two Liquid Phase Decanter

Feed to the two liquid phase decanter is dominated by the rate and composition. Therefore point D has to be in two liquid phase region. Points E and R in Fig. 6.7 correspond to phase compositions of extract (light phase) and raffinate (heavy phase) phases. The tie line computed with NRTL and modified UNIQUAC (discussed in Section 2.1) parameters is reported in Fig. 4.6. Phase compositions and slope of the tie line estimated by NRTL are in better agreement with the experimental LLE data (Morachevskii, 1958) at 35°C. Tables 4.16 and 4.17 show the comparison of results of tie line predicted by various sets of UNIQUAC parameters with that of NRTL. Hence in the further research work, the tie line data was estimated using the NRTL equation and LLE parameters reported by Sorensen (1979).

The light phase from the decanter is dominant in benzene and correspond to 0.88 mole fraction of the total incoming liquid. This benzene rich phase (28.1 mole % ethanol, 11.8 mole % water, and 60.1 mole % benzene) is returned back to the azeotropic column. Thus points B, D, E, and R of Fig. 6.7 are practically fixed and therefore they provide excellent stream values to initialize the process simulation.

6.1.3 Benzene Recovery System and Make-up Benzene

The aqueous phase from the two liquid decanter (composition, 35.78 mole % ethanol, 55.63 mole % water, and 8.59 mole % benzene) is fed to a recovery section. This stream composition and the associated rate are fixed because of inflexibility in point D on Fig. 6.7. The rate of this aqueous stream is dependent upon the ethanol-water feed composition to the azeotropic tower. It can be observed in Tables 5.2-5.4 and Fig 5.2 that the entrainer rate and bottoms rate of the azeotropic column are tied together to maintain column product within specifications.

There are two functions of the stripping column: first, to recover the benzene completely and second, to purge water and balance the plant's ethanol as its bottoms product. Behavior of the stripping column with various ethanol-water feed compositions is discussed in the subsequent section. It is observed that the vapor distillate composition is bounded by the predicted vapor phase ethanol-water-benzene azeotrope at that column pressure. The published ternary azeotropic composition (Weast, 1975) at atmospheric pressure is 22.80 mole % ethanol, 23.30 mole % water, and 53.90 mole % benzene, and the corresponding temperature is 64.86 °C. This restricts the amount of benzene that can be stripped at atmospheric pressure. Therefore at atmospheric pressure the dual objective just stated is not achieved, but the reduction of operating pressure to approximately 4.8 psia results in benzene stripping and the producing the required material balance on ethanol and water as bottoms product.

6.2 Sensitivity of Water Recovery with Respect to the Azeotropic Column Binary Feed Concentration

In order to study the benzene stripping column results with varying azeotropic column feed concentration, a dummy distillation block (SBOX) was incorporated in PROSIM. The system description of SBOX block is described in section 2.4. The feed to this column or block is the heavy (aqueous) phase from the decanter. SBOX was used to attain the desired split which would lead to convergence in the simulation calculations. For a given feed condition, the bottoms rate of benzene stripping column is the summation of excess ethanol, and water which is fed with the ethanol feed to the azeotropic column.

This study was introduced because the actual stripping column (DIST block) lead to no solution and was oscillating for most of the azeotropic column feed concentrations. In other words, the distillation column fails to perform the desired separation as obtained by SBOX. It depicts that for the process configuration shown in Fig. 6.6, there has to be a range, probably small, of azeotropic column feed concentrations which can make the process work. Figs. 6.8 to 6.14 show the results obtained using SBOX, this being an azeotropic column feed concentrations from 70:30 to 83.5:16.5 mole % alcohol-water mixture. In addition, results of actual distillation column simulation are reported in Tables 6.1 - 6.7 with the same range of azeotropic column feed concentration, and column pressure as the manipulative variable. For all these cases the dry ethanol product specification was fixed as 99+ mole % ethanol, less than 10 ppm (mole) water, and a small amount of benzene (entrainer).

As discussed in section 6.1.3, ternary azeotrope

Fig. 6.8: Effect of Azeotropic Column Feed Concentration (70 mole % ethanol) on the Benzene Stripping Section (using Block SBOX)

The following results are obtained using PROSIM, with ethanol-water feed composition of 70.0 mole % alcohol to the azeotropic column. Dry ethanol specifications: 99 % + (E).

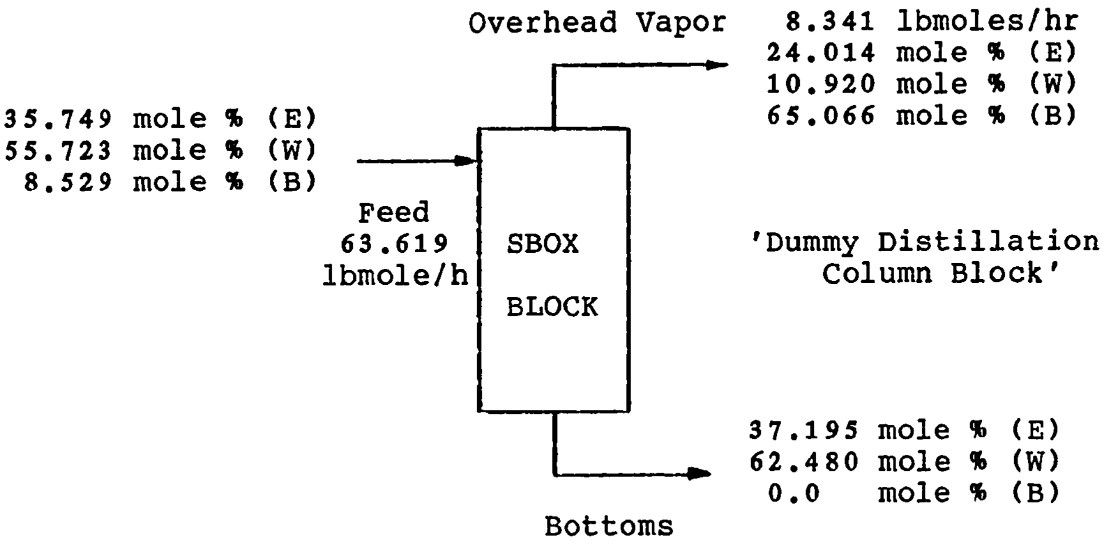


Table 6.1: Effect of Azeotropic Column Feed Concentration (70 mole % ethanol) and Operating Pressure on the Benzene Stripping Column

Distillation column performance with ABDIS

Ser. #	P (psia)	Vapor Distillate			Bottoms		
		EtOH	Wtr	Bz	EtOH	Wtr	Bz
1	14.696	22.928	21.027	56.045	37.683	60.958	1.358
2	6.0	21.980	18.441	59.579	37.827	61.348	0.825
3	1.0	22.720	15.955	61.325	37.715	61.724	0.562
4	0.5	24.039	15.984	59.977	37.516	61.719	0.765
5	0.25	25.780	16.426	57.793	37.253	61.652	1.095

Note: All the compositions are in mole %

Fig. 6.9: Effect of Azeotropic Column Feed Concentration (78 mole % ethanol) on the Benzene Stripping Section (using block SBOX)

The following results are obtained using PROSIM, with ethanol-water feed composition of 78.0 mole % alcohol to the azeotropic column. Dry ethanol specifications: 99 % + (E).

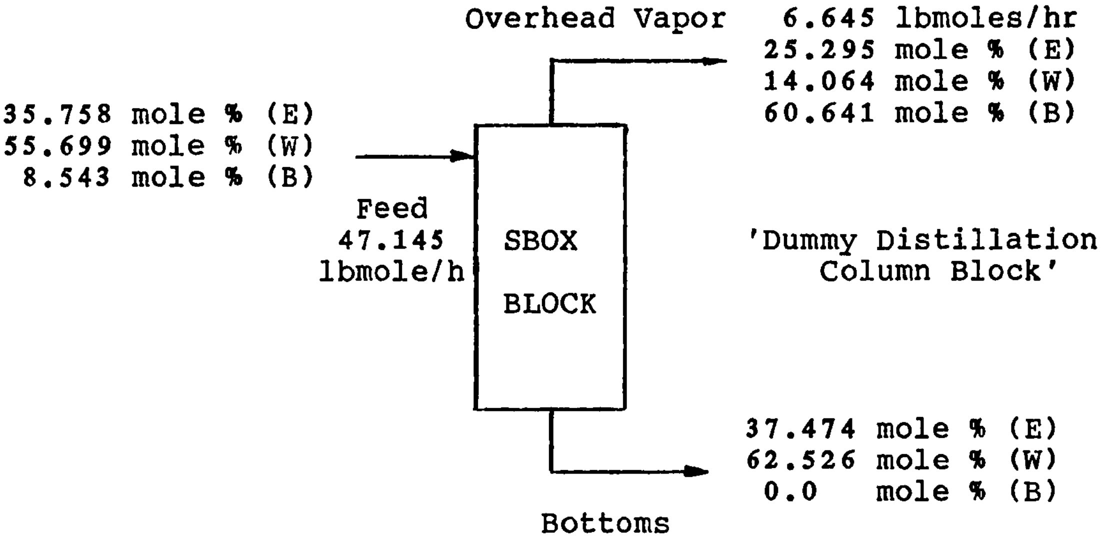


Table 6.2: Effect of Azeotropic Column Feed Concentration (78 mole % ethanol) and Operating Pressure on the Benzene Stripping Column

Distillation column performance with ABDIS

Ser. #	P (psia)	Vapor Distillate			Bottoms		
		EtOH	Wtr	Bz	EtOH	Wtr	Bz
1	14.696	22.934	21.023	56.025	37.837	61.358	0.751
2	6.0	22.019	18.449	59.532	37.985	61.778	0.178
3	1.0	23.250	16.192	60.555	37.787	62.148	0.010
4	0.5	24.062	15.997	59.938	37.664	62.197	0.110
5	0.3	25.266	16.267	58.463	37.466	62.148	3.529
6	0.1	28.336	17.366	54.295	36.948	61.975	1.037
7	0.05	33.240	17.034	47.011	36.158	61.580	2.230

Note: All the compositions are in mole %

Fig. 6.10:Effect of Azeotropic Column Feed Concentration (82.5 mole % ethanol) on the Benzene Stripping Section (using block SBOX)

The following results are obtained using PROSIM, with ethanol-water feed, composition of 82.5 mole % alcohol, to the azeotropic column. Dry ethanol specifications: 99 % + (E).

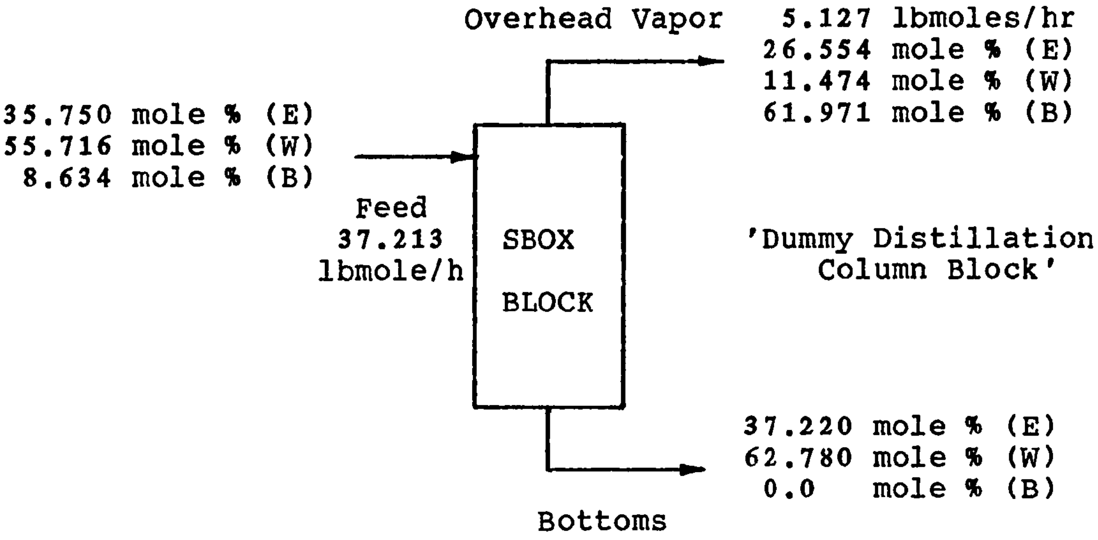


Table 6.3: Effect of Azeotropic Column Feed Concentration (82.5 mole % ethanol) and Operating Pressure on the Benzene Stripping Column

Distillation column performance with ABDIS

Ser. #	P (psia)	Vapor Distillate			Bottoms		
		EtOH	Wtr	Bz	EtOH	Wtr	Bz
1	14.696	22.936	21.025	56.034	37.797	61.261	0.942
2	6.0	22.000	18.445	59.565	37.953	61.666	0.380
3	1.0	22.761	15.976	61.261	37.828	62.040	0.108
4	0.5	24.029	15.979	59.994	37.610	62.040	0.311
5	0.35	24.887	16.165	58.941	37.486	62.008	0.477
6	0.25	25.765	16.165	58.941	37.486	62.008	0.477

Note: All the compositions are in mole %

Fig. 6.11: Effect of Azeotropic Column Feed Concentration (83.0 mole % ethanol) on the Benzene Stripping Section (using block SBOX)

The following results are obtained using PROSIM, with ethanol-water feed composition of 83.0 mole % alcohol to the azeotropic column. Dry ethanol specifications: 99 % + (E).

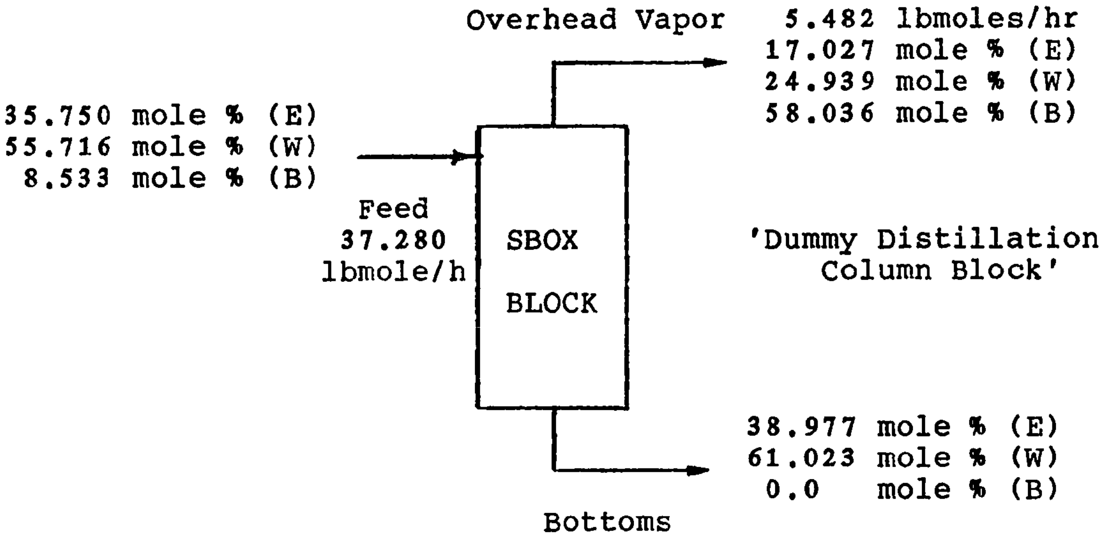


Table 6.4: Effect of Azeotropic Column Feed Concentration (83.0 mole % ethanol) and Operating Pressure on the Benzene Stripping Column

Distillation column performance with ABDIS

Ser. #	P (psia)	Vapor Distillate			Bottoms		
		EtOH	Wtr	Bz	EtOH	Wtr	Bz
1	14.696	22.930	21.033	56.040	37.957	61.700	0.342
2	6.0	23.186	18.808	58.028	37.926	62.078	0.000

Note: All the compositions are in mole %

Fig. 6.12: Effect of Azeotropic Column Feed Concentration (83.5 mole % ethanol) on the Benzene Stripping Section (using block SBOX)

The following results are obtained using PROSIM, with ethanol-water feed composition of 83.5 mole % alcohol to the azeotropic column. Dry ethanol specifications: 99 % + (E).

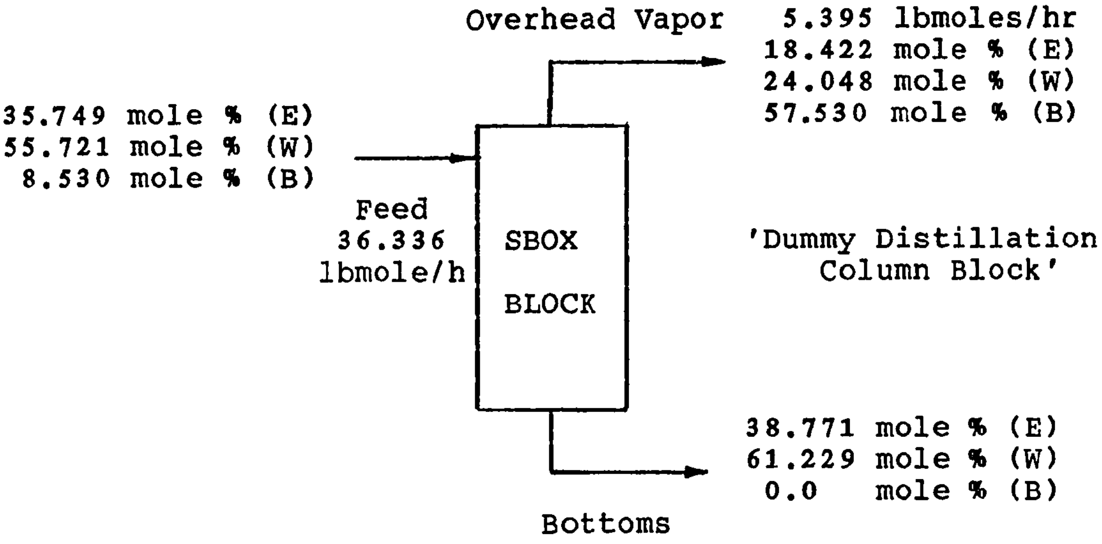


Table 6.5: Effect of Azeotropic Column Feed Concentration (83.5 mole % ethanol) and Operating Pressure on the Benzene Stripping Column

Distillation column performance with ABDIS

Ser. #	P (psia)	Vapor Distillate			Bottoms		
		EtOH	Wtr	Bz	EtOH	Wtr	Bz
1	14.696	22.928	21.019	56.051	37.982	61.773	0.245
2	6.0	23.633	18.925	57.440	37.885	62.161	0.000
3	1.0	25.375	17.177	57.441	37.562	62.450	0.000

Note: All the compositions are in mole %

Fig. 6.13: Effect of Azeotropic Column Feed Concentration (82.82 mole % ethanol) on the Benzene Stripping Section (using block SBOX)

The following results are obtained using PROSIM, with ethanol-water feed composition of 82.82 mole % alcohol to the azeotropic column. Dry ethanol specifications: 99 % + (E).

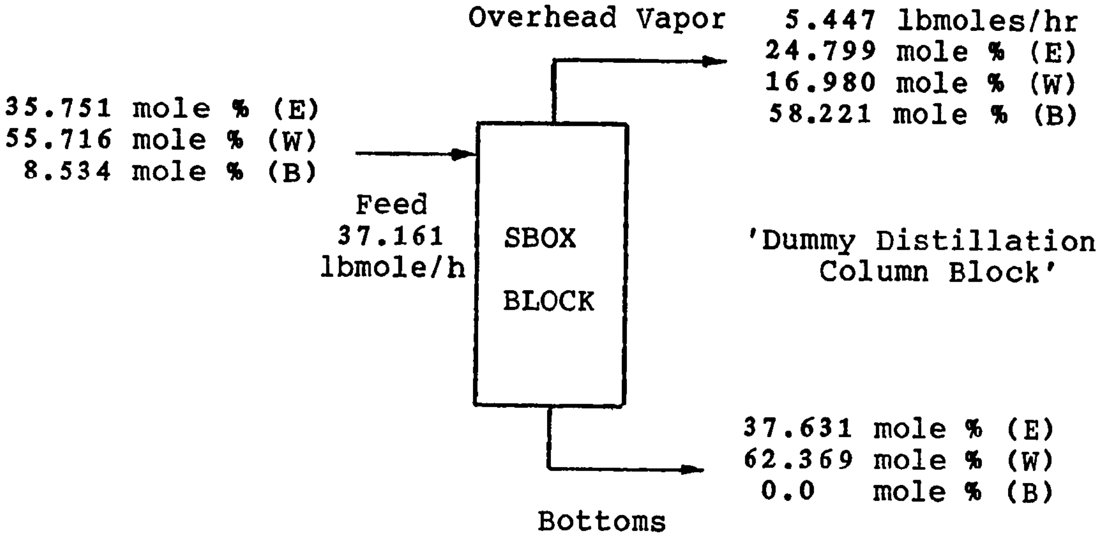


Table 6.6: Effect of Azeotropic Column Feed Concentration (82.82 mole % ethanol) and Operating Pressure on the Benzene Stripping Column

Distillation column performance with ABDIS

Ser. #	P (psia)	Vapor Distillate			Bottoms		
		EtOH	Wtr	Bz	EtOH	Wtr	Bz
1	14.696	22.930	21.021	56.050	37.959	61.668	0.373
2	6.0	23.040	18.744	58.216	37.928	62.046	0.000
3	1.0	24.858	16.931	58.216	37.612	62.361	0.000

Note: All the compositions are in mole %

Fig. 6.14: Effect of Azeotropic Column Feed Concentration (82.89 mole % ethanol) on the Benzene Stripping Section (using block SBOX)

The following results are obtained using PROSIM, with ethanol-water feed composition of 82.89 mole % alcohol to the azeotropic column. Dry ethanol specifications: 99 % + (E).

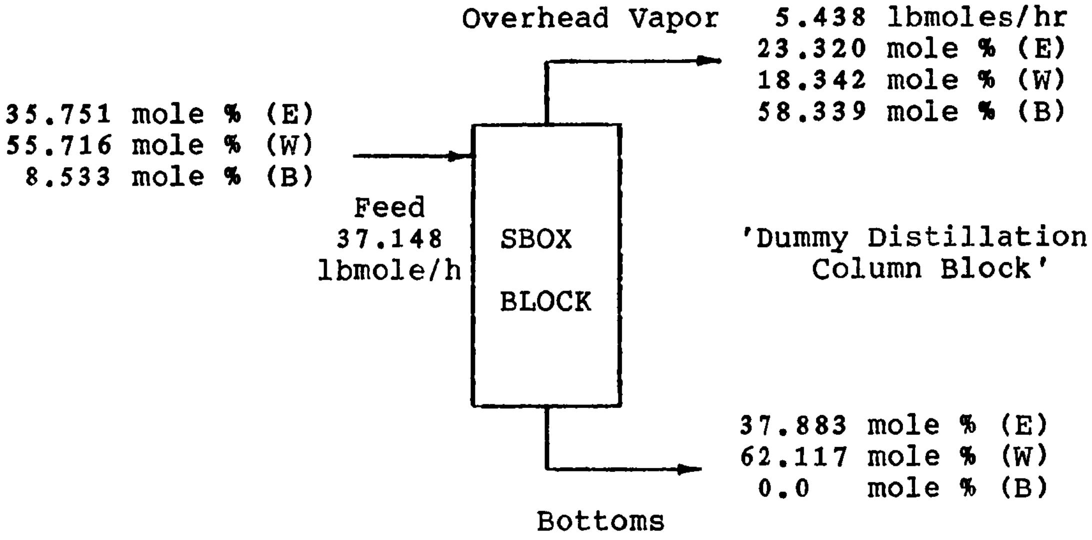


Table 6.7: Effect of Azeotropic Column Feed Concentration (82.89 mole % ethanol) and Operating Pressure on the Benzene Stripping Column

Distillation column performance with ABDIS

Ser. #	P (psia)	Vapor Distillate			Bottoms		
		EtOH	Wtr	Bz	EtOH	Wtr	Bz
1	14.696	22.931	21.019	56.050	37.947	61.667	0.386
2	5.0	23.262	18.444	58.293	37.915	62.109	0.000
3	4.8	23.320	18.387	58.293	37.883	62.117	0.000
4	4.0	23.556	18.145	58.293	37.852	62.172	0.000

Note: All the compositions are in mole %

formation locks the stripper overhead vapor composition. For example, in the Fig. 6.8 and Table 6.1, at atmospheric pressure, the column predicts much different overhead and bottoms compositions for the same material balance. The change in pressure from 14.7 psia to 1 psia causes the benzene concentration in the overhead vapor to increase from 56 mole % to 61.3 mole %, which shows that vacuum column operation is nearer to the desired solution than that of the profile generated by atmospheric column. A continual search in the increasing direction of the azeotropic column feed concentration lead to a possible solution with 82.82 mole % (ethanol) feed with a column pressure of 1 psia, which is shown in Fig. 6.13 and Table 6.6.

After the addition of ethanol concentrator in the flow-scheme, Fig. 6.6, the use of SBOX block in place of benzene stripper leads to solution shown in Fig. 6.14. In this case the benzene stripping column represents the desired separation at approximately 4.8 psia column pressure, reported in Table 6.7. The optimum azeotropic column aqueous ethanol feed concentration has been established to be about 82.89 mole % ethanol and 17.11 mole % water.

6.3 Sensitivity of Dry Ethanol Product Specification on the Benzene Stripping Column

Simulation of process plant is feasible around 82.9 mole % ethanol feed to the azeotropic column, as discussed in section 6.2. Thus, the feed concentration range for further study has been established to be between 82.5 to 83.0 mole %

ethanol. The benzene stripping column results, with ethanol specification of 99.75+ mole %, and azeotropic column feed concentration between 82.5 to 83.0 mole % are summarized in Figs. 6.15 to 6.19, and Tables 6.8 to 6.12.

Alcohol and water contents in the azeotropic column overhead stream change drastically, with constant feed concentration, as alcohol product purity is increased. Moreover benzene concentration in the overhead vapor, approximately 65 mole %, is far from the ternary azeotropic composition predicted by stripper. This shows that the complete process operates under very narrow operating conditions. A small perturbation in the azeotropic column aqueous alcohol feed may lead to an unsteady and oscillating process, which would demand a stiff process control scheme.

For the constant feed concentration of 82.82 mole %, increase in ethanol specifications from 99+ to 99.75+ mole % shifts the overhead vapor composition from 24.80 (E) - 16.98 (W) - 58.22 (B) to 14.72 (E) - 20.81 (W) - 65.08 (B) mole %, which in effect is driven away from the azeotropic composition at atmospheric pressure. The results of the effect of ethanol product specification on the benzene stripper product streams are presented in Figs. 6.13, 6.17 and 6.19, and in Tables 6.6, 6.10 and 6.12.

6.4 Discussion on the Development of the Flowscheme and Block Diagram

The flowscheme configurations obtained from the published literature is covered in the beginning of this

Fig. 6.15: Benzene Stripping Section (using block SBOX) Results with Ethanol Product Specifications of 99.75 + mole % and Azeotropic Column Feed Concentration of 82.5 mole % Ethanol

The following results are obtained using PROSIM.

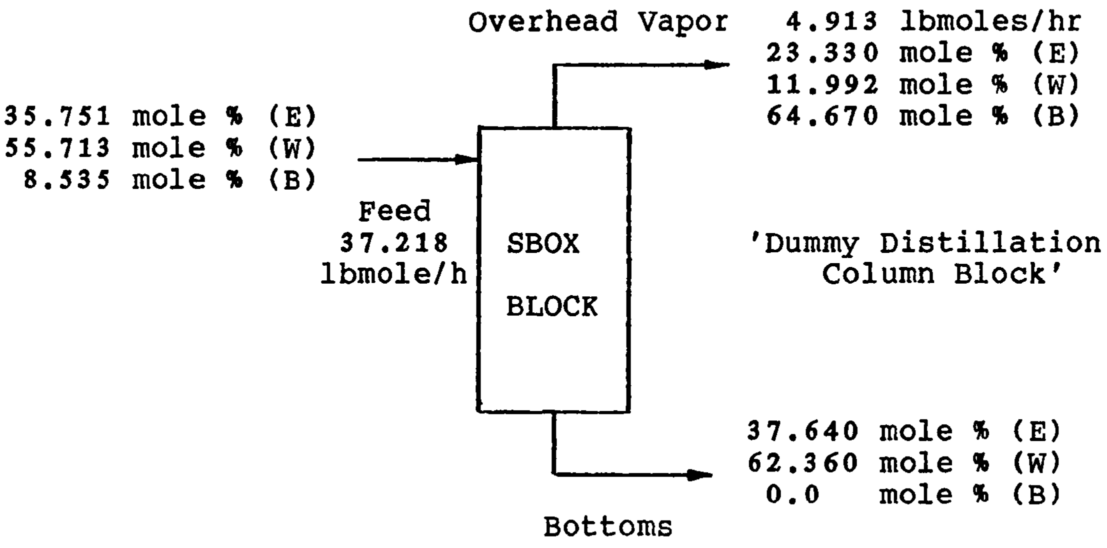


Table 6.8: Benzene Stripping Column Results with Ethanol Product Specifications of 99.75 + mole % and Azeotropic Column Feed Concentration of 82.5 mole % Ethanol

Distillation column performance with ABDIS

Ser. #	P (psia)	Vapor Distillate			Bottoms		
		EtOH	Wtr	Bz	EtOH	Wtr	Bz
1	14.696	22.918	21.025	56.053	37.705	60.985	1.309
2	1.0	22.714	15.951	61.345	37.736	61.759	0.505
3	0.5	24.037	15.977	60.002	37.551	61.759	0.702
4	0.25	25.767	16.419	57.824	37.272	61.697	1.041
5	0.1	28.352	17.382	54.262	36.870	61.542	1.581

Note: All the compositions are in mole %

Fig. 6.16: Benzene Stripping Section (using block SBOX) Results with Ethanol Product Specifications of 99.75 + mole % and Azeotropic Column Feed Concentration of 82.75 mole % Ethanol

The following results are obtained using PROSIM.

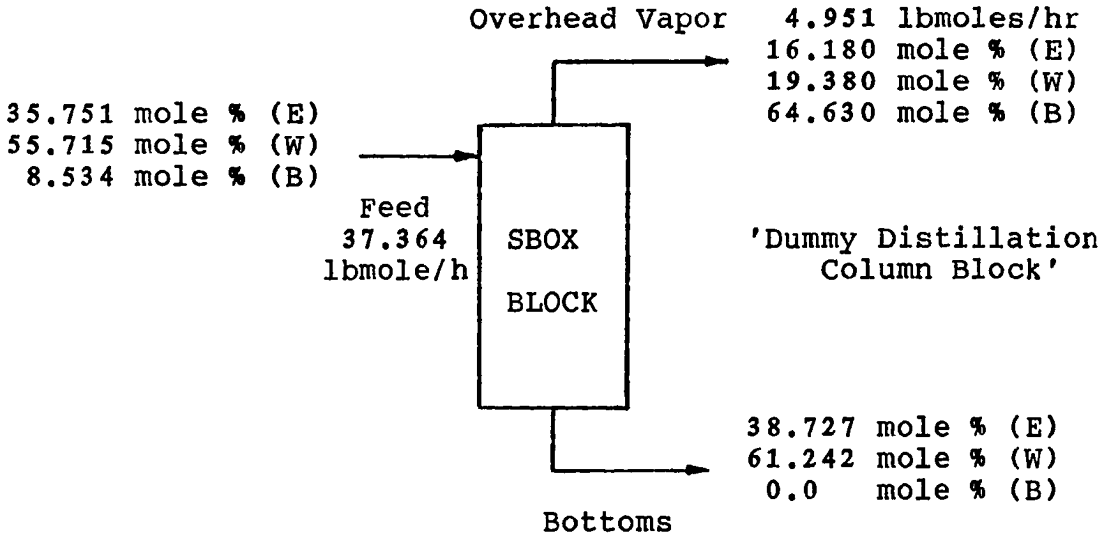


Table 6.9: Benzene Stripping Column Results with Ethanol Product Specifications of 99.75 + mole % and Azeotropic Column Feed Concentration of 82.75 mole % Ethanol

Distillation column performance with ABDIS

Ser. #	P (psia)	Vapor Distillate			Bottoms		
		EtOH	Wtr	Bz	EtOH	Wtr	Bz
1	14.696	22.925	21.026	56.049	37.700	61.023	1.277
2	10.0	22.420	19.851	57.726	37.792	61.177	1.019
3	8.0	22.218	19.247	58.534	37.823	61.270	0.896
4	6.0	21.975	18.439	59.584	37.854	61.393	0.736
5	1.0	22.723	15.952	61.341	37.731	61.794	0.469

Note: All the compositions are in mole %

Fig. 6.17: Benzene Stripping Section (using block SBOX) Results with Ethanol Product Specifications of 99.75 + mole % and Azeotropic Column Feed Concentration of 82.82 mole % Ethanol

The following results are obtained using PROSIM.

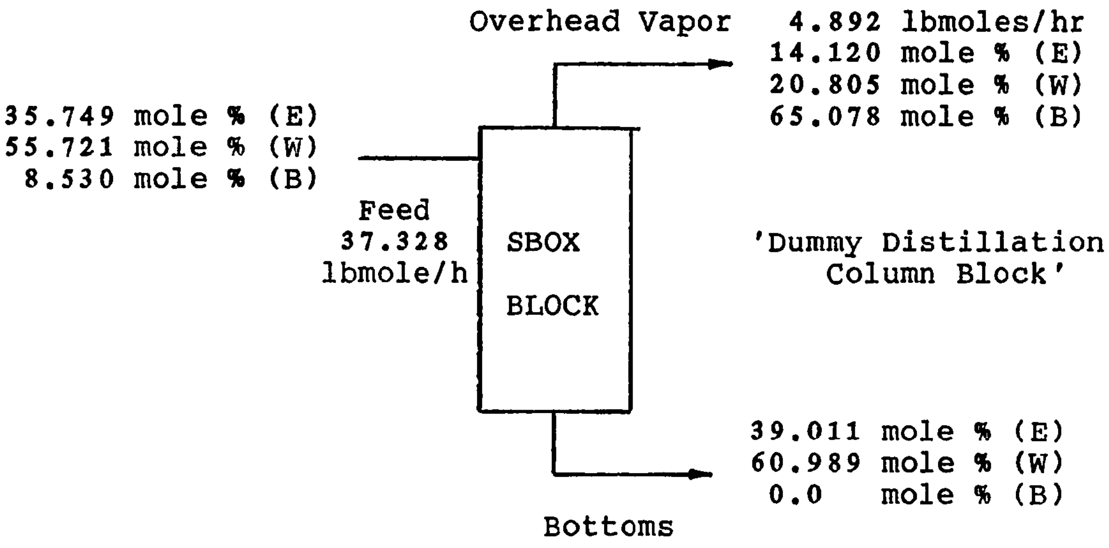


Table 6.10: Benzene Stripping Column Results with Ethanol Product Specifications of 99.75 + mole % and Azeotropic Column Feed Concentration of 82.82 mole % Ethanol

Distillation column performance with ABDIS

Ser. #	P (psia)	Vapor Distillate			Bottoms		
		EtOH	Wtr	Bz	EtOH	Wtr	Bz
1	14.696	22.935	21.034	56.051	37.680	60.958	1.364
2	6.0	21.975	18.440	59.587	37.833	61.359	0.830
3	1.0	22.711	15.955	61.325	37.709	61.729	0.567

Note: All the compositions are in mole %

Fig. 6.18: Benzene Stripping Section (using block SBOX) Results with Ethanol Product Specifications of 99.75 + mole % and Azeotropic Column Feed Concentration of 83.0 mole % Ethanol

The following results are obtained using PROSIM.

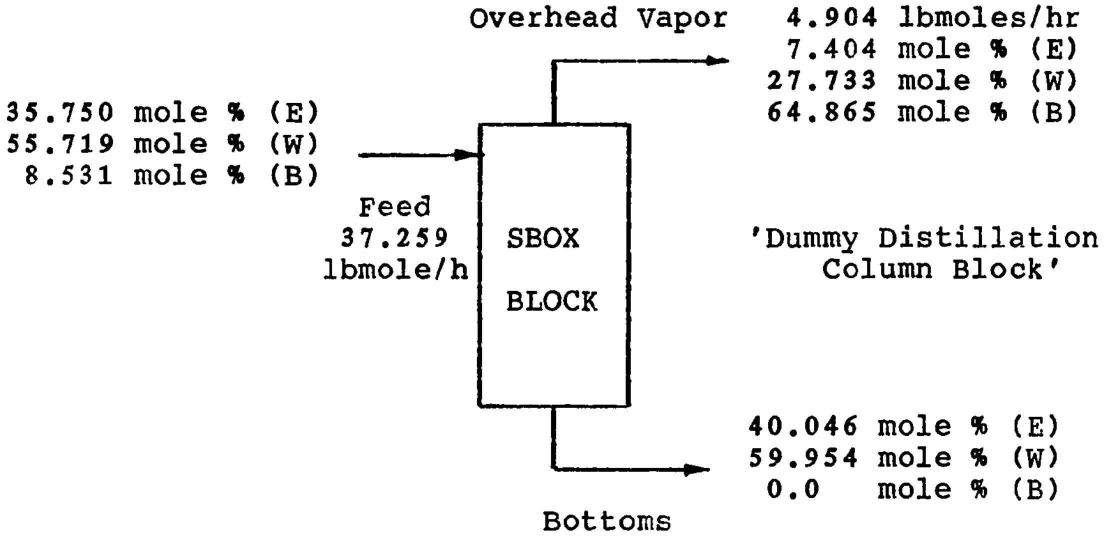


Table 6.11: Benzene Stripping Column Results with Ethanol Product Specification of 99.75+ mole % and Azeotropic Column Feed Concentration of 83.0 mole % Ethanol

Distillation column performance with ABDIS

Ser. #	P (psia)	Vapor Distillate			Bottoms		
		EtOH	Wtr	Bz	EtOH	Wtr	Bz
1	14.696	22.919	21.023	56.054	37.700	60.970	1.329
2	0.5	24.041	15.982	59.989	37.515	61.743	0.732

Note: All the compositions are in mole %

Fig. 6.19: Benzene Stripping Section (using block SBOX) Results with Ethanol Product Specifications of 99.25 + mole % and Azeotropic Column Feed Concentration of 82.82 mole % Ethanol

The following results are obtained using PROSIM.

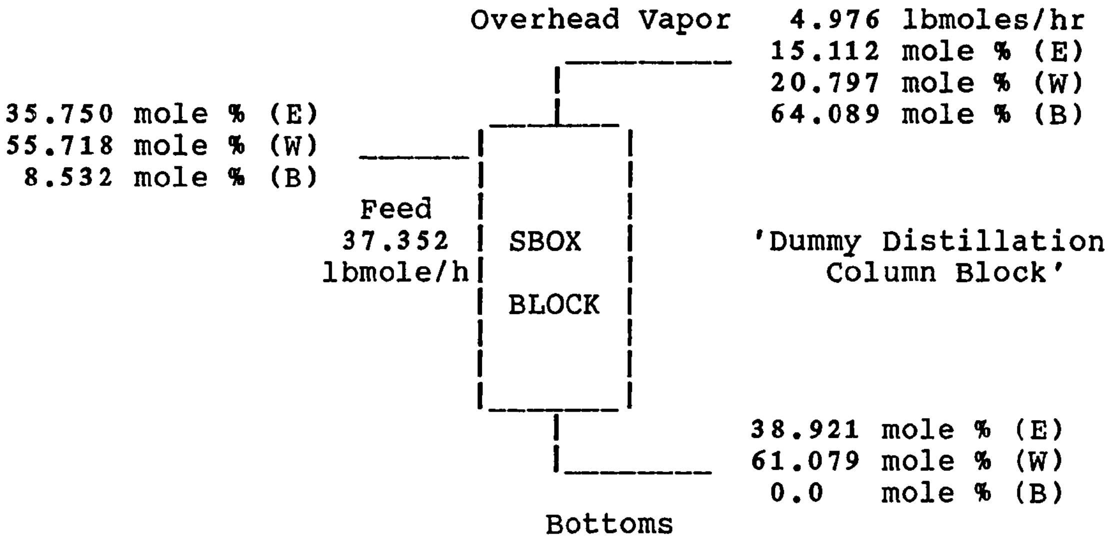


Table 6.12: Benzene Stripping Section Results with Ethanol Product Specifications of 99.75 + mole % and Azeotropic Column Feed Concentration of 82.82 mole % Ethanol

Distillation column performance with ABDIS

Ser. #	P (psia)	Vapor Distillate			Bottoms		
		EtOH	Wtr	Bz	EtOH	Wtr	Bz
1	14.696	22.925	21.026	56.049	37.718	61.052	1.230
2	6.0	21.976	18.440	59.584	37.864	61.449	0.687
3	1.0	22.713	15.952	61.335	37.751	61.832	0.418

Note: All the compositions are in mole %

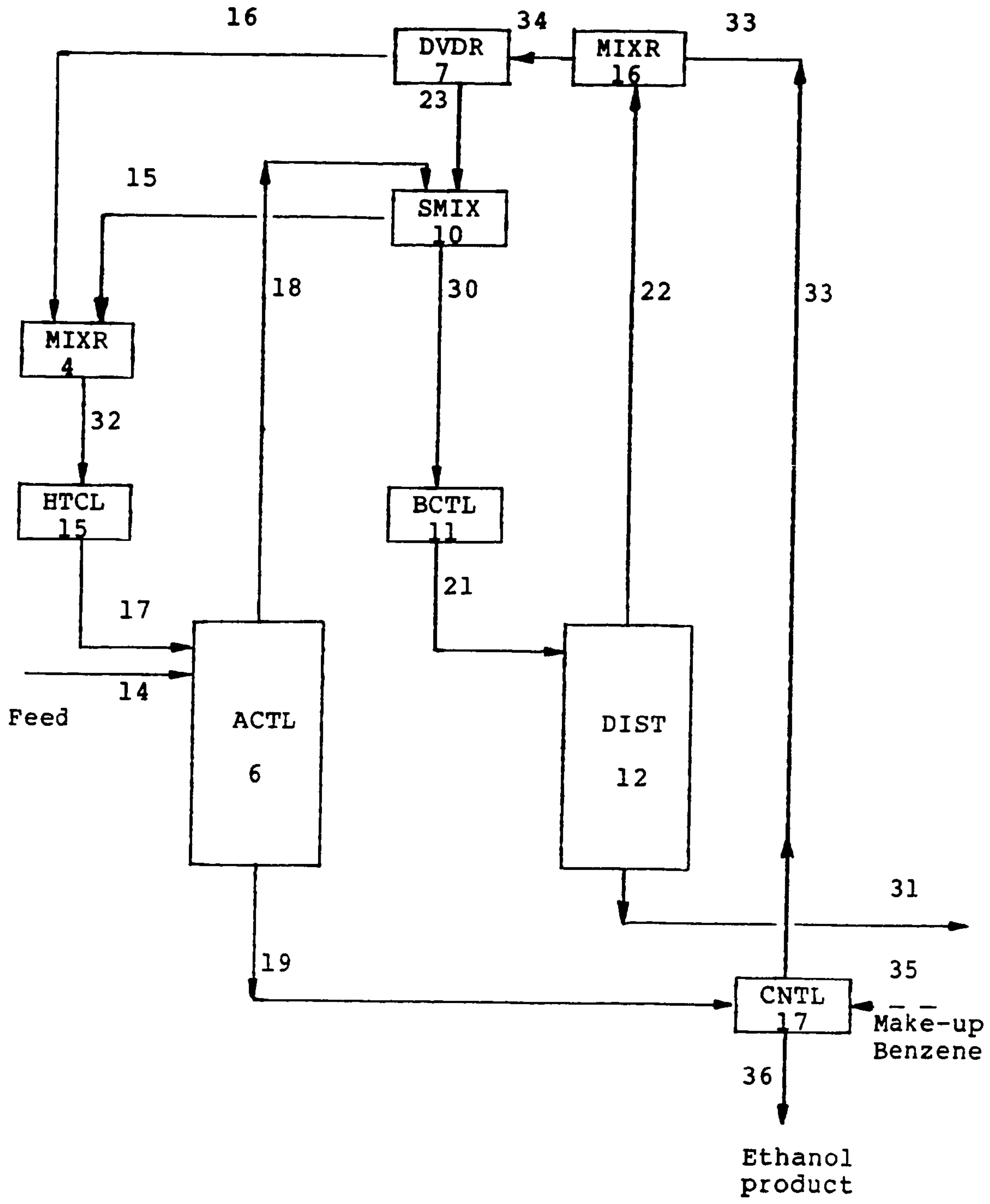


Fig. 6.20 Block Diagram (Type A Scheme) for Industrial Ethanol Azeotropic Distillation Process

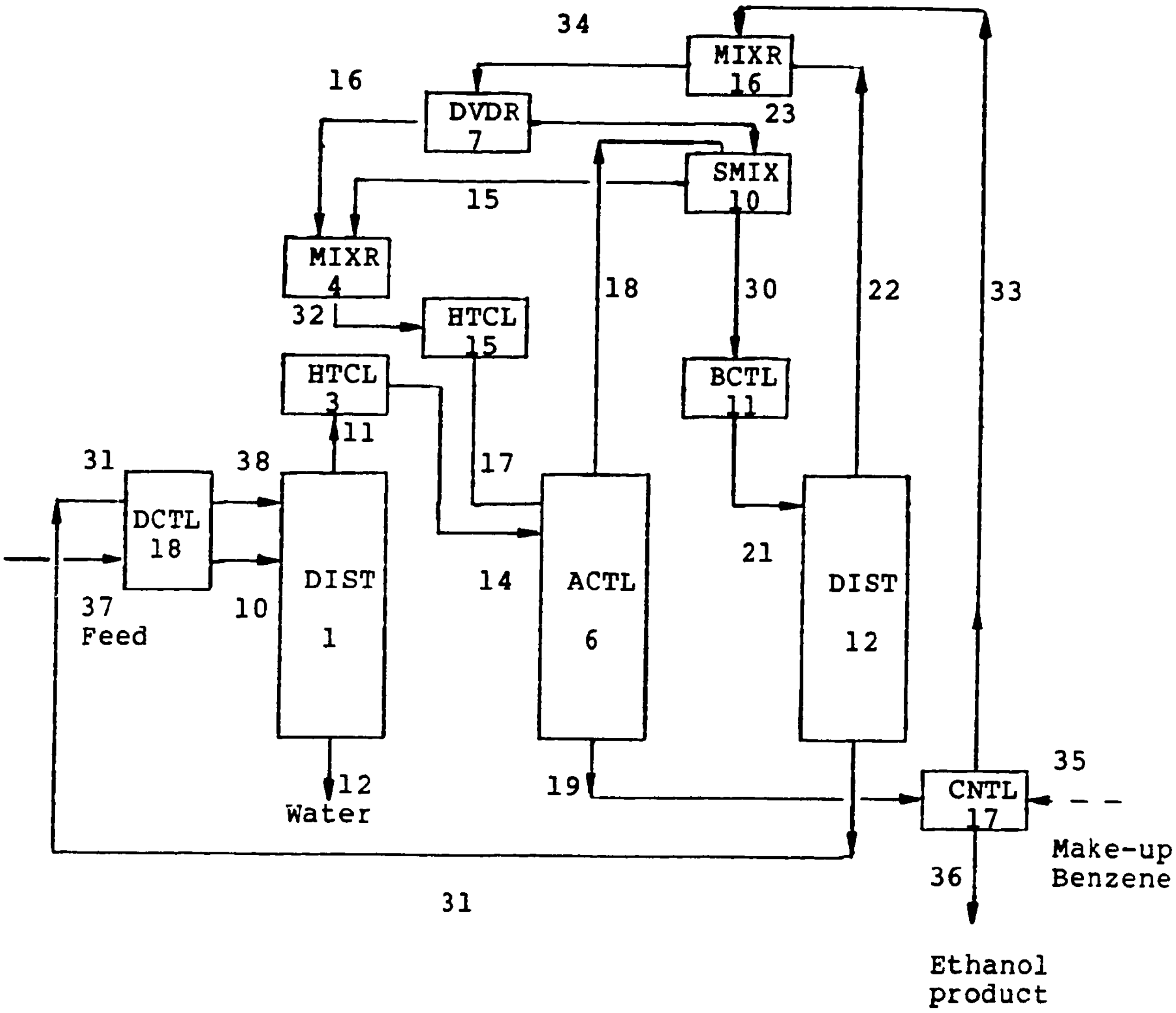


Fig 6.21 Block Diagram (Type B Scheme) for Industrial Ethanol Azeotropic Distillation Process

Chapter (Fig. 6.1 - 6.5). The research was focused on the two primary configurations (Type A and B) given in the form of block diagrams in Figs. 6.20 and 6.21. The Type A flowscheme is a subset of Type B flowscheme, but from a process analysis standpoint they are considered as different configurations. The Type A flowscheme includes only two distillation columns, the azeotropic column and the benzene stripping column. The Type B scheme includes three columns, an additional one is the ethanol concentrator.

- Scheme A (Fig. 6.20) assumes the main process feed is concentrated ethanol (approximately 82.8 mole %). The primary dry ethanol product stream (36) is withdrawn as the bottoms from the azeotropic column (Block 6) and the other output stream (31) contains significant amount of ethanol.
- The objective of Scheme B (Fig. 6.21) is to process a very dilute alcohol feed stream (37) with ethanol concentration of approximately 3.2 mole % (7.79 wt. %) and simultaneously recover ethanol from Stream 31.

Based on the analysis of the major segments of the flowscheme and the sensitivity studies reported in Sections 6.1-6.3, new blocks were introduced in PROSIM. The system description of these blocks is covered in Section 2.4.1. Since Scheme A is a subset of Scheme B, the discussion would be based on Scheme B as represented by the block diagram in Fig. 6.21. The simulation results are reported in the following Section 6.5. The stream numbers in Figs. 6.20 and 6.21 are consistent.

Azeotropic Distillation Block

The overhead vapor composition in the single phase region and the production of wet alcohol are the main problems encountered during the recycle calculations. The use of either block BCTL, DCTL, or DSPT (Section 2.4.2), for controlling the distillation rate, in conjunction with the distillation block has been found to yield instability in the flowsheet calculations. Because of this fact blocks ACTL and ECTL (discussed in Section 2.4.1) were introduced.

The ACTL block has been designed to manipulate the azeotropic column overhead vapor rate. The bottoms product specification of 99+ mole % ethanol, less than 10 ppm (mole) water, and less than 1 mole % benzene is built into this block. ACTL provides computational stability from the stand point of overhead and bottoms compositions. It was experienced that the use of the distillation (DIST) block, for the azeotropic tower, introduces problems after the first or second trial of the process plant recycle calculations. The computational instability in using DIST may be due to the fact that the distillate rate requires a dynamic change because of the change in the recycle (entrainer) rate in the iterative calculation procedure.

Two-Liquid Phase Decanter Block

Introduction of SMIX block in the place of a condenser and a two-liquid phase separator reduces the number of blocks in the flow scheme and therefore reduces the affiliated computational efforts. Moreover the old version of CHESS (Chemical Engineering Simulation System) was not equipped with any module to represent two liquid phase processes. It should be noted that the two liquid streams leaving this SMIX block are always in equilibrium with each other at a constant temperature.

It was experienced that the use of inappropriate parameters, in either NRTL or UNIQUAC equations, introduced severe errors in the composition and rate of each of the streams (Streams 15 and 30 in Fig 6.21) leaving the block SMIX. Since these two streams are in equilibrium, a simultaneous incorrect prediction of both the streams makes the recycle calculations diverge. On the other hand, error in the prediction of (Streams 15 and 30) compositions may generate another set of incorrect simulation results. Selection of Streams 15 and 30 as tear streams for the recycle calculations provides a better control because its initial estimate is made based on the composition of the overhead vapor stream from the azeotropic column.

Benzene Stripping Section Configuration

The behavior of the benzene stripper was observed to be very stiff. This may be attributed to the following facts:

A. Inflexibility in the composition of the feed (Stream 30) to the stripper, as discussed in the Section 6.1.3.

B. Predicted overhead composition as the ethanol-water-benzene azeotrope at the column pressure.

C. Simultaneous operation of recovering benzene as distillate, and material balancing ethanol and water as the bottoms.

Because of azeotrope formation, the overhead composition in the stripping is constrained and this in effect sets the bottoms (Stream 31) composition. Because of above stated constraints the use of DIST block as a stripper at the atmospheric pressure leads to divergence in the flowsheet calculations. A detailed investigation of the effect of ethanol-water feed (to the azeotropic column) composition on the benzene stripper is reported in Section 6.3. To obtain the preliminary solution and suitable stripping operating conditions a dummy column block (SBOX) was introduced in the flowscheme, Fig. 6.21. The system description of SBOX is covered in the Section 2.4. The use of SBOX establishes the material balance constraints for the real benzene stripping column.

Benzene Stripper Overhead Vapor Stream Recycle Location

The Stream 22 leaving the stripper has a composition of approximately 23.5 mole % ethanol, 18.4 mole %, and 58.3 mole % benzene, which will form two liquid phases after condensation to 35 ^{o}C temperature. Therefore the best process choice would be to direct Stream 22 towards the SMIX block, by forcing Stream 16 from the DVDR (Block 7) to be a null stream. Since the rate ratio of Stream 18 over Stream

23 is approximately 57 (for 82.9 mole % ethanol feed to the azeotropic column), the rate of Stream 22 does not adversely affect the rate and composition of Streams 15 and 30 (Fig. 6.21) significantly.

Make-up Benzene Location

In the flowscheme calculations the make-up benzene was introduced in the two liquid phase decanter, by mixing it with the vapor distillate from the benzene stripper (Block 12). Since the rate of make-up benzene stream is not significant, its location is chosen to minimize a process upset. The addition of make-up stream as shown in Fig. 6.21 would cooperate in the liquid-liquid separation phenomena, which is a very desirable feature in this process plant. A special block CNTL, Fig. 6.21, estimates the amount of the make-up benzene on the basis of benzene losses in the dry ethanol product (Stream 19). The system description of the CNTL block is covered in Section 2.4.1.

Ethanol Concentrator and Ethanol Recovery

Ethanol leaving in Stream 31 (Fig. 6.21) is about 37 mole %, therefore its recovery is economically important. This objective is achieved by introducing an ethanol concentrator into the Type B process flowscheme. Thus Stream 31 is recycled to the process via an ethanol-water column (Block 1). Introduction of a two feed binary distillation column serves two purposes:

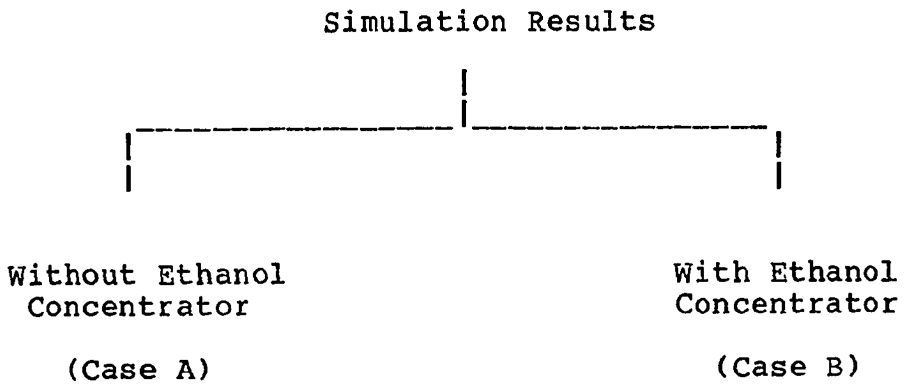
a) It concentrates the primary aqueous alcohol feed (approximately 3.25 mole % or 7.79 wt. %) to the desired concentration near the azeotrope.

b) It recovers the ethanol from the recycle Stream 31.

In such a developed flowscheme (Type B) high purity dry ethanol (99+ mole %) is produced as the bottoms from the azeotropic column and gross water is purged from the ethanol concentration column as the bottoms product. The simulation results of two cases are presented in the following section.

6.5 Simulation of Industrial Ethanol Azeotropic Distillation Process using PROSIM (PROcess SIMulator)

The simulation studies were conducted foran industrial ethanol azeotropic distillation process using PROSIM as a tool, developed as part of the research. The simulation results are classified as shown below:



The Cases A and B correspond to Type A and Type B flowschemes respectively as discussed in Section 6.4.

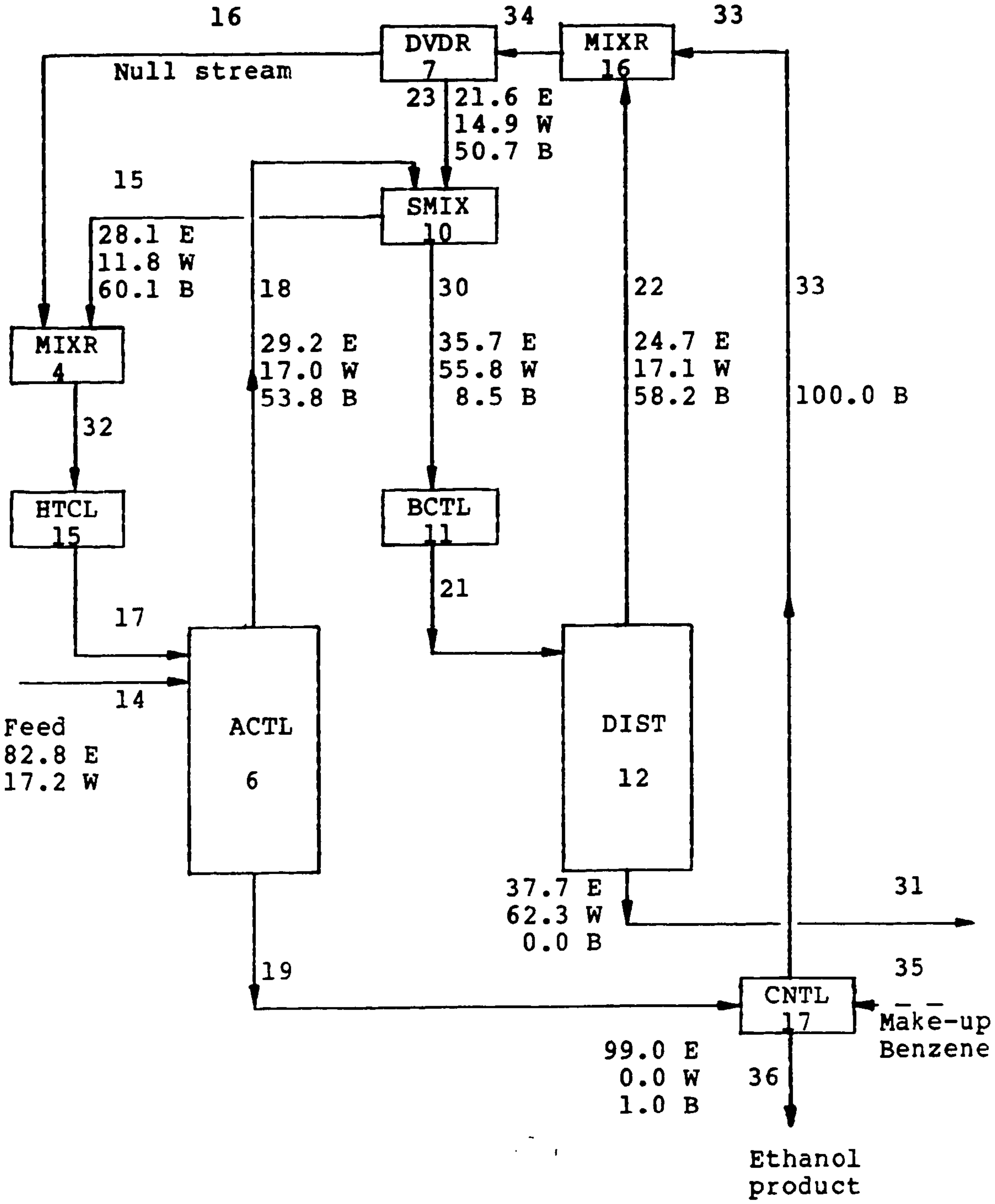
6.5.1 Simulated Process without Ethanol Concentrator (Case A)

PROSIM is based on sequential modular calculation approach. The final results obtained after iterative recycle calculations using Type A block diagram shown in Fig. 6.22 and Table 6.13. The final stream conditions of the simulated process plant are reported in Table 6.13. Appendix F consists of a complete set of process and design variables as input, and the final results obtained for Case A.

Streams 15 and 30 were selected as the tear streams. The calculations demand very good initialization values, which are also given in Appendix F. A concentrated ethanol-water (82.8 mole % ethanol) feed is introduced into the process via azeotropic tower and dry ethanol (99 mole %) is withdrawn as the main product. The azeotropic column (Block 6) operates at the atmospheric pressure whereas the benzene stripper (Block 12) operates at 1 psia in the Type A scheme. It is observed that overhead vapor Streams 18 and 22 (from distillation column blocks 6 and 12 respectively) are azeotropic mixtures as estimated by VLE NRTL parameters (Gmehling et al., 1977). This fact provides stability in the two liquid phase decanter (Block SMIX), where liquid-liquid equilibria calculations are done using LLE NRTL parameters (Sorensen et al., 1979) at 35°C.

6.5.2 Simulated Process Including Ethanol Concentrator (Case B)

Simulation of Type B scheme introduces more complexities as compared to that of the Type A scheme discussed in the Section 6.5.1. The final results are shown in the Fig. 6.23 and Table 6.14. A complete computer simulation, including process conditions, initial values, and final computed



Note: All the compositions are in mole %
E - Ethanol, W - Water, B - Benzene

Fig 6.22 Simulated Industrial Ethanol Azeotropic Distillation Process without Ethanol Concentrator (Case A)

Table 6.13

Simulation Results: Industrial Ethanol Azeotropic Distillation Process

```
*** CHEMICAL ENGINEERING PROCESS FLOWSHEET SIMULATION ***

                  PROSIM VERSION ONE

                      MARCH  1985

CASE A : INDUSTRIAL ETHANOL AZEOTROPIC DISTILLATION PROCESS

SYSTEM:    ETHANOL-WATER-BENZENE

VLE AND LLE EQUATIONS: NRTL** AND IDEAL GAS

STREAM NUMBER           14          15          16          17

EQUIP CONXION        0 TO  6    10 TO  4     7 TO  4    15 TO  6

VAPOR FRACTION        0.0000      0.0000      0.9098      0.0000
TEMPERATURE, F       95.0000     95.0000     45.7580     95.0000
PRESSURE, PSIA       14.6960     14.6960      1.0000     14.6960
ENTHALPY, K-BTU    -238.6199   -669.5720      0.0000   -668.7388
L/H LIQUID FRAC       1.0000      1.0000      1.0000      1.0000

           COMPONENTIAL FLOWRATES, LB-MOLES/UNIT TIME

ETOH                95.36771    78.76645     0.00000    78.57763
WATER               19.78290    33.08500     0.00000    32.94643
BENZENE              0.00000   168.15891     0.00000   168.11349

           TOTAL   115.15060   280.01035     0.00000   279.63757

STREAM NUMBER           18          19          22          23

EQUIP CONXION        6 TO 10     6 TO 17    12 TO 16     7 TO 10

VAPOR FRACTION        1.0000      0.0000      1.0000      0.9098
TEMPERATURE, F      149.1139    171.6422     52.4409     45.7580
PRESSURE, PSIA       14.6960     14.6960      1.0000      1.0000
ENTHALPY, K-BTU    4497.7769     -1.5666     69.4771     67.3723
L/H LIQUID FRAC       1.0000      1.0000      1.0000      1.0000

           COMPONENTIAL FLOWRATES, LB-MOLES/UNIT TIME

ETOH                90.60188    83.34265     1.35585     1.35585
WATER               52.72929     0.00000     0.93700     0.93700
BENZENE            167.30380     0.80902     3.18826     3.99728

           TOTAL   310.63498    84.15167     5.48111     6.29012
```

```
STREAM NUMBER          30          31          32          33

EQUIP CONXION       10 TO 11    12 TO  0     4 TO 15    17 TO 16

VAPOR FRACTION        0.0000      0.0000      0.0000      0.0000
TEMPERATURE, F       95.0000     75.8444     94.9984     95.0000
PRESSURE, PSIA       14.6960      1.0000     14.6960     14.6960
ENTHALPY, K-BTU     -78.7528    -79.4617   -668.7445     -2.1034
L/H LIQUID FRAC       1.0000      1.0000      1.0000      1.0000

         COMPONENTIAL FLOWRATES, LB-MOLES/UNIT TIME

ETOH                13.19192    11.97723    78.57763     0.00000
WATER               20.58685    19.83069    32.94643     0.00000
BENZENE              3.13598     0.00002   168.11349     0.80902

         TOTAL      36.91476    31.80794   279.63757     0.80902



STREAM NUMBER          34          35          36

EQUIP CONXION       16 TO  7     0 TO 17    17 TO  0

VAPOR FRACTION        0.9098      0.0000      0.0000
TEMPERATURE, F       45.7580     95.0000    171.6422
PRESSURE, PSIA        1.0000     14.6960     14.6960
ENTHALPY, K-BTU      67.3723     -2.1034     -1.5666
L/H LIQUID FRAC       1.0000      1.0000      1.0000

         COMPONENTIAL FLOWRATES, LB-MOLES/UNIT TIME

ETOH                 1.35585     0.00000    83.34265
WATER                0.93700     0.00000     0.00000
BENZENE              3.99728     0.80902     0.80902

         TOTAL       6.29012     0.80902    84.15167
```

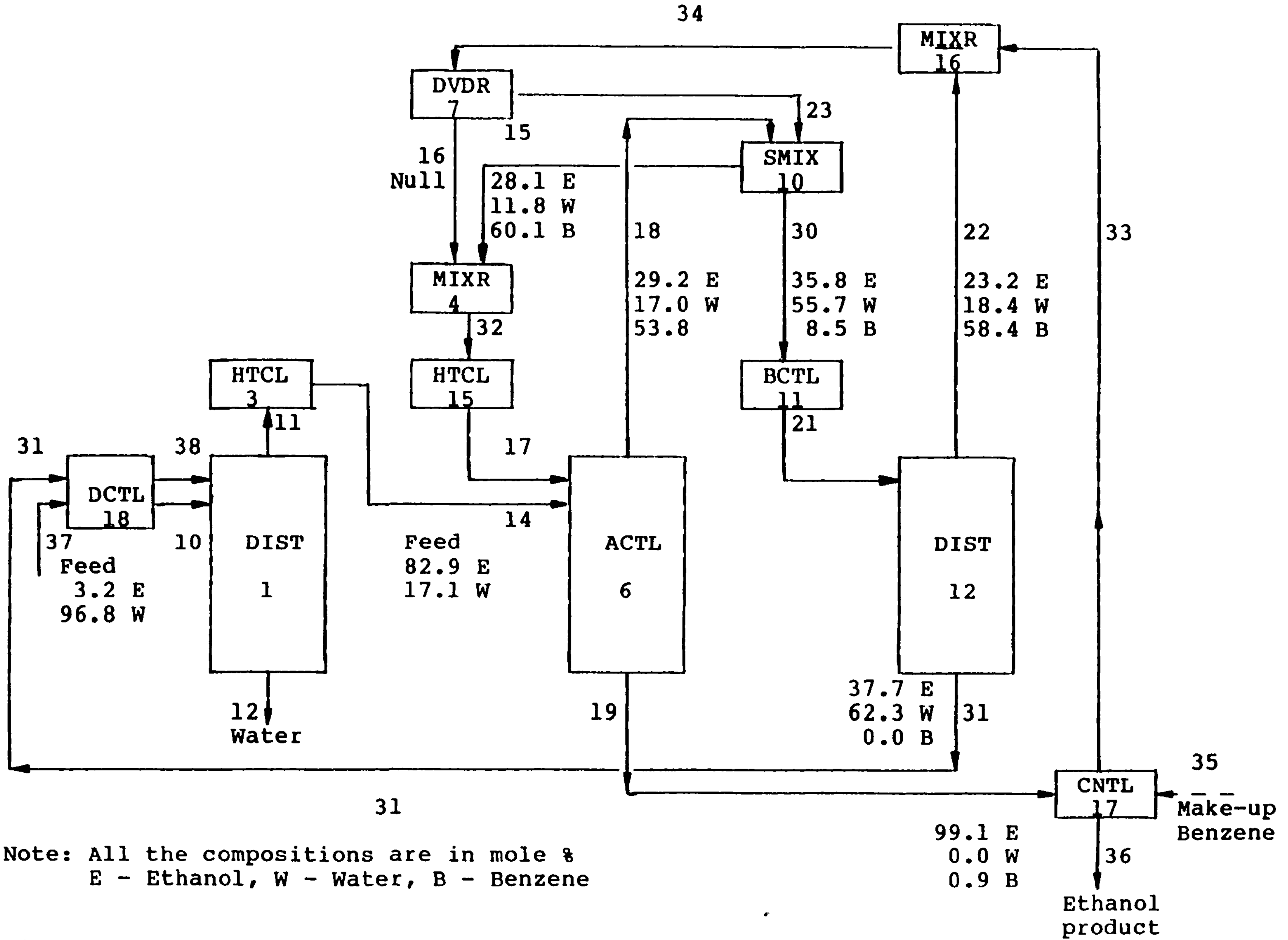
Note: ** - VLE and LLE NRTL parameters were used in the VLE and LLE systems respectively.

stream variables, is presented in Appendix F.

The aqueous alcohol feed to the process consists of approximately 3.2 mole % (7.79 wt. %) ethanol, with concentration to 82.8 % ethanol being accomplished in an ethanol concentration column. In addition to Streams 15 and 30, Stream 14 was also used as the tear stream. A good estimate of the tear stream values were established by preliminary flowsheet calculations using SBOX instead of DIST as Block 12. The rate of Stream 11 was maintained at a constant value bypassing DCTL (Block 18) calculations which provided flexibility to the compositions of Stream 14.

It should be noted that the feed (Stream 14) to the azeotropic column in Fig. 6.23 attains an ethanol concentration of 82.9 mole % as compared to 82.8 mole % in Fig. 6.21. Based on the componential rates of Streams 14 and 19 (Fig. 6.23), the ethanol concentration in Stream 31 increases from 37.7 to 37.9 mole %. At the same time a comparison between Fig. 6.22 and 6.23 show an increase in ethanol concentration from 35.7 to 35.8 mole % takes place in Stream 30. The above changes have a relatively significant effect on the composition of the overhead vapor (Stream 22) from the stripping column (Block 12). It has been stated earlier in Section 6.4 that composition of Stream 22 is constrained by the ternary azeotrope formation at the column pressure conditions. Therefore to satisfy the component material balance of the benzene stripping column (Block 12), it was required to maintain the column pressure at 4.8 psia.

The design pressure of 1 atmosphere in the benzene



Note: All the compositions are in mole %
E - Ethanol, W - Water, B - Benzene

Fig 6.23 Simulated Industrial Ethanol Azeotropic Distillation Process (Case B)

Table 6.14

Simulation Results: Industrial Ethanol Azeotropic Distillation Process (Case B)

```
*** CHEMICAL ENGINEERING PROCESS FLOWSHEET SIMULATION ***

                    PROSIM VERSION ONE

                        MARCH  1985

CASE B: INDUSTRIAL ETHANOL AZEOTROPIC DISTILLATION PROCESS

SYSTEM:  ETHANOL-WATER-BENZENE

VLE AND LLE EQUATIONS: NRTL** AND IDEAL VAPOR


STREAM NUMBER        10          11          12          14

EQUIP CONXION      0 TO  1     1 TO  3     1 TO  0     3 TO  6

VAPOR FRACTION      0.0000      0.0000      0.0000      0.0000
TEMPERATURE, F    184.0000    153.8289    211.9922     95.0000
PRESSURE, PSIA     14.6960     14.6960     14.6960     14.6960
ENTHALPY, K-BTU -1250.2102    -67.7280     -3.6281   -238.5979
L/H LIQUID FRAC     1.0000      1.0000      1.0000      1.0000

          COMPONENTIAL FLOWRATES, MOLES/UNIT TIME

ETOH              83.43170    95.45193     0.00037    95.45193
WATER           2528.23047    19.69789  2528.23340    19.69789
BENZENE            0.00000     0.00008     0.00000     0.00008

         TOTAL  2611.66187   115.14990  2528.23364   115.14990


STREAM NUMBER        15          16          17          18

EQUIP CONXION     10 TO  4     7 TO  4    15 TO  6     6 TO 10

VAPOR FRACTION      0.0000      0.8775      0.0000      1.0000
TEMPERATURE, F     95.0000     99.6651     95.0000    149.1172
PRESSURE, PSIA     14.6960      4.8000     14.6960     14.6960
ENTHALPY, K-BTU   -668.9789      0.0000   -669.0304   4498.3696
L/H LIQUID FRAC     1.0000      1.0000      1.0000      1.0000

          COMPONENTIAL FLOWRATES, MOLES/UNIT TIME

ETOH               78.62567     0.00000    78.63961    90.65314
WATER              32.98320     0.00000    32.99416    52.69683
BENZENE           168.12511     0.00000   168.12692   167.32634

         TOTAL    279.73398     0.00000   279.76068   310.67633
```

```
STREAM NUMBER          19          21          22          23

EQUIP CONXION        6 TO 17    11 TO 12    12 TO 16     7 TO 10

VAPOR FRACTION        0.0000      0.0000      1.0000      0.8775
TEMPERATURE, F      171.6569     95.0000    101.9489     99.6651
PRESSURE, PSIA       14.6960     14.6960      4.8000      4.8000
ENTHALPY, K-BTU      -1.5339    -79.2645     73.4274     71.3476
L/H LIQUID FRAC       1.0000      1.0000      1.0000      1.0000

          COMPONENTIAL FLOWRATES, MOLES/UNIT TIME

ETOH                83.43219    13.28153     1.26078     1.26078
WATER                0.00000    20.70020     0.99885     0.99885
BENZENE              0.79995     3.16979     3.16971     3.96967

         TOTAL      84.23215    37.15152     5.42935     6.22930




STREAM NUMBER          30         31          32          33

EQUIP CONXION       10 TO 11   12 TO  1     4 TO 15    17 TO 16

VAPOR FRACTION        0.0000     0.0000      0.0000      0.0000
TEMPERATURE, F       95.0000   129.9099     94.9976     95.0000
PRESSURE, PSIA       14.6960     4.8000     14.6960     14.6960
ENTHALPY, K-BTU     -79.3082   -42.7308   -669.0167     -2.0798
L/H LIQUID FRAC       1.0000     1.0000      1.0000      1.0000

          COMPONENTIAL FLOWRATES, MOLES/UNIT TIME

ETOH                13.28933   12.02075    78.63961     0.00000
WATER               20.70906   19.70135    32.99416     0.00000
BENZENE              3.17323    0.00008   168.12692     0.79995

         TOTAL      37.17162   31.72217   279.76068     0.79995
```

```
STREAM NUMBER          34          35          36

EQUIP CONXION      16 TO  7     0 TO 17    17 TO  0

VAPOR FRACTION       0.8775      0.0000      0.0000
TEMPERATURE, F      99.6651     95.0000    171.6569
PRESSURE, PSIA       4.8000     14.6960     14.6960
ENTHALPY, K-BTU     71.3476     -2.0798     -1.5339
L/H LIQUID FRAC      1.0000      1.0000      1.0000

          COMPONENTIAL FLOWRATES, MOLES/UNIT TIME

ETOH                1.26078     0.00000    83.43219
WATER               0.99885     0.00000     0.00000
BENZENE             3.96967     0.79995     0.79995

          TOTAL     6.22930     0.79995    84.23215
```

Note: ** - The VLE and LLE parameters were used to represent vapor-liquid and liquid-liquid equilibria respectively.

stripping column causes divergence in the sequential modular recycle calculations. Hence the analysis of the two flowschemes (Type A and B) demonstrates the sensitivity of the process conditions. The comments made by Keister (1982) and Black (1980) about the stripping column design flexibility are contrary to the results obtained in this research study. The flexibility in the stripping column may exist if the composition of Stream 30 is erroneous.

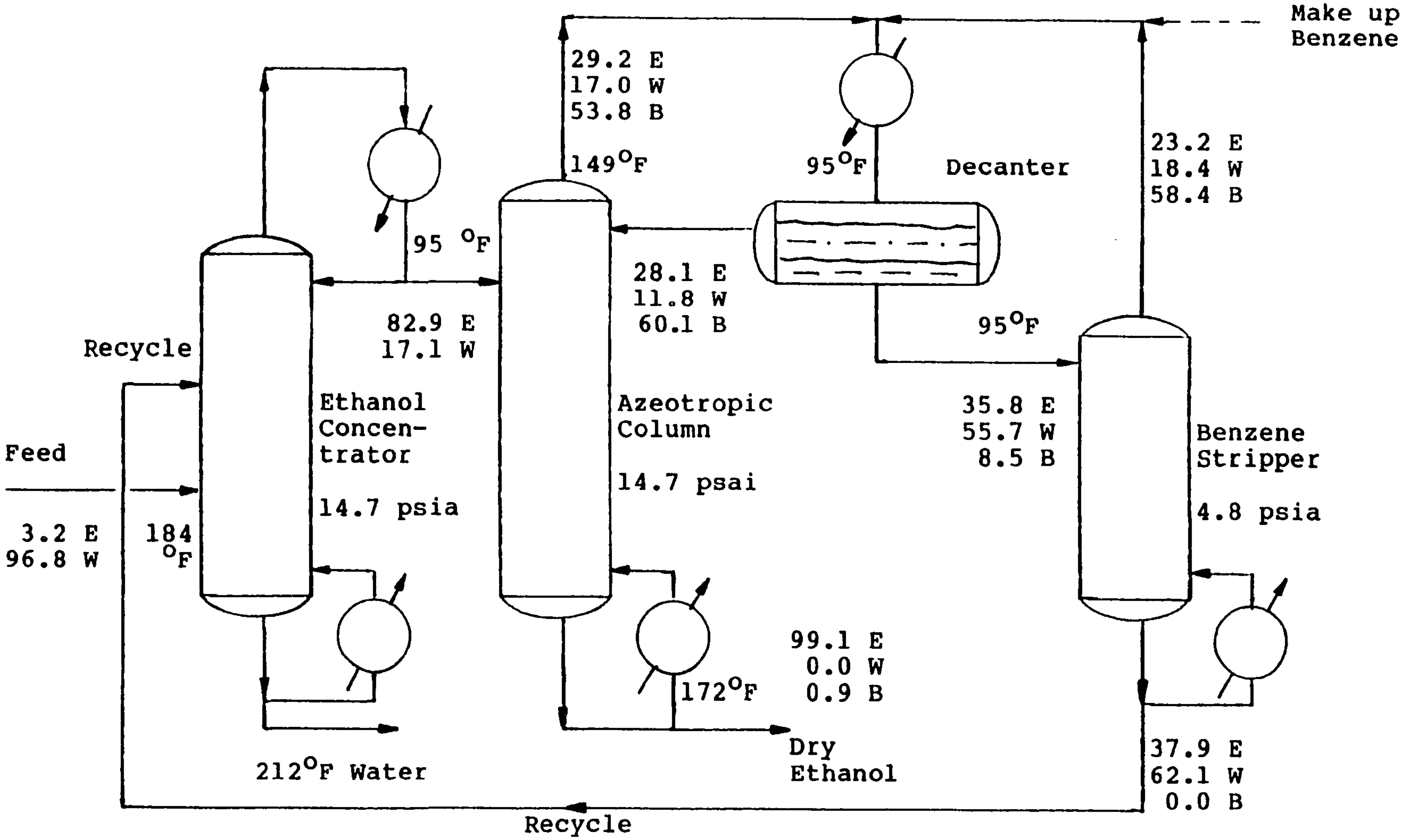
An incorrect prediction of the composition (Stream 30) is possible if either an incorrect set of parameters or an inferior equation is used for ternary liquid-liquid equilibria calculations in the decanter (Block 10). A comparison of ties line calculated (Table 4.17) by NRTL and UNIQUAC equations demonstrate the superiority of the NRTL over UNIQUAC for this system. Because of this fact the NRTL equation was used for the two liquid phase calculations (Block 10). This is very evident from the investigation that the complete process operates under very narrow operating conditions.

6.6 Conclusions

A detailed analysis and simulation of an industrial ethanol azeotropic distillation process using benzene as an entrainer reveals that the individual units as well as the complete process plant operate within very a narrow range of operating conditions. The process simulator (PROSIM) developed as part of the research work was used to attain the viable simulation results. PROSIM includes elegant process modules to simulate highly non-ideal distillation, liquid-liquid systems, and various control blocks to aid in obtaining the solution in the desired operating region.

The research concludes that a scheme (Type B) involving three distillation columns (ethanol concentrator, azeotropic column, and benzene stripping) and a two-liquid phase decanter, shown in Fig. 6.24, is the most suitable configuration for producing dry ethanol. The ethanol-water feed to the azeotropic column is a key process variable and a detailed study in Chapters 5 and 6 show that a very small window (82.8-82.9 mole % ethanol) of feed composition to the azeotropic column can make the process simulation feasible. The ethanol concentration in the binary (ethanol-water) azeotrope at 1 atmosphere is 89.43 mole % (Weast, 1975). The effect of this binary feed composition on the azeotropic column is covered in Chapter 5. The investigation of binary feed composition on the benzene stripping column is discussed in the Section 6.2.

A similarity has been observed in the azeotropic tower and the benzene stripper in terms of their overhead vapor compositions being ternary (ethanol-water-benzene) azeotropic mixtures. This phenomena invites the strategy of combining these two streams and then condensing to form two liquid phases in the decanter. Representation of vapor-liquid and liquid-liquid equilibria using different sets of parameters, in the NRTL equation, obtained from the respective ternary experimental data is of utmost importance.



Note: E - Ethanol; W - Water; B - Benzene; All the compositions are in mole %

Fig. 6.24 Simulated Industrial Ethanol Azeotropic Distillation Process Flowscheme (Case B)

The presence of 8.5 mole % benzene in the water phase from the two liquid phase decanter restricts the operatibility of the benzene stripping process. Therefore a design pressure of 4.8 psia (Fig. 6.23) is required to achieve the required material balance in the benzene stripper. The dry alcohol product specification of 99+ mole %, less than 10 ppm (mole) water, and less than 1 mole % is also an important variable. The effect of product specification on the benzene stripping column is discussed in the Section 6.3. The product specification of 99.75+ mole % ethanol, increases the benzene concentration in the overhead vapor from the benzene stripper. This phenomena places the benzene stripper in an infeasible operating region if benzene has to be completely recovered in that column. Simulation results of two process configurations (A and B) are reported and discussed in the Section 6.5.

CHAPTER 7

OVERALL CONCLUSIONS AND RECOMMENDATIONS FOR FUTURE RESEARCH

7.1 Overall Conclusions

A process simulator (PROSIM) of extensive process capabilities was developed based on the executive of CHESS program. Major features of PROSIM includes:

- A rigorous multi-stage distillation/absorption model based on Naphthali-Sandholm (1972) method.
- A capability of simulating three phase (vapor-liquid-liquid) processes.
- New and advanced control blocks for a wide range of process applications.

A comprehensive analysis and simulation, using PROSIM, of the industrial ethanol azeotropic distillation process using benzene as the entrainer reveals that the individual process units as well as the complete process plant operate over very limited range of operating conditions. A suitable flowscheme has been developed incorporating an ethanol concentrator, an azeotropic tower, a two liquid phase decanter, and a benzene stripper as the key process units. An optimum azeotropic column aqueous feed concentration of 82.9 mole % ethanol and 17.1 mole % water has been established for the simulated process plant.

The composition of the overhead vapor from azeotropic and benzene stripping columns falls in the two liquid phase region, after condensation to 35°C. The dry ethanol product specification of 99+ mole % requires the benzene stripping column pressure to be at 4.8 psia. The increase in product specification value from 99+ mole % to 99.75+ mole % (ethanol), for a constant aqueous ethanol feed composition to the azeotropic column, increases the benzene to ethanol ratio, in the stripper overhead vapor, from 2.4 to 4.4. This fact, determined by using the dummy separation module, introduces difficulty in the simulation calculations because in the actual benzene stripper the overhead composition is restricted by the ethanol-water-benzene azeotrope formation.

An extensive study of azeotropic column shows the existence of multiple solutions. The desired solution can be achieved by manipulating the column material balance. Relationships between entrainer to feed rate ratio and bottoms rate versus ethanol concentration in the aqueous alcohol feed to the azeotropic tower have been established. It is concluded that for a constant ethanol-water feed to the azeotropic column, a very narrow range of entrainer and distillate rates can make the azeotropic column operational in the desired region with the overhead vapor in the required two liquid phase envelope and dry high purity ethanol as bottoms.

In another part of the research, a global set of modified UNIQUAC interaction parameters have been estimated, after the rigorous thermodynamic analysis of the ethanol-water-benzene system. The simultaneous regression of two isobaric binary vapor-liquid systems (ethanol-water and ethanol-benzene) and a single tie line (ethanol-water-benzene liquid-liquid system) yielded a set of parameters which can simulate the azeotropic column and the two liquid phase decanter in the process. The analysis was conducted using a regression package developed as part of this research work. Various minimization objective functions, including new ones, for vapor-liquid and liquid-liquid equilibria were evaluated in the selection process.

Finally, the performance of twelve potential entrainers was evaluated using the UNIFAC group contribution activity coefficient equation. The study shows that the following entrainers can be used in the ethanol dehydration process: benzene, cyclohexane, methyl cyclopentane, n-hexane, 2-methyl pentane, 1-hexene, and 2,2,3-trimethyl butane. In a study performed by Black (1980), n-pentane and diethyl ether can be used as the potential entrainers but unfortunately neither the thermodynamic parameters nor the experimental VLE data reported in the public literature.

7.2 Recommendations for Future Research

The future research can be conducted in the various areas related to the alcohol dehydration processes. Recommendations can be broadly classified into six areas:

- Process simulator -- expansion of the present version of PROSIM
- Steady state simulation of alternate alcohol dehydration processes, for example ethanol drying via liquid-liquid extraction process

- Simulation methods and computational algorithms
- Non-linear regression analysis of VLE and LLE data
- Phase equilibria calculation techniques
- Dynamic simulation of the process plant

7.2.1 Process Simulator

The following recommendations are made as enhancements to the process simulator (PROSIM):

1. The introduction of analytical, numerical, or direct search optimization techniques to study process optimization with respect to various variables.
2. Expansion of the rigorous computational algorithm to incorporate occurrence of chemical reaction in the distillation column as discussed by Murthy (1984).
3. Extension of distillation model to simulation three phase systems.
4. Incorporation of an liquid-liquid extraction algorithm proposed by Roche (1984).
5. Incorporation of the batch distillation model proposed by Clarke (1985) and Springer (1985).
6. Expansion of process modeling approach, using equation of state, reported by Banerjee (1985).
7. Inclusion of a broad component property database.

7.2.2 Steady State Simulation of Alcohol Dehydration Processes

Simulation of the alternate industrial alcohol dehydration processes using sophisticated techniques like liquid-liquid extraction and supercritical extraction can be considered as the potential future research work.

7.2.3 Simulation Methods and Computational Algorithms

Alternate process simulation approaches like

- Random sequential modular approach, and
- Simultaneous solution of equations approach

should be considered for the future work.

The multicomponent absorption/distillation program (ABDIS) should be investigated in the following areas:

1. Study of the sensitivity on the separation in the azeotropic distillation column with respect to numerical and analytical solution of partial derivatives.
2. New and efficient techniques to solve sparse matrices described by Holland (1981).

7.2.4 Non-linear Regression Analysis VLE and LLE data

The research work should be continued on the subject discussed in Chapter 3 of this dissertation. It is recommended to investigate the following areas for the estimation of interaction parameters.

1. Investigation of Murthy's non-linear regression algorithm (Roth, 1985) and maximum likelihood method (Anderson et al., 1978).
2. Improvement of Marquardt's regression package, with respect to the driver program and affiliated

subroutines.

3. Estimation of temperature dependent parameters for various activity coefficient model.
4. Global thermodynamic parameters estimation and their evaluation in the alcohol dehydration processes using entrainers other than benzene.

7.2.5 Phase Equilibria Calculation Techniques

The future studies should also concentrate on the following topics:

1. Investigation of the Knox (1984) activity coefficient model in the vapor-liquid and liquid-liquid process.
2. Entrainer study using a new group contribution model proposed by Knox (1982) for the prediction of liquid phase activity coefficients.
3. Incorporation of the equations of state proposed by Peng and Robinson (1976), Soave (1971), and Chao and Seader (1961) for the computation of vapor and liquid phase via single equation calculation approach as reported by Banerjee (1985).

7.2.6 Dynamic Simulation of the Alcohol Dehydration Processes

Dynamic simulation of the integrated process plant to incorporate the startup, shutdown and process variable change effects.

APPENDIX A

THERMODYNAMICS: LIQUID PHASE MODELS FOR NON-IDEAL SYSTEMS

A.1 Liquid Phase Activity Coefficient Models

  A.1.1 NRTL Equation

  A.1.2 Modified UNIQUAC Equation

  A.1.3 UNIFAC Equation

A.2 Modified UNIQUAC Model for Heats of Mixing

A.3 UNIFAC VLE Interaction Parameters Databank

A.1 Liquid Phase Activity Coefficient Equations

The NRTL (Non Random Two Liquid) equation developed by Renon (1968) and the modified UNIQUAC (UNIversal QUAsi Chemical) equation proposed by Anderson (1978) are used for the estimation of liquid phase activity coefficients in vapor-liquid and liquid-liquid systems. Whereas the UNIFAC (UNIQUAC Functional-group Activity Coefficients) group contribution method is used for the prediction of activity coefficients. NRTL and UNIQUAC equations consists of three and two temperature independent adjustable parameters, respectively for each pair of components.

A.1.1 NRTL Equation

For a multicomponent mixture activity coefficient of component i is represented by

$$\ln \gamma_i = \frac{\sum_i \tau_{ji} G_{ji} x_j}{\sum_k G_{ki} x_k} + \sum_j \frac{x_j G_{ij}}{\sum_k G_{kj} x_k} \left(\tau_{ij} - \frac{\sum_k \tau_{kj} G_{kj} x_k}{\sum_k G_{kj} x_k} \right) \tag{A.1}$$

where $\tau_{ji} = (\lambda_{ji} - \lambda_{ii})/RT$ $\quad G_{ji} = \exp(-\alpha_{ji}\tau_{ji})$ (A.2,A.3)

$\tau_{ij} = (\lambda_{ij} - \lambda_{jj})/RT$ $\quad G_{ij} = \exp(-\alpha_{ij}\tau_{ij})$ (A.4,A.5)

$\alpha_{ij} = \alpha_{ji}$ (A.6)

A.1.2 Modified UNIQUAC Equation

For any component i, the activity coefficient is given by

$$\ln \gamma_i = \ln \frac{\phi_i}{x_i} + (\frac{Z}{2})q \ln \frac{\theta_i}{\phi_i} + l_i - \frac{\phi_i}{x_i} \sum_j x_j l_j - q_i' \ln (\sum_j \theta_j' \tau_{ji}) + q_i' - q_i' \sum_j \frac{\theta_j' \tau_{ij}}{\sum_k \theta_k' \tau_{kj}} \qquad (2.1)$$

where segment fraction ϕ and area fractions θ and θ' are given by

$$\phi_i = r_i x_i / (\sum_j r_j x_j) \qquad \theta_i = q_i x_i / (\sum_j q_j x_j) \qquad (A.7, A.8)$$

$$\theta_i' = q_i' x_i / (\sum_j q_j' x_j) \qquad l_j = \frac{Z}{2} (r_j - q_j) - (r_j - 1) \qquad (A.9, A.10)$$

A.1.3 UNIFAC Equation

The UNIFAC method, developed by Fredenslund et al. (1975), is based on the UNIQUAC equation

$$\ln \gamma_i = \ln \gamma_i^C + \ln \gamma_i^R \qquad (2.4)$$

where the superscripts C and R refer to the combinatorial and residual parts of the activity coefficient respectively.

The combinatorial part of the activity coefficient is represented by

$$\ln \gamma_i^C = \ln \frac{\phi_i}{x_i} + (\frac{Z}{2})q \ln \frac{\theta_i}{\phi_i} + l_i - \frac{\phi_i}{x_i} \sum_j x_j l_j \qquad (2.5)$$

where $l_i = \frac{Z}{2} (r_i - q_i) - (r_i - 1)$ (A.11)

$$r_i = \sum v_{ki} R_k \qquad q_i = \sum v_{ki} Q_k \qquad \text{(A.12,A.13)}$$

$$\emptyset_i = r_i x_i / (\sum_j r_j x_j) \qquad \theta_i = q_i x_i / (\sum_j q_j x_j) \qquad \text{(A.14,A.15)}$$

x_i = mole fraction of component i in the mixture

v_{ki} = count of k th group in component i

R_k = a measure of Van der Waals volume ratio for group k

Q_k = a measure of Van der Waals area ratio for group k

The residual part of the activity coefficient is computed as follows

$$\ln \gamma_i^R = \sum_k v_{ki} (\ln \Gamma_k - \ln \Gamma_{k,i}) \qquad (2.6)$$

where the summation are over all groups, and

Γ_k = activity coefficient for group k in the mixture

$\Gamma_{k,i}$= activity coefficient for group k in pure component i

The activity coefficient Γ_k is computed as follows

$$\ln \Gamma_k = Q_k \left[1 - \ln \left(\sum_m \beta_m \xi_{mk}\right) - \sum_m \left(\frac{\beta_m \xi_{km}}{\sum_n \beta_m \xi_{km}}\right)\right] \qquad (2.7)$$

where the summations are over all groups, and

$\beta_m = X_m Q_m / \sum_n X_n Q_n$, area fraction of group m (A.16)

$X_m = \sum_j x_j v_{mj} / \sum_n \sum_j x_j v_{nj}$, mole fraction of group m (A.17)

$\xi_{mn} = \exp(-a_{mn}/T)$ (A.18)

$\{a_{mn}\}$= set of group interaction parameters, $a_{mn} \neq a_{mn}$

The activity coefficient $\ln \Gamma_{ki}$ is computed as follows

$$\ln \Gamma_{ki} = Q_k \left[1 - \ln \left(\sum_m \beta_{mi}\xi_{mk}\right) - \sum_m \left(\frac{\beta_{mi}\xi_{km}}{\sum_n \beta_{ni}\xi_{nm}}\right)\right] \tag{2.8}$$

where the summations are over all groups in component i, and

$$\beta_{mi} = X_{mi}Q_m / \sum_n X_{ni}Q_n, \text{ area fraction of group m in i} \tag{A.19}$$

$$X_{mi} = v_{mi} / \sum_n v_{ni}, \text{ mole fraction of group m in i} \tag{A.20}$$

Values of R_k, Q_k, and a_{mn} are given in Appendix (A.3)

A.2 Modified UNIQUAC Equation for Heats of Mixing

The relationship between excess heats of mixing and activity coefficient of component i in the mixture is given by

$$h^E = -RT^2 \sum x_i \left(\frac{\partial \ln \gamma_i}{\partial T}\right)_{P,x} \tag{2.2}$$

If $\tau_{ji} = \exp\left(-\frac{a_{ji} + b_{ji}/T}{T}\right)$ (2.1A)

then

$$h^E = R \sum_i \left[\frac{q_i' x_i}{\sum_j \theta_j' \tau_{ji}} \sum_j \theta_j' \tau_{ji} (a_{ji} + 2b_{ji}/T) \right] \tag{2.3}$$

A.3 UNIFAC VLE Interaction Parameters Databank

The following databank consists of constants, R_k and Q_k, for 77 secondary groups, and interaction parameters a_{mn} for 41 primary groups reported by Ghemling et al. (1982).

```
4177
 0.8480 0.9011 1CH3          0.5400 0.6744 1CH2          0.2280 0.4469 1CH          QR
 0.0000 0.2195 1C            1.1760 1.3454 2CH2=CH       0.8670 1.1167 2CH=CH       QR
 0.9880 1.1173 2CH2=C        0.6760 0.8886 2CH=C         0.4850 0.6605 2C=C         QR
 0.4000 0.5313 3ACH          0.1200 0.3652 3AC           0.9680 1.2663 4ACCH3       QR
 0.6600 1.0396 4ACCH2        0.3480 0.8121 4ACCH         1.2000 1.0000 5OH          QR
 1.4320 1.4311 6CH3OH        1.4000 0.9200 7H2O          0.6800 0.8952 8ACOH        QR
 1.4880 1.6724 9CH3CO        1.1800 1.4457 9CH2CO        0.9480 0.998010CHO         QR
 1.7280 1.903111CH3COO       1.4200 1.676411CH2COO       1.1880 1.242012HCOO        QR
 1.0880 1.145013CH3O         0.7800 0.918313CH2O         0.4680 0.690813CH-O        QR
 1.1000 0.918313FCH2O        1.5440 1.595914CH3NH2       1.2360 1.369214CH2NH2      QR
 0.9240 1.141714CHNH2        1.2440 1.433715CH3NH        0.9360 1.207015CH2NH       QR
 0.6240 0.979515CHNH         0.9400 1.186516CH3N         0.6320 0.959716CH2N        QR
 0.8160 1.060017ACNH2        2.1130 2.999318C5H5N        1.8330 2.833218C5H4N       QR
 1.5530 2.667018C5H3N        1.7240 1.870119CH3CN        1.4160 1.643419CH2CN       QR
 1.2240 1.301320COOH         1.5320 1.528020HCOOH        1.2640 1.465421CH2CL       QR
 0.9520 1.238021CHCL         0.7240 1.006021CCL          1.9880 2.256422CH2CL2      QR
 1.6840 2.060622CHCL2        1.4480 1.801622CCL2         2.4100 2.870023CHCL3       QR
 2.1840 2.640123CCL3         2.9100 3.390024CCL4         0.8440 1.156225ACCL        QR
 1.8680 2.008626CH3NO2       1.5600 1.781826CH2NO2       1.2480 1.554426CHNO2       QR
 1.1040 1.419927ACNO2        1.6500 2.057028CS2          1.6760 1.877029CH3SH       QR
 1.3680 1.651029CH2SH        2.4810 3.168030FURFURAL     2.2480 2.408831(CH2OH)2    QR
 0.9920 1.264032I            0.8320 0.949233BR           1.0880 1.292034CH C        QR
 0.7840 1.061334C≡C          2.4720 2.826635ME2SO        2.0520 2.314436ACRY        QR
 0.7240 0.791037CL(C=C)      0.5240 0.694838ACF          2.7360 3.085639DMF-1       QR
 2.1200 2.632239DMF-2        1.3800 1.406040CF3          0.9200 1.010540CF2         QR
 0.4600 0.615040CF           1.2000 1.380041COO                                     QR
```

```
   0.00     86.02     61.13     76.50    986.50    697.20  1318.00CH2    1- 7
1333.00    476.40    677.00    232.10    741.40    251.50   391.50CH2    8-14
 255.70    206.60   1245.00    287.70    597.00    663.50    35.93CH2   15-21
  53.76     24.90    104.30    321.50    661.50    543.00   153.60CH2   22-28
 184.40    354.50   3025.00    335.80    479.50    298.90   526.50CH2   29-35
 689.00     -4.19    125.80    485.30     -2.86    387.10         CH2   36-42
 -35.36      0.00     38.81     74.15    524.10    787.60   270.60C=C    1- 7
 526.10    182.60      0.       37.85    449.10    214.50   240.90C=C    8-14
 163.90     61.11      0.        0.      336.90    318.90   204.60C=C   15-21
   5.89    -13.99   -109.70    393.10    357.50      0.      76.30C=C   22-28
   0.        0.        0.        0.        0.       31.14  -137.40C=C   29-35
   0.      -66.46      0.      -70.45      0.       48.33         C=C   36-42
 -11.12      3.45      0.0     167.00    636.10    637.30   903.80ACH    1- 7
1329.00     25.77      0.        5.99      0.       32.14   161.70ACH    8-14
 122.80     90.49    668.20     -4.45    212.50    537.40   -18.81ACH   15-21
-144.40   -231.90      3.00    538.20    168.00    194.90    52.07ACH   22-28
 -10.43    -64.69    210.40    113.30    -13.59      0.     169.90ACH   29-35
   0.     -259.10    389.30    245.60      0.      103.50         ACH   36-42
 -69.70   -113.60   -146.80      0.0     803.20    603.20  5695.00ACCH2 1- 7
 884.90    -52.10      0.     5688.00      0.      213.10     0.  ACCH2 8-14
 -49.29     23.50    764.70     52.80   6096.00    603.80  -114.10ACCH215-21
   0.      -12.14   -141.30   -126.90   3629.00   4448.00    -9.45ACCH222-28
   0.      -20.36   4975.00      0.     -171.30      0.    4284.00ACCH229-35
   0.        0.      101.40   5629.00      0.       69.26         ACCH236-42
 156.40    457.00     89.60     25.82      0.0    -137.10   353.50OH     1- 7
-259.70     84.00    441.80    101.10    193.10     28.06    83.02OH     8-14
  42.70   -323.00   -348.20    170.00      6.71    199.00    75.62OH    15-21
-112.10    -98.12    143.10    287.80     61.11    157.10   477.00OH    22-28
 147.50   -120.50   -318.90   -313.50    133.40      0.    -202.10OH    29-35
   0.      225.80     44.78   -143.90      0.      190.30         OH    36-42
  16.51    -12.52    -50.00    -44.50    249.10      0.0   -181.00CH3OH 1- 7
-101.70     23.39    306.40    -10.72    193.40   -180.60   359.30CH3OH 8-14
 266.00     53.90    335.50    580.50     36.23   -289.50   -38.32CH3OH15-21
-102.50   -139.40    -67.80     17.12     75.14      0.     -31.09CH3OH22-28
  37.84      0.        0.        0.        0.        0.    -399.30CH3OH29-35
   0.       33.47    -48.25   -172.40      0.      165.70         CH3OH36-42
```

```
 300.00    496.10    362.30    377.60   -229.10    289.60      0.00H2O    1- 7
 324.50   -195.40   -257.30     14.42     0.       540.50     48.89H2O    8-14
 168.00    304.00    213.00    459.00    112.60    -14.09    325.40H2O   15-21
 370.40    353.70    497.50    678.20    220.60    399.50    887.10H2O   22-28
   0.      188.00      0.0       0.        0.        0.     -139.00H2O   29-35
 160.80      0.        0.      319.00      0.     -197.50           H2O   36-42
 275.80    217.50     25.34    244.20   -451.60   -265.20   -601.80ACOH   1- 7
   0.0    -356.10      0.     -449.40      0.        0.         0.  ACOH  8-14
   0.        0.        0.     -305.50      0.        0.         0.  ACOH 15-21
   0.        0.     1827.00      0.        0.        0.         0.  ACOH 22-28
   0.        0.     -687.10      0.        0.        0.         0.  ACOH 29-35
   0.        0.        0.        0.        0.     -494.20           ACOH 36-42
  26.76     42.92    140.10    365.80    164.50    108.70    472.50CH2CO 1- 7
-133.10      0.0     -37.36   -213.70      0.        5.20      0.  CH2CO 8-14
   0.        0.      937.90    165.10    481.70    669.40   -191.70CH2CO15-21
-284.00   -354.60    -39.20    174.50    137.50      0.      216.10CH2CO22-28
 -46.28   -163.70      0.       53.59    245.20   -246.60    -44.58CH2CO29-35
   0.      -34.57      0.      -61.70      0.      -18.80           CH2CO36-42
 505.70      0.        0.        0.     -404.80   -340.20    232.70CHO    1- 7
   0.      128.00      0.0       0.        0.      304.10      0.  CHO    8-14
   0.        0.        0.        0.        0.        0.      751.90CHO   15-21
   0.        0.        0.        0.        0.        0.         0.  CHO   22-28
   0.        0.        0.        0.        0.        0.         0.  CHO   29-35
   0.        0.        0.        0.        0.        0.              CHO   36-42
 114.80    132.10     85.84   -170.00    245.40    249.60  10000.00CCOO   1- 7
 -36.72    372.20      0.        0.0     372.90   -235.70      0.  CCOO   8-14
 -73.50      0.        0.        0.      494.60    660.20      0.  CCOO  15-21
 108.90   -209.70     54.47    629.00      0.        0.      183.00CCOO  22-28
   0.      202.30   -101.70    148.30      0.        0.       52.08CCOO  29-35
   0.      -83.30      0.        0.        0.      560.20           CCOO  36-42
  90.49    -62.55      0.        0.      191.20    155.70      0.  HCOO   1- 7
   0.        0.        0.     -261.10      0.0       0.         0.  HCOO   8-14
   0.        0.        0.        0.        0.     -356.30      0.  HCOO  15-21
   0.     -287.20      0.        0.        0.        0.         0.  HCOO  22-28
   4.34      0.        0.        0.        0.        0.         0.  HCOO  29-35
   0.        0.        0.        0.        0.      -70.24           HCOO  36-42
```

```
   83.36     26.51     52.13     65.69    237.70    339.70   -314.70CH2O  1- 7
    0.       52.38     -7.84    461.30      0.        0.0       0.  CH2O  8-14
  141.70      0.        0.        0.        0.      664.60    301.10CH2O 15-21
  137.80   -154.30     47.67      0.       95.18      0.      140.90CH2O 22-28
   -8.54      0.      -20.11   -149.50   -202.30      0.      172.10CH2O 29-35
    0.      240.20      0.      254.80      0.      417.00          CH2O 36-42
  -30.48      1.16    -44.85      0.     -164.00   -481.70   -330.40CNH2  1- 7
    0.        0.        0.        0.        0.        0.        0.00CNH2  8-14
   63.72    -41.11      0.        0.        0.        0.        0.  CNH2 15-21
    0.        0.      -99.81     68.81      0.        0.        0.  CNH2 22-28
  -70.14      0.        0.        0.        0.        0.        0.  CNH2 29-35
    0.        0.        0.        0.        0.        0.            CNH2 36-42
   65.33    -28.70    -22.31    223.00   -150.00   -500.40   -448.20CNH   1- 7
    0.        0.        0.      136.00      0.      -49.30    108.80CNH   8-14
    0.0    -189.20      0.        0.        0.        0.        0.  CNH  15-21
    0.        0.       71.23   4350.00      0.        0.        0.  CNH  22-28
    0.        0.        0.        0.        0.        0.        0.  CNH  29-35
    0.        0.        0.        0.        0.      -38.77          CNH  36-42
  -83.98    -25.38   -223.90    109.90     28.60   -406.80   -598.80C3N   1- 7
    0.        0.        0.        0.        0.        0.       38.89C3N   8-14
  865.90      0.0       0.        0.        0.        0.        0.  C3N  15-21
  -73.85   -352.90     -8.28    -86.36      0.        0.        0.  C3N  22-28
    0.        0.        0.        0.        0.        0.        0.  C3N  29-35
    0.        0.        0.        0.        0.        0.            C3N  36-42
 5339.00      0.      650.40    979.80    529.00      5.18   -339.50ACNH2 1- 7
    0.     -399.10      0.        0.        0.        0.        0.  ACNH2 8-14
    0.        0.        0.0       0.     -216.80      0.        0.  ACNH215-21
    0.        0.     8455.00    699.10      0.      -62.73      0.  ACNH222-28
    0.        0.      125.30      0.        0.        0.        0.  ACNH229-35
    0.        0.        0.     -293.10      0.        0.            ACNH236-42
 -101.60      0.       31.87     49.80   -132.30   -378.20   -332.90PYRID 1- 7
 -341.60    -51.54      0.        0.        0.        0.        0.  PYRID 8-14
    0.        0.        0.        0.0    -169.70   -153.70      0.  PYRID15-21
 -351.60   -114.70   -165.10      0.        0.        0.        0.  PYRID22-28
    0.        0.        0.        0.        0.        0.        0.  PYRID29-35
    0.        0.        0.        0.        0.        0.            PYRID36-42
```

```
   24.82     -40.62     -22.97    -138.40     185.40     157.80     242.80CCN   1- 7
    0.      -287.50      0.       -266.60       0.          0.         0.  CCN   8-14
    0.         0.       617.10     134.30      0.0         0.          0.  CCN  15-21
    0.       -15.62     -54.86      52.31       0.          0.       230.90CCN  22-28
   21.37       0.         0.          0.        0.       -203.0        0.  CCN  29-35
   81.57       3.51       0.          0.        0.        120.30           CCN  36-42
  315.30    1264.00      62.32     268.20    -151.00    1020.00     -66.17COOH  1- 7
    0.      -297.80      0.       -256.30     312.50    -338.50        0.  COOH  8-14
    0.         0.         0.      -313.50       0.         0.0       44.42COOH 15-21
 -183.40      76.75     212.70       0.         0.          0.         0.  COOH 22-28
    0.         0.         0.          0.        0.          0.         0.  COOH 29-35
    0.       -11.16       0.          0.        0.       -337.00           COOH 36-42
   91.46      97.51       4.68     122.90     562.20     529.00     698.20CCL   1- 7
    0.       286.30     -47.51       0.         0.        225.40       0.  CCL   8-14
    0.         0.         0.          0.        0.        326.40       0.0 CCL  15-21
  108.30     249.20      62.42     464.40       0.          0.       450.10CCL  22-28
   59.02       0.         0.          0.     -125.90        0.         0.  CCL  29-35
    0.      -245.40       0.          0.        0.          0.             CCL  36-42
   34.01      18.25     121.30       0.       747.70     669.90     708.70CCL2  1- 7
    0.       423.20       0.      -132.90       0.       -197.70       0.  CCL2  8-14
    0.      -141.40       0.       587.30       0.       1821.00     -84.53CCL2 15-21
    0.0        0.0       56.33       0.         0.          0.         0.  CCL2 22-28
    0.         0.         0.       177.60       0.          0.       215.00CCL2 29-35
    0.         0.         0.          0.        0.        -96.87           CCL2 36-42
   36.70      51.06     288.50      33.61     742.10     649.10     826.70CCL3  1- 7
    0.       552.10       0.       176.50     488.90     -20.93        0.  CCL3  8-14
    0.      -293.70       0.        18.98      74.04    1346.00    -157.10CCL3 15-21
    0.0        0.0      -30.10       0.         0.          0.       116.60CCL3 22-28
    0.       -64.38       0.        86.40       0.          0.       363.70CCL3 29-35
    0.       111.20       0.          0.        0.        255.80           CCL3 36-42
  -78.45     160.90      -4.70     134.70     856.30     860.10    1201.00CCL4  1- 7
10000.00     372.00       0.       129.50       0.        113.90     261.10CCL4  8-14
   91.13    -126.00    1301.00     309.20     492.00     689.00      11.80CCL4 15-21
   17.97      51.90       0.0      475.80     490.90     534.70     132.20CCL4 22-28
    0.       546.70       0.       247.80      41.94        0.       337.70CCL4 29-35
    0.       187.10     215.20     498.60       0.        256.50           CCL4 36-42
```

```
 -141.30   -158.80   -237.70    375.50    246.90    661.60    920.40ACCL  1- 7
    0.      128.10      0.     -246.30      0.        0.      203.50ACCL  8-14
 -108.40   1088.00    323.30      0.      356.90      0.     -314.90ACCL 15-21
    0.        0.     -255.40      0.0    -154.50      0.        0.  ACCL 22-28
    0.        0.        0.        0.      -60.70      0.        0.  ACCL 29-35
    0.        0.        0.        0.        0.     -145.10          ACCL 36-42
  -32.69     -2.00     10.38    -97.05    341.70    252.60    417.90CNO2  1- 7
    0.     -142.60      0.        0.        0.      -94.49      0.  CNO2  8-14
    0.        0.        0.        0.        0.        0.        0.  CNO2 15-21
    0.        0.      -34.68    794.40      0.0     533.20      0.  CNO2 22-28
    0.        0.      139.80    304.30     10.17    -27.70      0.  CNO2 29-35
    0.       10.76      0.        0.        0.        0.          CNO2 36-42
 5541.00      0.     1824.00   -127.80    561.60      0.      360.70ACNO2 1- 7
    0.        0.        0.        0.        0.        0.        0.  ACNO2 8-14
    0.        0.     5250.00      0.        0.        0.        0.  ACNO215-21
    0.        0.      514.60      0.      -85.12      0.0       0.  ACNO222-28
    0.        0.        0.        0.        0.        0.        0.  ACNO229-35
    0.        0.        0.        0.        0.        0.          ACNO236-42
  -52.65     16.62     21.50     40.68    823.50    914.20   1081.00CS2   1- 7
    0.      303.70      0.      243.80      0.      112.40      0.  CS2   8-14
    0.        0.        0.        0.      335.70      0.      -73.09CS2  15-21
    0.      -26.06    -60.71      0.        0.        0.        0.00CS2  22-28
    0.        0.        0.        0.        0.        0.        0.  CS2  29-35
    0.      -47.37      0.        0.        0.      469.80          CS2  36-42
   -7.48      0.       28.41      0.      461.60    382.80      0.  CH3SH 1- 7
    0.      160.60      0.        0.      239.80     63.71    106.70CH3SH 8-14
    0.        0.        0.        0.      125.70      0.      -27.94CH3SH15-21
    0.        0.        0.        0.        0.        0.        0.  CH3SH22-28
    0.0       0.        0.        0.        0.        0.       31.66CH3SH29-35
    0.        0.        0.       78.92      0.        0.          CH3SH36-42
  -25.31      0.      157.30    404.30    521.60      0.       23.48FURFU 1- 7
    0.      317.50      0.     -146.30      0.        0.        0.  FURFU 8-14
    0.        0.        0.        0.        0.        0.        0.  FURFU15-21
    0.       48.48   -133.10      0.        0.        0.        0.  FURFU22-28
    0.        0.0       0.        0.        0.        0.        0.  FURFU29-35
    0.        0.        0.        0.        0.        0.          FURFU36-42
```

```
  140.00       0.       221.40     150.60     267.60       0.          0.0 DOH    1- 7
  838.40       0.         0.       152.00       0.         9.21        0.  DOH    8-14
    0.         0.       164.40       0.         0.         0.          0.  DOH   15-21
    0.         0.         0.         0.       481.30       0.          0.  DOH   22-28
    0.         0.         0.0        0.         0.         0.     -417.20DOH   29-35
    0.         0.         0.       302.20       0.         0.             DOH   36-42
  128.00       0.        58.68       0.       501.30       0.          0.  I      1- 7
    0.       138.00       0.        21.92       0.       476.60        0.  I      8-14
    0.         0.         0.         0.         0.         0.          0.  I     15-21
  -40.82      21.76      48.49       0.        64.28       0.          0.  I     22-28
    0.         0.         0.         0.         0.         0.          0.  I     29-35
    0.         0.         0.         0.         0.        68.55            I     36-42
  -31.52       0.       155.60     291.10     721.90       0.          0.  BR     1- 7
    0.      -142.60       0.         0.         0.       736.40        0.  BR     8-14
    0.         0.         0.         0.         0.         0.       1169.00BR    15-21
    0.         0.       225.80     224.00     125.30       0.          0.  BR    22-28
    0.         0.         0.         0.         0.0        0.          0.  BR    29-35
    0.         0.         0.         0.         0.         0.             BR    36-42
  -72.88      41.38       0.         0.         0.         0.          0.  C C    1- 7
    0.       443.60       0.         0.         0.         0.          0.  C C    8-14
    0.         0.         0.         0.       329.10       0.          0.  C C   15-21
    0.         0.         0.         0.       174.40       0.          0.  C C   22-28
    0.         0.         0.         0.         0.         0.0         0.  C C   29-35
    0.         0.         0.      -119.80       0.         0.             C C   36-42
   50.49     422.40      -2.50    -143.20     -25.87     695.00     -240.00ME2SO 1- 7
    0.       110.40       0.        41.57       0.      -122.10        0.  ME2SO 8-14
    0.         0.         0.         0.         0.         0.          0.  ME2SO15-21
 -215.00    -343.60     -58.43       0.         0.         0.          0.  ME2SO22-28
   85.70       0.       535.80       0.         0.         0.          0.0 ME2SO29-35
    0.         0.         0.       -97.71       0.       153.70            ME2SO36-42
 -165.90       0.         0.         0.         0.         0.        386.60ACRY  1- 7
    0.         0.         0.         0.         0.         0.          0.  ACRY  8-14
    0.         0.         0.         0.       -42.31       0.          0.  ACRY 15-21
    0.         0.         0.         0.         0.         0.          0.  ACRY 22-28
    0.         0.         0.         0.         0.         0.          0.  ACRY 29-35
    0.0        0.         0.         0.         0.       423.40            ACRY 36-42
```

```
  47.41    124.20    395.80      0.      738.90    528.00       0.  CLCC  1- 7
   0.      -40.90      0.       16.99      0.     -217.90       0.  CLCC  8-14
   0.        0.        0.        0.      304.00    898.20     428.50CLCC 15-21
   0.     -149.80   -134.20      0.      379.40      0.       167.90CLCC 22-28
   0.        0.        0.        0.        0.        0.         0.  CLCC 29-35
   0.        0.0       0.        0.        0.      730.80           CLCC 36-42
  -5.13      0.     -237.20   -157.30    649.70    645.90       0.  ACF   1- 7
   0.        0.        0.        0.        0.        0.         0.  ACF   8-14
   0.        0.        0.        0.        0.        0.         0.  ACF  15-21
   0.        0.     -124.60      0.        0.        0.         0.  ACF  22-28
   0.        0.        0.        0.        0.        0.         0.  ACF  29-35
   0.        0.        0.0       0.        0.        0.             ACF  36-42
 -31.95    249.00   -133.90   -240.20     64.16    172.20    -287.10DMF   1- 7
   0.       97.04      0.        0.        0.     -158.20       0.  DMF   8-14
   0.        0.      335.60      0.        0.        0.         0.  DMF  15-21
   0.        0.     -186.70      0.        0.        0.         0.  DMF  22-28
 -71.00      0.     -191.70      0.        0.        6.70     136.60DMF  29-35
   0.        0.        0.        0.0       0.        0.             DMF  36-42
-147.30      0.        0.        0.        0.        0.         0.  CF2   1- 7
   0.        0.        0.        0.        0.        0.         0.  CF2   8-14
   0.        0.        0.        0.        0.        0.         0.  CF2  15-21
   0.        0.        0.        0.        0.        0.         0.  CF2  22-28
   0.        0.        0.        0.        0.        0.         0.  CF2  29-35
   0.        0.        0.        0.        0.0       0.             CF2  36-42
 529.00   1397.00    317.60    615.80     88.63    171.00     284.40COO   1- 7
-167.30    123.40      0.     -234.90     65.37   -247.80       0.  COO   8-14
 284.50      0.        0.        0.      -61.60   1179.00       0.  COO  15-21
 305.40   -193.00    335.70   1107.00      0.        0.       885.50COO  22-28
   0.        0.        0.      288.10      0.        0.       -29.34COO  29-35
 -53.91   -198.00      0.        0.        0.        0.0            COO  36-42
```

APPENDIX B

DISTILLATION ALGORITHM AND SIMULATOR -- PROCESS EQUIPMENT PARAMETER DATA SPECIFICATION

B.1 Generalized Absorption/Distillation Algorithm (ABDIS)

B.1.1 Linearized Discrepancy Function

B.1.2 Solution Algorithm

B.2 Process Simulator (PROSIM) - Process Equipment Parameters Specification

B.2.1 ADBF - General Purpose Three Phase Flash Package

B.2.2 ACTL - Azeotropic Column Control Block, Variable Distillate Rate

B.2.3 BCTL - Benzene Stripping Column Control Block, Variable Distillate Rate - I

B.2.4 BZTL - Benzene Stripping Column Control Block, Variable Distillate Rate - II

B.2.5 CNTL - Stream Rate Control Block - I

B.2.6 DCTL - Control Block, Feed-Forward Control of the Split - I

B.2.7 DIST - Rigorous Absorption/Distillation Package

B.2.8 DSPT - Control Block, Feed-Forward Control of the Split - II

B.2.9 ECTL - Azeotropic Column Control Block, Variable Entrainer Rate

B.2.10 RCTL - Stream Rate Control Block - II

B.2.11 SBOX - Dummy Separation Block

B.2.12 SMIX - Special Mixer-Splitter Block

B.1 Generalized Absorption/Distillation Algorithm (ABDIS)

B.1.1 Linearized Discrepancy Function

The discrepancy function (Eq. 2.26 through 2.30) can be linearized using Taylor's series expansion, neglecting the quadratic terms, about a known set of variables. The linearization process generates a new set of independent variables, namely $l_{n,i}$, $v_{n,i}$, and T_n. For each of the discrepancy functions, the resulting equations in the restructured mode will have the following form according to Roche (1978) and Tsai (1982):

Main equation -

$$F(x_1,x_2,x_3) = 0 \tag{B.1}$$

Linearized equation in the restructured mode

$$\frac{\partial F}{\partial x_1} \Delta x_1 + \frac{\partial F}{\partial x_2} \Delta x_2 + \frac{\partial F}{\partial x_3} \Delta x_3 + \ldots\ldots = -F \tag{B.2}$$

The linearization of each of the discrepancy functions is given below:

Component Material Balance

$$F_{1(n,i)} = (1 + \frac{S_n^L}{L_n}) l_{n,i} + (1 + \frac{S_n^V}{V_n}) v_{n,i} + v_{n-1,i} - l_{n+1,i} - f_{n,i} = 0 \tag{2.26}$$

Linearization of Equation 2.26 leads to

$$- \Delta v_{n-1,i} + (1 + \frac{S_n^L}{L_n}) \Delta l_{n,i} - \frac{S_n^V}{V_n^2} l_{n,i} \sum_k \Delta l_{n,k} + (1 + \frac{S_n^V}{V_n}) \Delta v_{n,i}$$

$$- \frac{S_n^V}{V_n^2} l_{n,i} \sum_k \Delta v_{n,k} - \Delta l_{n+1,i} = -F_{1(n,i)} \tag{B.3}$$

Equilibrium Relationship coupled with the Murphree stage efficiency, η

$$F_{2(n,i)} = \eta_n \frac{K_{n,i} V_n}{L_n} l_{n,i} - v_{n,i} + (1 - \eta_n) \frac{V_n}{V_{n-1}} = 0 \qquad (2.27)$$

The above equation can be linearized as follows:

$$(1 - \eta) \frac{V_n}{V_{n-1}} \Delta v_{n-1,i} - (1 - \eta) \frac{V_n}{V_{n-1}^2} v_{n-1,i} \sum_k \Delta v_{n-1,k}$$

$$+ \eta_n K_{n,i} \frac{V_n}{L_n} \Delta l_{n,i} - \eta_n K_{n,i} \frac{V_n}{L_{n-1}^2} l_{n,i} \sum_k l_{n,k}$$

$$+ \eta_n K_{n,i} \frac{l_{n,i}}{L_n} \sum_k \Delta v_{n,k} + (1 - \eta) \frac{v_{n-1,i}}{V_{n-1}} \sum_k \Delta v_{n,k}$$

$$+ \eta_n \frac{V_n}{L_n} l_{n,i} \sum_k \frac{\partial K_{n,i}}{\partial l_{n,k}} \Delta l_{n,k} + \eta_n \frac{V_n}{L_n} l_{n,i} \sum_k \frac{\partial K_{n,i}}{\partial v_{n,k}} v_{n,k}$$

$$+ \eta_n \frac{V_n}{L_n} l_{n,i} \frac{\partial K_{n,i}}{\partial T_n} \Delta T_n - \Delta v_{n,i} = -F_{2(n,i)} \qquad (B.4)$$

Energy Balance

$$F_{3(n)} = \left(1 + \frac{S_n^L}{L_n}\right) h_n + \left(1 + \frac{S_n^V}{V_n}\right) H_n - H_{n-1} - h_{n+1} - h_n^F - Q_n +$$

$$h_n^{mix} - h_{n+1}^{mix} = 0 \qquad (2.30)$$

Linearized Eq. 2.30 is given below:

$$- \sum_k \frac{H_{n-1}}{V_{n-1,k}} \Delta v_{n-1,k} - \frac{\partial H_{n-1}}{\partial T_{n-1}} \Delta T_{n-1} + \left(1 + \frac{S^L_n}{L_n}\right) \sum_k \frac{\partial h_n}{\partial l_{n,k}} \Delta l_{n,k}$$

$$+ \left(1 + \frac{S^L_n}{L_n}\right) \frac{\partial h_n}{\partial T_n} \Delta l_n + \left(1 + \frac{S^V_n}{V_n}\right) \sum_k \frac{\partial H_n}{\partial v_{n,k}} \Delta v_{n,k} - \frac{S^V_n}{V^2_n} H_n \sum_k \Delta v_{n,k}$$

$$+ \left(1 + \frac{S^V_n}{V_n}\right) \frac{\partial H_n}{\partial T_n} \Delta T_n - \sum_k \frac{\partial h_{n+1}}{\partial l_{n+1,k}} \Delta l_{n+1,k} + \frac{\partial h_{n+1}}{\partial T_{n+1}} \Delta T_{n+1} +$$

$$\sum_k \frac{\partial h^{mix}_n}{\partial l_{n,k}} \Delta l_{n,k} + \sum_k \frac{\partial h^{mix}_n}{\partial T_n} \Delta T_n - \sum_k \frac{\partial h^{mix}_n}{\partial l_{n+1,k}} \Delta l_{n+1,k} -$$

$$\sum_k \frac{\partial h^{mix}_{n+1}}{\partial T_{n,k}} \Delta T_n = -F_3(n) \qquad (B.5)$$

B.1.2 Solution Algorithm

Stagewise arrangement of linearized discrepancy functions result in the formation of tridiagonal matrix (NxN) as shown in Fig. B.1. Each of the submatrices, within the big matrix, is of 2c+1 x 2c+1 dimension, where c is defined as the number of components. Thomas algorithm is employed to attain the solution. The computation procedure is as follows:

1) Initialization of B-matrix and D-matrix for the N stage column.
2) Inversion procedure to eliminate A-matrix and C-matrix, starting with stage 2:
   - o Perform Gaussian elimination on

$$B^T_{m-1} * S^T = A^T_m \qquad (B.6)$$

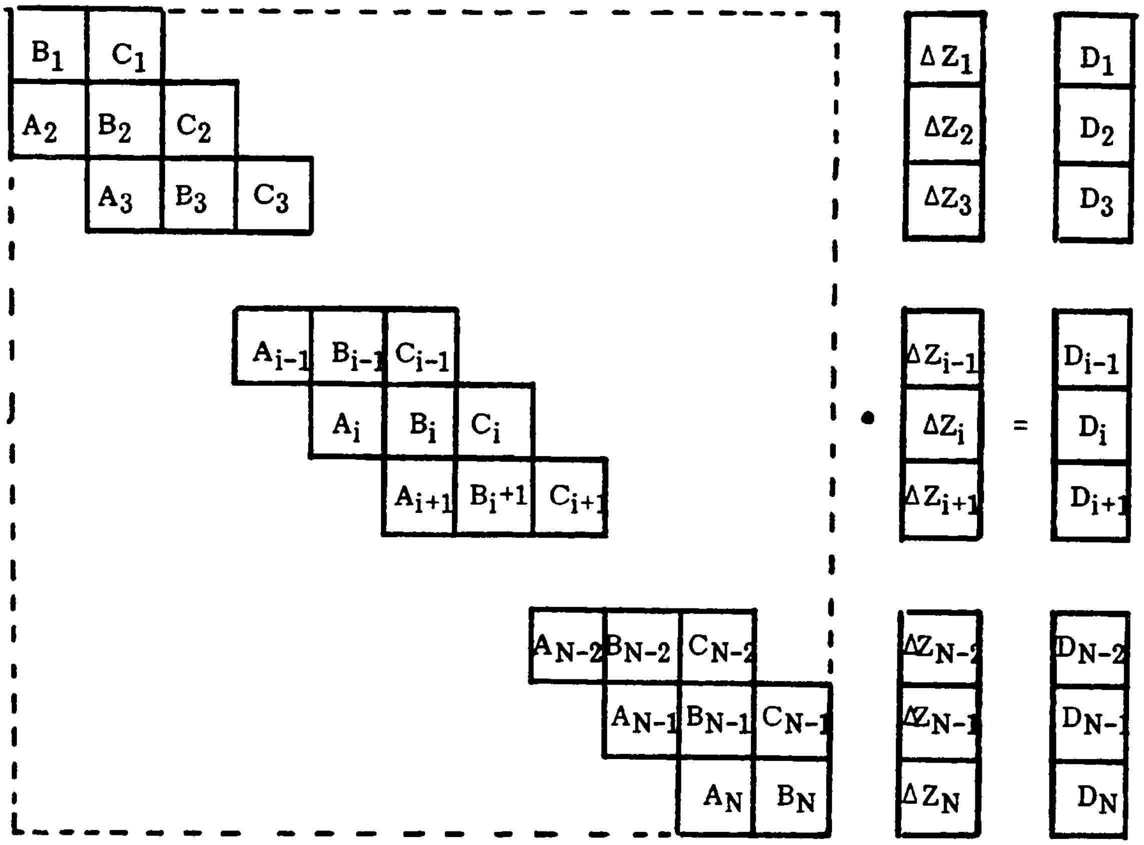


Figure B.1 Schematic Representation of the Column's Linearized Discrepancy Functions and retain the results in S after transposing.

- Eliminate A_m (by induction) by modifying B_m and D_m(subtraction of product of $S.C_{m-1}$ from B_m and product of $S.D_{m-1}$ from D_m).
- The back substitution is initiated with m=N, by performing Gaussian elimination on:

  $$B_N * S = D_N$$

  The result of this operation is the set of flow and temperature corrections for the stage N.
- Cm is eliminated in the process of back substitution for m= N-1, N-2, etc. The process is thus:
  - a) Eliminate C by subtracting from D the product of $C_m * D_{m+1}$
  - b) Perform Gaussian elimination on $_mB * S=D_m$ to obtain the set of corrections associated with stage m.

The matrix C is not defined explicitly and the unique structure is exploited to minimize the iterative computational effort.

B.2 Process Simulator (PROSIM) - Equipment Parameters Specification

Every process block/node in the system must have its operational parameters defined through the use of the equipment parameter (EQPAR) vector. EQPAR vectors for the new or improved blocks are given below, whereas the detailed definitions are covered elsewhere (Andreyuk, 1983).

B.2.1 ACTL - Azeotropic Column Control Block, Variable Distillate Rate

EQPAR(J,NE) = NE, N_s, N_R, Ncase, E_s, E_R, T_t, T_b, P_t, P_b, ΔT, ΔF, F, N_1, N_2, N_3, N_4, D_v, D_l, R, D_c, I_M, V_F, I_{MA}, 0.0.

I_{MA} = Maximum value of iterations within ACTL block

Refer to definition of other variables in EQPAR description of DIST block.

B.2.2 ADBF - General Purpose 3 Phase Flash Package

EQPAR(J,NE) = NE, Mode, 23*0.0,

NE = Equipment block/node number

Mode = Type of calculations

1 Dew point temperature
2* Bubble point temperature
3 All vapor enthalpy with prior dew point
4* All liquid enthalpy with prior bubble point
5 All vapor enthalpy
6* All liquid enthalpy
7* Isothermal flash
8* Isothermal flash ... no dew/bubble point

9* Adiabatic flash

10* Adiabatic flash ... no dew/bubble point

11 Dew point pressure

12* Bubble point pressure

13* Liq - liq seperation below bubble point

* Types applicable for either one or two liquid phases

B.2.3 BCTL - Benzene Stripping Column Control Block, Variable Distillate Rate - I

EQPAR(J,NE) = NE, NE_D, D_C, V_F, S_{R1}, S_{R2}, S_{R3}, S_{R4}, C_1, C_2, C_3, C_4, 13*0.0,

NE = Equipment block/node number

NE_D = Distillation column block/node number

D_C = Distillate code

-1 subcooled liquid

0 vapor/liquid distillate

+1 liquid at bubble point

V_F = Vapor fraction in distillate

S_{Ri} = i th reference stream number

C_j = j th reference component number

B.2.4 BZTL - Benzene Stripping Column Control Block, Variable Distillate Rate - II

EQPAR(J,NE) = NE, N_S, N_R, Ncase, E_S, E_R, T_t, T_b, P_t, P_b, ΔT, ΔF, F, N_1, S_{R1}, S_{R2}, S_{R3}, D_v, D_l, R, D_c, I_M, V_F, 2*0.0,

S_{R1} = First reference stream number

S_{R2} = Second reference stream number

S_{R3} = Third reference stream number

Refer to definition of other variables in EQPAR description of DIST block.

B.2.5 CNTL - Stream Rate Control Block - I

EQPAR(J,NE) = NE, I_o, I_c, MINR, MAXR, MAXF, 19*0.0,

NE = Equipment block/node number

I_o = Option code

1 Manipulation of componential flow based on difference of two stream rates

2 Manipulation of componential flow based on ratio of two stream rates

I_c = Component code

MINR = Minimum ratio for option 2

MAXR = Maximum ratio for option 2

MAXF = Maximum allowable of selected component

B.2.6 DCTL - Control Block, Feed-Forward Control of the Split - I

EQPAR(J,NE) = NE, NE_D, D_c, V_F, x_{d1}, x_{d2}, x_{d3}, x_{d4}, x_{b1}, x_{b2}, x_{b3}, x_{b4}, 13*0.0,

NE = Equipment block/node number

NE_D = Distillation column block/node number

D_c = Distillate code

-1 subcooled liquid

0 vapor/liquid distillate

+1 liquid at bubble point

V_F = Vapor fraction in distillate

x_{di} = Mole fraction guess of ith component in distillate

x_{bi} = Mole fraction guess of ith component in bottoms

If EQPAR(5,NE) < 0 no change is made in the block

>= 2 default mole fractions are used

B.2.7 DIST - Rigorous Absorption/Distillation Package

EQPAR(J,NE) = NE, N_S, N_R, Ncase, E_S, E_R, T_t, T_b, P_t, P_b, ΔT, ΔF, F, N_1, N_2, N_3, N_4, D_V, D_l, R, D_C, I_M, V_F, 2*0.0,

NE = Equipment block/node number

N_S = Number of stages in the stripping section

N_R = Number of stages in the rectifying section

Ncase = Type of process unit

3 Distillation column (refux ratio specified)

4 Distillation column (Boilup ratio specified)

5 Self refluxing column (Boilup ratio specified)

6 Self reboiling column (reflux ratio specified)

E_S = Murphree stage efficiency stripping section

E_R = Murphree stage efficiency rectifying section

T_t = Temperature at top of column, ^oF

T_b = Temperature at bottom of column, ^oF

P_t = Pressure at top of column, ^oF

P_b = Pressure at bottom of column, ^oF

ΔT = Temp. tolerance for convergence (default = 0.01)

ΔF = Flow tolerance for convergence (default = 0.0005)

F = Number of feeds to the column (maximum of four)

$N_1..N_4$= Stage for first to fourth feeds

D_v = Vapor distillate rate

D_l = Liquid distillate rate

R = Reflux ratio or boilup ratio

D_c = Distillate code

-1 subcooled liquid

0 vapor/liquid distillate

+1 liquid at bubble point

I_M = Maximum value for iterations

V_F = Vapor fraction in distillate

B.2.8 DSPT - Control Block, Feed-Forward Control of the Split - II

EQPAR(J,NE) = NE, NE_D, D_c, V_F, M_1, M_2,...., M_{10}, 11*0.0,

NE = Equipment block/node number

NE_D = Distillation column block/node number

D_c = Distillate code

-1 subcooled liquid

0 vapor/liquid distillate

+1 liquid at bubble point

V_F = Vapor fraction in distillate

M_i = Feed multiplier of the ith component, $0 < M_i < 1$

B.2.9 ECTL - Azeotropic Column Control Block, Variable Entrainer Rate

EQPAR(J,NE) = NE, N_S, N_R, Ncase, E_S, E_R, T_t, T_b, P_t, P_b, ΔT, ΔF, F, N_1, N_2, N_3, N_4, D_v, D_l, R, D_c, I_M, V_F, B, 0.0,

B = Bottoms rate, lbmoles/hr

Refer to definition of other variables in EQPAR description of DIST block.

B.2.10 RCTL - Stream Rate Control Block - II

EQPAR(J,NE) = NE, 3*0.0, S_{R1}, S_{R2}, S_{R3}, S_{R4}, C_1, C_2, C_3, C_4, 13*0.0,

NE = Equipment block/node number

S_{Ri} = i th reference stream number

C_j = j th reference component number

B.2.11 SBOX - Dummy Separation Block

EQPAR(J,NE) = NE, 0.0, H, I_o, S_{R1}, S_{R2}, S_{R3}, S_{R4}, C_1, C_2, C_3, C_4, T_d, P_d, V_d, T_b, P_b, 8*0.0,

NE = Equipment block/node number

H = Heat (out-in) stored

I_o = Output target stream number (default = 2)

S_{Ri} = i th reference stream number

C_j = j th reference component number

T_d = Distillate temperature, ^oF

P_d = Distillate pressure, psia

V_d = Distillate vapor fraction

T_b = Bottoms temperature, ^oF

P_b = Bottoms pressure, psia

B.2.12 SMIX - Special Mixer-Splitter Block

EQPAR(J,NE) = NE,T, P, H, Mode, 20*0.0,

NE = Equipment block/node number

T = Output streams temperature, ^oF

P = Output streams pressure, psia

H = Heat (out-in) stored

Mode = Type of flash calculations

The 'Mode' option codes are described in Appendix B.2.2

APPENDIX C

ENTRAINER STUDY: SAMPLE INPUT AND RESULTS

C.1 Sample Input and Azeotropic Column Results for Ethanol-Water-Benzene System

Table C.1.1 Input for Ethanol-Water-Benzene System

```
ETOH-WTR-BENZ DEHYD ... NCASE=5: UNIFAC & VIRIAL (EX #4A)
3, 7, 1, 2, 0, 0, 0, 1, 0, 0, 0,
ETOH
0, 46.1, 351.1, 516.2, 63.0, 167.0, 0.248, 58.39, 0.635,
0.0, 0.0, 2.1055, 1.9720, 0.92, 0.0, 0.0, 0.252,
2.25, 1.70, 1.40,
202.1, 351.1,
-0.8469, 0.1152E-01, -0.3535E-04, 0.4462E-07,
2.153, 5.113E-02, -2.004E-05, 0.328E-09,
12.0457, -3667.705, -46.976, 3*0.0,
WATER
0, 18.0, 373.2, 647.6, 217.3, 56.0, 0.348, 18.05, 0.344,
0.0, 0.0, 0.92, 1.40, 1.00, 0.0, 0.0, 0.238,
0.615, 1.84, 1.70,
538.7, 373.2,
-2.7133, 0.27235E-01, -0.7271E-04, 0.7007E-07,
7.701, 4.595E-04, 2.521E-06, -0.859E-09,
11.9516, -3984.923, -39.734, 3*0.0,
BENZENE
0, 78.1, 353.3, 562.1, 48.3, 259.0, 0.210, 88.26, 0.212,
0.0, 0.0, 3.1878, 2.4, 0.0, 0.0, 0.0, 0.2696,
3.004, 0.00, 0.00,
94.1, 353.3,
0.3049, -0.6510E-04, 0.5858E-06, 0.1717E-08,
-8.101, 1.133E-1, -7.206E-05, 1.703E-08,
9.2082, -2755.644, -53.999, 3*0.0,
1.40, 1.55, 0.0,
1.55, 1.70, 0.0,
3*0.0,
 3 ETHANOL
 1 WATER
 1 BENZENE

1, 1, 1, 2, 1, 15,
1, 17,
6, 10,
SIMULATION OF ETOH-ETR-BZ AZEO COLUMN: UNIFAC MODEL
5, 0, 40, 2, 0, 0, 40, 1, 0,
1.0, 0.0, 0.0,
726.9, 0.0, 6.015, 150.0, 175.0, 14.696, 0.0,
40, 0, 98, 0, 169.2, 22.65, 400.0,
37, 0, 96, 0, 191.9, 66.6, 0.0,
```

Table C.1.2 <u>Azeotropic Distillation Column Bottoms Results</u>

System: Ethanol - Water - Benzene

Models : UNIFAC and Virial (Hayden & O'Connell) vapor

Variable Process Parameters : Pressure and Boilup ratio

Case No.	Top Stage Pressure (psia)	Boilup Ratio	Bottoms Product Composition		
			Ethanol	Water	Benzene
4A5	12.0	6.015	98.3647	1.7457E-09	1.6353
4A2 *	14.7	6.015	92.0354	8.3129E-08	7.9646
4A3	30.0	6.015	70.9312	1.0176E-09	29.0688
4A12	12.0	5.714	98.6547	1.1806E-09	1.3453
4A13	12.0	5.113	99.4347	3.6523E-09	0.5653
4A9	14.7	3.910	97.9300	3.5514E-08	2.2691
4A10	14.7	3.760	98.6654	1.7547E-07	1.3346
4A11	14.7	3.680	99.2402	4.5488E-07	0.7598

* Base case

Table C.1.3: Comparison of T and X Profiles in the Azeotropic Column Using NRTL and UNIFAC Models

Models: UNIFAC, NRTL for liquid phase and ideal vapor
System: (1) Ethanol - (2) Water - (3) Benzene

	NRTL				UNIFAC			
Stg #	T(F)	(1)	(2)	(3)	T(F)	(1)	(2)	(3)
40	150.66	29.15	4.43	66.42	149.36	30.22	2.55	67.23
39	150.69	29.37	4.41	66.23	149.92	30.69	2.20	67.11
38	150.68	30.94	4.75	64.31	150.00	32.30	2.32	65.38
37	150.69	45.05	8.86	46.09	150.00	48.14	5.27	46.59
36	151.32	46.97	6.91	46.11	151.69	50.49	2.68	46.83
35	151.96	48.68	5.13	46.18	152.76	51.74	1.26	47.00
34	152.54	50.08	3.65	46.28	153.33	52.33	0.57	47.09
33	153.02	51.14	2.50	46.36	153.61	52.61	0.25	47.14
32	153.38	51.89	1.67	46.43	153.74	52.73	0.11	47.16
31	153.65	52.42	1.10	46.49	153.79	52.78	0.49E-1	47.17
30	153.83	52.77	0.71	46.53	153.82	52.81	0.22E-1	47.17
29	153.95	52.99	0.46	46.55	153.83	52.82	0.95E-2	47.17
28	154.03	53.14	0.29	46.57	153.84	52.82	0.42E-2	47.17
27	154.09	53.24	0.19	46.58	153.84	52.82	0.18E-2	47.17
26	154.12	53.30	0.12	46.59	153.84	52.83	0.80E-3	47.17
25	154.14	53.34	0.75E-1	46.59	153.84	52.83	0.36E-3	47.17
24	154.15	53.36	0.47E-1	46.59	153.84	52.83	0.15E-3	47.18
23	154.16	53.38	0.30E-1	46.59	153.84	52.83	0.67E-4	47.18
22	154.17	53.39	0.19E-1	46.60	153.84	52.83	0.29E-4	47.18
20	154.17	53.40	0.76E-2	46.60	153.84	52.83	0.56E-5	47.18
19	154.18	53.40	0.48E-2	46.60	153.84	52.83	0.25E-5	47.18
18	154.18	53.40	0.30E-2	46.60	153.84	52.83	0.11E-5	47.18
16	154.18	53.40	0.12E-2	46.60	153.84	52.83	0.21E-6	47.18
13	154.18	53.40	0.31E-3	46.60	153.84	52.83	0.16E-7	47.18
12	154.18	53.40	0.20E-3	46.60	153.84	52.83	0.63E-8	47.18
11	154.18	53.40	0.12E-3	46.60	153.84	52.83	0.20E-8	47.18
10	154.18	53.40	0.78E-4	46.60	153.84	52.83	0.17E-9	47.18
9	154.18	53.41	0.49E-4	46.60	153.84	52.83	0.39E-8	47.17
8	154.18	53.42	0.31E-4	46.58	153.84	52.83	0.39E-8	47.17
7	154.18	53.48	0.19E-4	46.52	153.84	52.83	0.39E-8	47.17
6	154.19	53.74	0.12E-4	46.26	153.84	52.85	0.39E-8	47.15
5	154.23	54.89	0.76E-5	45.11	153.84	52.95	0.39E-8	47.06
4	154.47	59.28	0.52E-5	40.74	153.86	53.39	0.39E-8	46.61
3	155.83	70.59	0.43E-5	29.42	153.93	55.38	0.42E-8	44.62
2	160.57	85.21	0.40E-5	14.80	154.38	62.72	0.55E-8	37.29
1	166.96	94.49	0.37E-5	5.509	157.11	78.03	0.89E-8	21.97
R	170.82	98.27	0.32E-5	1.731	164.03	91.66	0.13E-7	8.337

Note: All the compositions are in mole %

C.2 Sample Input and Azeotropic Column Results for Ethanol-Water-Cyclohexane System

Table C.2.1 Input Data for Ethanol-Water-Cyclohexane System

```
ETOH-WTR-CYHEXAN DEHYD: NCASE=5, UNIFAC & VIRIAL VAPOR(EX #4B)
3, 7, 1, 2, 0, 0, 0, 1, 0, 0, 0,
ETOH
0, 46.1, 315.10, 516.2, 63.0, 167.0, 0.248, 58.39, 0.635,
0.0, 0.0, 2.1055, 1.9720, 0.92, 0.0, 0.0,0.252,
2.25, 1.70, 1.40,
202.1, 351.1,
-0.3499, 9.559E-03, -37.86E-06, 54.59E-09,
2.153, 5.113E-02, -2.004E-05, 0.328E-09,
12.0457, -3667.705, -46.976, 3*0.0,
WATER
0, 18.0, 373.2, 647.6, 217.3, 56.0, 0.348, 18.05, 0.344,
0.0, 0.0, 0.92, 1.40, 1.00, 0.0, 0.0, 0.238,
0.615, 1.84, 1.70,
538.7, 373.2,
0.6741, 2.825E-03, -8.371E-06, 8.601E-09,
7.701, 4.595E-04, 2.521E-06, -0.859E-09,
11.9516, -3984.923, -39.734, 3*0.0,
CYHEXANE
0, 84.162, 353.9, 553.4, 40.2, 308.0, 0.273, 108.04, 0.213,
0.0, 0.0, 3.97, 3.01, 3.01, 0.0, 0.0, 0.2729,
3.261, 0.0, 0.0,
85.07, 353.9,
-1.284, 13.39E-03, -35.10E-06, 32.27E-09,
-13.027, 1.460E-01, -6.027E-05, 3.156E-09,
9.1194, -2766.63, -50.50, 3*0.0,
1.40, 1.55, 0.0,
1.55, 1.70, 0.0,
3*0.0,
 3 ETHANOL
 1 WATER
 1 CYCLOHEXANE

1, 1, 1, 2, 1, 15,
1, 17,
6, 2,
ETOH-WTR-CYCLOHEXANE AZEO DIST COLUMN SIMULATION: UNIFAC
5, 0, 40, 2, 0, 0, 60, 1, 0,
1.0, 0.0, 0.0,
726.9, 0.0, 6.015, 130.0, 170.0, 14.7, 0.10,
40, 0, 98, 0, 169.2, 22.65, 400.0,
37, 0, 96, 0, 191.9, 66.6, 0.0,
```

Table C.2.2 Azeotropic Distillation Column Results

System: Ethanol - Water - Cyclohexane

Models : UNIFAC and Virial (Hayden & O'Connell)

Variable Process Parameters : Pressure and Boilup ratio

Case No.	Top Stage Pressure (psia)	Boilup Ratio	Bottoms Product Composition(mole%)		
			Ethanol	Water	Cyclohexane
4B10	12.0	6.015	97.6896	6.1519E-12	2.3104
4B2 *	14.7	6.015	89.6853	3.6724E-09	10.3147
4B3	30.0	6.015	63.2043	2.5085E-11	36.7957
4B14	12.0	7.100	99.0900	1.0111E-09	0.9100
4B5	14.7	6.917	91.0483	2.4229E-09	8.9517
4B6	14.7	7.218	91.4067	4.5065E-10	8.5933
4B7	14.7	7.820	92.0196	2.8018E-06	7.9804
4B8	14.7	15.038	95.0216	9.9259E-12	4.9784
4B9	14.7	27.068	96.1805	1.6044E-09	3.8195

* Base case

Table C.1.3: Comparison of T and x Profiles in the Azeotropic Column Using NRTL and UNIFAC Models

Models: UNIFAC, NRTL for liquid phase and ideal vapor
System: (1) Ethanol - (2) Water - (3) Cyclohexane

	NRTL				UNIFAC			
Stg #	T(F)	(1)	(2)	(3)	T(F)	(1)	(2)	(3)
40	134.44	30.51	1.89	67.60	143.72	29.74	3.05	67.22
39	135.61	30.90	1.54	67.56	144.37	30.25	2.80	66.96
38	136.10	30.02	1.39	68.59	144.72	28.46	2.41	69.13
37	136.56	47.00	3.82	49.18	145.20	45.00	5.98	49.01
36	139.16	48.98	1.50	49.51	146.92	47.39	3.46	49.15
35	140.58	49.81	0.56	49.63	148.27	48.88	1.84	49.28
34	141.37	50.15	0.21	49.65	149.24	49.72	0.93	49.35
33	141.90	50.31	0.74E-1	49.62	149.92	50.17	0.46	49.37
32	142.32	50.39	0.27E-1	49.58	150.42	50.41	0.22	49.36
31	142.71	50.45	0.97E-2	49.54	150.83	50.55	0.11	49.34
30	143.09	50.50	0.35E-2	49.49	151.18	50.64	0.52E-01	49.31
29	143.45	50.55	0.13E-2	49.45	151.51	50.70	0.25E-01	49.27
28	143.81	50.60	0.46E-3	49.40	151.83	50.75	0.12E-01	49.24
27	144.17	50.65	0.17E-3	49.35	152.14	50.79	0.57E-02	49.20
26	144.53	50.69	0.60E-4	49.31	152.45	50.84	0.27E-02	49.16
25	144.88	50.74	0.22E-4	49.26	152.76	50.87	0.13E-02	49.12
22	145.93	50.87	0.10E-5	49.13	153.66	50.99	0.14E-03	49.01
21	146.28	50.91	0.38E-6	49.09	153.95	51.02	0.69E-04	48.98
19	146.96	51.00	0.50E-7	49.00	154.54	51.10	0.16E-04	48.90
18	147.30	51.05	0.18E-7	48.96	154.83	51.13	0.76E-05	48.87
17	147.64	51.09	0.68E-8	48.91	155.12	51.17	0.37E-05	48.83
16	147.97	51.13	0.26E-8	48.87	155.41	51.20	0.18E-05	48.80
15	148.30	51.17	0.11E-8	48.83	155.70	51.24	0.84E-06	48.76
13	148.97	51.26	0.30E-9	48.74	156.27	51.31	0.19E-06	48.69
12	149.29	51.30	0.22E-9	48.70	156.56	51.35	0.93E-07	48.65
10	149.94	51.38	0.19E-9	48.62	157.12	51.42	0.21E-07	48.58
9	150.26	51.42	0.18E-9	48.58	157.40	51.45	0.10E-07	48.55
8	150.59	51.46	0.18E-9	48.54	157.68	51.49	0.49E-08	48.52
7	150.90	51.50	0.18E-9	48.50	157.96	51.52	0.24E-08	48.48
6	151.22	51.54	0.18E-9	48.46	158.23	51.55	0.11E-08	48.45
5	151.54	51.59	0.18E-9	48.41	158.51	51.59	0.54E-09	48.41
4	151.85	51.68	0.18E-9	48.32	158.78	51.65	0.26E-09	48.35
3	152.17	52.22	0.19E-9	47.79	159.06	52.00	0.12E-09	48.00
2	152.57	56.11	0.22E-9	43.89	159.39	55.57	0.63E-10	44.43
1	154.29	72.28	0.41E-9	27.73	161.00	71.94	0.49E-10	28.06
R	163.28	91.35	0.42E-4	8.65	170.24	90.88	0.47E-10	9.12

Note: All the compositions are in mole %

NRTL parameters are shown in Table 3.2

C.3 Sample Input and Azeotropic Column Results for Ethanol-Water-Pentane System

Table C.3.1 Input for Ethanol-Water-Pentane System

```
ETOH-WTR-PENTANE DEHYD. NCASE=5: UNIFAC & VIRIAL (EX#4C)
3, 7, 1, 2, 0, 0, 0, 1, 0, 0, 0,
ETOH
0, 46.1, 351.10, 516.2, 63.0, 167.0, 0.248, 58.39, 0.635,
0.0, 0.0, 2.1055, 1.9720, 0.92, 0.0, 0.0,0.252,
2.25, 1.70, 1.40,
202.1, 351.1,
-0.3499, 9.559E-03, -37.86E-06, 54.59E-09,
2.153, 5.113E-2, -2.004E-5, 0.328E-9,
12.0457, -3667.705, -46.976, 3*0.0,
WATER
0, 18.0, 373.2, 647.6, 217.3, 56.0, 0.348, 18.05, 0.344,
0.0, 0.0, 0.92, 1.40, 1.00, 0.0, 0.0, 0.238,
0.615, 1.84, 1.70,
538.7, 373.2,
0.6741, 2.825E-03, -8.371E-06, 8.601E-09,
7.701, 4.595E-4, 2.521E-6, -0.859E-9,
11.9516, -3984.923, -39.734, 3*0.0,
PENTANE
0, 72.151, 309.2, 469.6, 33.3, 304.0, 0.262, 115.257, 0.251,
0.0, 0.0, 3.82, 3.31, 3.31, 0.0, 0.0, 0.2685,
3.385, 0.0, 0.0,
85.38, 309.2,
0.2904, 1.7109E-03, -6.2396E-06, 11.5436E-09,
-0.866, 1.164E-1, -6.163E-5, 1.267E-8,
9.20, -2477.07, -39.94, 3*0.0,
1.40, 1.55, 0.0,
1.55, 1.70, 0.0,
3*0.0,
 3 ETHANOL
 1 WATER
 2 PENTANE

1, 1, 1, 2, 1, 15,
1, 17,
2, 1, 3, 2,
ETOH-WTR-PENTANE AZEO DIST COLUMN SIMULATION: USING UNIFAC
5, 1, 40, 2, 0, 0, 50, 1, 0,
1.0, 0.0, 0.0,
726.9, 0.0, 6.015, 175.0, 220.0, 30.0, 0.10,
40, 0, 98, 0, 169.2, 22.65, 400.0,
37, 0, 96, 0, 191.9, 66.6, 0.0,
239.91, 87.24, 399.85,
83.0, 20.0, 20.0,
```

Table C.3.2 Azeotropic Distillation Column Bottoms Results

System: Ethanol - Water - n-Pentane

Models : UNIFAC and Virial (Hayden & O'Connell) vapor

Variable Process Parameters : Pressure and Boilup ratio

Case No.	Top Stage Pressure (psia)	Boilup Ratio	Bottoms Product Composition (mole%)		
			Ethanol	Water	Pentane
4C23	30.0	6.015	67.8646	32.1354	4.3795E-14
4C38	35.0	6.015	68.4082	31.5218	1.3476E-20
4C7	125.0	6.015	72.6582	27.3418	6.4379E-20
4C14	125.0	4.812	71.8436	28.1564	7.5500E-12

Note : All the compositions are in mole % .

Table C.3.3: T and x Profiles in the Azeotropic Column Using UNIFAC Models

Models: UNIFAC for liquid phase and Virial for vapor Phase
System: (1) Ethanol - (2) Water - (3) n-Pentane
Case #: 4C23

Stage		Liquid Phase Compositions in Mole %		
#	T(F)	(1)	(2)	(3)
40	170.61	80.722	13.285	5.9935
39	204.67	83.723	15.987	0.28941
38	207.25	81.921	18.066	0.13045E-01
37	207.65	79.629	20.371	0.55674E-03
36	207.82	79.627	20.373	0.34465E-04
35	207.99	79.624	20.376	0.21366E-05
34	208.16	79.622	20.378	0.13265E-06
33	208.33	79.619	20.381	0.82464E-08
32	208.49	79.617	20.383	0.51338E-09
31	208.66	79.615	20.385	0.32005E-10
30	208.83	79.612	20.388	0.19969E-11
29	208.99	79.610	20.390	0.12365E-12
28	209.16	79.608	20.392	0.65592E-14
27	209.32	79.605	20.395	0.20865E-11
25	209.65	79.601	20.399	0.15960E-11
24	209.81	79.598	20.402	0.70992E-13
23	209.97	79.596	20.404	0.55418E-14
22	210.14	79.594	20.406	0.13601E-14
21	210.30	79.591	20.409	0.12039E-14
19	210.62	79.587	20.413	0.40193E-12
18	210.78	79.584	20.416	0.30380E-13
17	210.94	79.581	20.419	0.29601E-14
16	211.10	79.578	20.422	0.15653E-14
15	211.26	79.573	20.427	0.44268E-09
14	211.42	79.568	20.432	0.31300E-10
12	211.74	79.549	20.451	0.44278E-13
11	211.90	79.531	20.469	0.22460E-07
10	212.05	79.503	20.497	0.38527E-11
9	212.21	79.458	20.542	0.39235E-07
8	212.37	79.384	20.616	0.38409E-07
7	212.54	79.261	20.739	0.37505E-10
6	212.70	79.057	20.943	0.13965E-11
5	212.88	78.714	21.286	0.19807E-16
4	213.07	78.133	21.867	0.33631E-16
3	213.29	77.136	22.864	0.33740E-16
2	213.57	75.383	24.616	0.32328E-16
1	213.99	72.187	27.813	0.11114E-13
R	214.77	65.956	34.044	0.48220E-15

Note: Profiles computed on Vax 11/780 without floating point extender and in single precision mode.

C.4 Sample Input and Azeotropic Column Results for Ethanol-Water-Cyclopentane System

Table C.4.1 Input for Ethanol-Water-Cyclopentane System

```
ETOH-WTR-CYCLO-C5 DEHYD. NCASE=5: UNIFAC & VIRIAL (EX #4D)
3, 7, 1, 2, 0, 0, 0, 1, 0, 0, 0,
ETOH
0, 46.1, 351.1, 516.2, 63.0, 167.0, 0.248, 58.39, 0.635,
0.0, 0.0, 2.1055, 1.9720, 0.92, 0.0, 0.0,0.252,
2.25, 1.70, 1.40,
202.1, 351.1,
-0.3499, 9.559E-03, -37.86E-06, 54.59E-09,
2.153, 5.113E-02, -2.004E-05, 0.328E-09,
12.0457, -3667.705, -46.976, 3*0.0,
WATER
0, 18.0, 373.2, 647.6, 217.3, 56.0, 0.348, 18.05, 0.344,
0.0, 0.0, 0.92, 1.40, 1.00, 0.0, 0.0, 0.238,
0.615, 1.84, 1.70,
538.7, 373.2,
0.6741, 2.825E-03, -8.371E-06, 8.601E-09,
7.701, 4.595E-04, 2.521E-06, -0.859E-09,
11.9516, -3984.923, -39.734, 3*0.0,
CYCLO-C5
0, 70.135, 322.4, 511.60, 44.50, 260.0, 0.276, 94.14, 0.192,
0.0, 0.0, 3.30, 2.47, 2.47, 0.0, 0.0, 0.2687,
3.12, 0.0, 0.0,
93.02, 322.4,
-0.08117, 4.146E-03, -13.16E-06, 15.95E-09,
-12.808, 1.296E-01, -7.239E-05, 1.549E-08,
9.2241, -2588.48, -41.79, 3*0.0,
1.40, 1.55, 0.0,
1.55, 1.70, 0.0,
3*0.0,
 3 ETHANOL
 1 WATER
 1 CYCLOPENTANE

1, 1, 1, 2, 1, 15,
1, 17,
5, 2,
ETOH-WTR-CYCLOPENTANE AZEO DIST COLUMN SIMULATION: UNIFAC
5, 0, 40, 2, 0, 0, 0, 1, 0,
1.0, 0.0, 0.0,
726.9, 0.0, 6.015, 150.0, 175.0, 30.0, 0.10,
40, 0, 98, 0, 169.2, 22.65, 400.0,
37, 0, 96, 0, 191.9, 66.6, 0.0,
```

C.4 Sample Input and Azeotropic Column Results for Ethanol-Water-Methyl Cyclopentane System

Table C.5.1 Input for Ethanol-Water-Methyl Cyclopentane System

```
ETOH-WTR-MTCYCLOC5 DEHYD. NCASE=5: UNIFAC & VIRIAL (EX#4E5)
3, 7, 1, 2, 0, 0, 0, 1, 0, 0, 0,
ETOH
0, 46.1, 351.1, 516.2, 63.0, 167.0, 0.248, 58.39, 0.635,
0.0, 0.0, 2.1055, 1.9720, 0.92, 0.0, 0.0,0.252,
2.25, 1.70, 1.40,
202.1, 351.1,
-0.3499, 9.559E-03, -37.86E-06, 54.59E-09,
2.153, 5.113E-2, -2.004E-5, 0.328E-9,
12.0457, -3667.705, -46.976, 3*0.0,
WATER
0, 18.0, 373.2, 647.6, 217.3, 56.0, 0.348, 18.05, 0.344,
0.0, 0.0, 0.92, 1.40, 1.00, 0.0, 0.0, 0.238,
0.615, 1.84, 1.70,
538.7, 373.2,
0.6741, 2.825E-03, -8.371E-06, 8.601E-09,
7.701, 4.595E-4, 2.521E-6, -0.859E-9,
11.9516, -3984.923, -39.734, 3*0.0,
MTCYCLC5
0, 84.162, 345.0, 532.7, 37.4, 319.0, 0.273, 111.62, 0.239,
0.0, 0.0, 3.97, 3.01, 3.01, 0.0, 0.0, 0.2700,
3.167, 0.0, 0.0,
82.58, 345.0,
-0.4414, 6.33489E-03, -16.5454E-06, 17.4712E-09,
-11.968, 1.524E-01, -8.699E-05, 1.914E-08,
9.1690, -2731.00, -47.11, 3*0.0,
1.40, 1.55, 0.0,
1.55, 0.0, 0.0,
3*0.0,
 3 ETHANOL
 1 WATER
 3 METHYL CYCLOPENTANE

1, 1, 1, 2, 1, 15,
1, 17,
1, 1, 4, 2, 1, 3,
ETOH-WTR-METHYL CYCLOPENTANE AZEO COLUMN SIMULATION: UNIFAC
5, 0, 40, 2, 0, 0, 50, 1, 0,
1.0, 0.0, 0.0,
726.9, 0.0, 6.015, 180.0, 215.0, 38.0, 0.10,
40, 0, 98, 0, 169.2, 22.65, 400.0,
37, 0, 96, 0, 191.9, 66.6, 0.0,
```

Table C.5.2 Azeotropic Distillation Column Bottoms Results

System: Ethanol - Water - Methyl Cyclopentane

Models : UNIFAC and Virial (Hayden & O'Connell) Vapor

Variable Process Parameters : Pressure and Boilup ratio

Case No.	Top Stage Pressure (psia)	Boilup Ratio	Bottoms Product Composition (mole%)		
			Ethanol	Water	CH3-Cyclo-C5
4E6	36.0	6.015	98.6898	1.1820E-08	1.3102
4E5	38.0	6.015	96.4856	5.2196E-13	3.5144
4E4	40.0	6.015	94.3885	1.9715E-06	5.6115
4E2	45.0	6.015	89.4979	1.2175E-10	10.5021
4E8	36.0	6.316	99.0059	2.9557E-11	0.9941
4E9	36.0	6.617	99.2887	5.4148E-12	0.7113
4E10	36.0	6.750	99.4025	6.9560E-11	0.5975
4E11	40.0	7.218	95.5285	1.7023E-10	4.4715

Table C.5.3: T and x Profile in the Azeotropic Column Using UNIFAC Model

Models: UNIFAC for liquid phase and Virial for vapor Phase
System: (1) Ethanol - (2) Water - (3) Methyl Cyclopentane
Case #: 4E5

Stage		Liquid Phase Compositions in Mole %		
#	T(F)	(1)	(2)	(3)
40	184.24	30.001	3.1356	66.863
39	184.88	30.429	2.7952	66.775
38	185.13	29.166	2.4808	68.353
37	185.38	44.966	5.8002	49.234
36	187.30	47.298	3.2781	49.424
35	188.73	48.706	1.7110	49.583
34	189.67	49.472	0.85120	49.677
33	190.24	49.868	0.41267	49.720
32	190.60	50.069	0.19749	49.733
31	190.86	50.175	0.93924E-01	49.731
30	191.05	50.235	0.44537E-01	49.720
29	191.23	50.272	0.21090E-01	49.706
28	191.38	50.299	0.99812E-02	49.691
27	191.53	50.321	0.47227E-02	49.674
25	191.83	50.358	0.10573E-02	49.641
24	191.98	50.376	0.50030E-03	49.624
23	192.12	50.393	0.23676E-03	49.607
22	192.26	50.410	0.11206E-03	49.590
21	192.41	50.427	0.53041E-04	49.573
20	192.55	50.444	0.25109E-04	49.556
18	192.84	50.478	0.56288E-05	49.522
17	192.98	50.495	0.26655E-05	49.505
16	193.13	50.511	0.12624E-05	49.489
15	193.27	50.528	0.59792E-06	49.472
14	193.41	50.545	0.28323E-06	49.455
12	193.69	50.578	0.63571E-07	49.422
11	193.83	50.595	0.30120E-07	49.405
10	193.97	50.611	0.14270E-07	49.389
9	194.12	50.628	0.67599E-08	49.372
8	194.26	50.644	0.32005E-08	49.356
7	194.40	50.661	0.15135E-08	49.339
6	194.54	50.681	0.71382E-09	49.319
5	194.68	50.747	0.33530E-09	49.253
4	194.82	51.364	0.15876E-09	48.636
3	195.12	56.930	0.87656E-10	43.070
2	198.15	75.914	0.74557E-10	24.086
1	210.70	92.643	0.71802E-10	7.3574
R	221.09	98.345	0.62770E-10	1.6546

Note: Profiles computed on Vax 11/780 without floating point extender and in single precision mode.

C.6 Sample Input and Azeotropic Column Results for Ethanol-Water-Isopentane System

Table C.6.1 Input for Ethanol-Water-Isopentane System

```
ETOH-WTR-IPENTANE DEHYD. NCASE=5: UNIFAC & VIRIAL (EX #4F)
3, 7, 1, 2, 0, 0, 0, 1, 0, 0, 0,
ETOH
0, 46.1, 351.1, 516.2, 63.0, 167.0, 0.248, 58.39, 0.635,
0.0, 0.0, 2.1055, 1.9720, 0.92, 0.0, 0.0,0.252,
2.25, 1.70, 1.40,
202.1, 351.1,
-0.3499, 9.559E-03, -37.86E-06, 54.59E-09,
2.153, 5.113E-02, -2.004E-05, 0.328E-09,
12.0457, -3667.705, -46.976, 3*0.0,
WATER
0, 18.0, 373.2, 647.6, 217.3, 56.0, 0.348, 18.05, 0.344,
0.0, 0.0, 0.92, 1.40, 1.00, 0.0, 0.0, 0.238,
0.615, 1.84, 1.70,
538.7, 373.2,
0.6741, 2.825E-03, -8.371E-06, 8.601E-09,
7.701, 4.595E-04, 2.521E-06, -0.859E-09,
11.9516, -3984.923, -39.734, 3*0.0,
IPENTANE
0, 72.151, 301.0, 460.4, 33.4, 306.0, 0.271, 116.37, 0.227,
0.0, 0.0, 3.82, 3.31, 3.31, 0.0, 0.0, 0.2716,
3.313, 0.13, 0.0,
81.77, 301.0,
-0.5019, 10.1929E-03, -36.5065E-06, 46.8004E-09,
-2.275, 1.210E-01, -6.519E-05, 1.367E-08,
9.0005, -2348.67, -40.05, 3*0.0,
1.40, 1.55, 0.0,
1.55, 0.0,  0.0,
3*0.0,
 3 ETHANOL
 1 WATER
 3 ISOPENTANE

1, 1, 1, 2, 1, 15,
1, 17,
3, 1, 1, 2, 1, 3,
ETOH-WTR-ISOPENTANE AZEO DIST COLUMN SIMULATION: USING UNIFAC
5, 0, 40, 2, 0, 0, 30, 1, 0,
1.0, 0.0, 0.0,
726.9, 0.0, 6.015, 200.0, 230.0, 85.0, 0.10,
40, 0, 98, 0, 169.2, 22.65, 400.0,
37, 0, 96, 0, 191.9, 66.6, 0.0,
```

C.7 Sample Input and Azeotropic Column Results for Ethanol-Water-n Hexane System

Table C.7.1 Input for Ethanol-Water-Hexane System

```
ETOH-WTR-HEXANE DEHYD: NCASE=5, UNIFAC & VIRIAL VAPCR(EX #4G)
3, 7, 1, 2, 0, 0, 0, 1, 0, 0, 0,
ETOH
0, 46.1, 351.1, 516.2, 63.0, 167.0, 0.248, 58.39, 0.635,
0.0, 0.0, 2.1055, 1.9720, 0.92, 0.0, 0.0,0.252,
2.25, 1.70, 1.40,
202.1, 351.1,
-0.3499, 9.559E-03, -37.86E-06, 54.59E-09,
2.153, 5.113E-02, -2.004E-05, 0.328E-09,
12.0457, -3667.705, -46.976, 3*0.0,
WATER
0, 18.0, 373.2, 647.6, 217.3, 56.0, 0.348, 18.05, 0.344,
0.0, 0.0, 0.92, 1.40, 1.00, 0.0, 0.0, 0.238,
0.615, 1.84, 1.70,
538.7, 373.2,
0.6741, 2.825E-03, -8.371E-06, 8.601E-09,
7.701, 4.595E-04, 2.521E-06, -0.859E-09,
11.9516, -3984.923, -39.734, 3*0.0,
N-HEXANE
0, 86.178, 341.9, 507.4, 29.3, 370.0, 0.260, 130.77, 0.296,
0.0, 0.0, 4.50, 3.86, 3.86, 0.0, 0.0, 0.2635,
3.812, 0.0, 0.0,
80.02, 341.9,
0.5357, -10.0356E-03, 3.6767E-06, -0.8608E-09,
-1.054, 1.390E-01, -7.449E-05, 1.551E-08,
9.2033, -2697.55, -48.78, 3*0.0,
1.40, 1.55, 0.0,
1.55, 1.70, 0.0,
3*0.0,
 3 ETHANOL
 1 WATER
 2 N-HEXANE

1, 1, 1, 2, 1, 15,
1, 17,
2, 1, 4, 2,
ETOH-WTR-N HEXANE AZEO DIST COLUMN SIMULATION: USING UNIFAC
5, 1, 40, 2, 0, 0, 150, 1, 0,
1.0, 0.0, 0.0,
726.9, 0.0, 6.015, 190.0, 230.0, 50.0, 0.10,
40, 0, 98, 0, 169.2, 22.65, 400.0,
37, 0, 96, 0, 191.9, 66.6, 0.0,
239.0, 80.0, 400.0,
```

Table C.7.2 Azeotropic Distillation Column Bottoms Results

System: Ethanol - Water - n-Hexane

Models : UNIFAC and Virial (Hayden & O'Connell) Vapor

Variable Process Parameters : Pressure and Boilup ratio

Case No.	Top Stage Pressure (psia)	Boilup Ratio	Bottoms Product Composition (mole%)		
			Ethanol	Water	Hexane
4G6	49.0	6.015	99.0563	1.3620E-08	0.9437
4G2	50.0	6.015	98.3822	1.3613E-08	1.6178
4G7	50.0	6.316	98.4755	1.7753E-09	1.5245
4G8	50.0	9.023	99.3803	3.8490E-10	0.6197
4G11	50.0	9.624	99.5394	9.7283E-09	0.4606

Table C.7.3: Comparison of T and x Profiles in the Azeotropic Column Using NRTL and UNIFAC Models

Models: UNIFAC for liquid and Virial for vapor phase
System: (1) Ethanol - (2) Water (3) n-Hexane
Case #: 4G6

Stage #	T(F)	Liquid Phase Comp. in Mole % (1)	(2)	(3)
40	195.71	26.162	2.468	71.371
38	195.30	23.793	2.421	73.785
36	197.05	47.027	6.158	46.814
34	200.02	50.661	2.423	46.867
32	201.05	52.260	0.814	46.926
30	202.55	52.825	0.247	46.927
28	202.97	53.026	0.733E-1	46.901
26	203.26	53.113	0.216E-1	46.864
24	203.51	53.167	0.635E-2	46.827
22	203.75	53.210	0.187E-2	46.788
20	203.99	53.250	0.552E-3	46.749
18	204.22	53.289	0.163E-3	46.710
16	204.46	53.328	0.483E-4	46.672
14	204.69	53.366	0.143E-4	46.633
12	204.92	53.404	0.424E-5	46.595
10	205.15	53.443	0.126E-5	46.557
8	205.38	53.481	0.372E-6	46.519
6	205.61	53.532	0.109E-6	46.468
4	205.88	54.905	0.307E-7	45.095
2	212.60	83.031	0.185E-7	16.969
R	235.45	99.056	0.136E-7	0.944

C.8 Sample Input and Azeotropic Column Results for Ethanol-Water-2 Methyl Pentane System

Table C.8.1 Input for Ethanol-Water-2 Methyl Pentane System

```
ETOH-WTR-2 METHYL C5 DYHYD:NCASE=5, UNIFAC & VIRIAL VAPOR(EX#4H)
3, 7, 1, 2, 0, 0, 0, 1, 0, 0, 0,
ETOH
0, 46.1, 351.1, 516.2, 63.0, 167.0, 0.248, 58.39, 0.635,
0.0, 0.0, 2.1055, 1.9720, 0.92, 0.0, 0.0,0.252,
2.25, 1.70, 1.40,
202.1, 351.1,
-0.3499, 9.559E-03, -37.86E-06, 54.59E-09,
2.153, 5.113E-02, -2.004E-05, 0.328E-09,
12.0457, -3667.705, -46.976, 3*0.0,
WATER
0, 18.0, 373.2, 647.6, 217.3, 56.0, 0.348, 18.05, 0.344,
0.0, 0.0, 0.92, 1.40, 1.00, 0.0, 0.0, 0.238,
0.615, 1.84, 1.70,
538.7, 373.2,
0.6741, 2.825E-03, -8.371E-06, 8.601E-09,
7.701, 4.595E-04, 2.521E-06, -0.859E-09,
11.9516, -3984.923, -39.734, 3*0.0,
2-MET-C5
0, 86.178, 333.4, 497.5, 29.7, 367.0, 0.267, 131.97, 0.279,
0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.2660,
3.809, 0.0, 0.0,
77.05, 333.4,
-0.3394, 8.3267E-03, -28.6794E-06, 35.3614E-09,
-2.524, 1.477E-01, -8.533E-05, 1.931E-08,
9.1143, -2614.38, -46.58, 3*0.0,
1.40, 1.55, 0.0,
1.55, 1.70, 0.0,
3*0.0,
 3 ETHANOL
 1 WATER
 3 2-METHYL PENTANE

1, 1, 1, 2, 1, 15,
1, 17,
3, 1, 2, 2, 1, 3,
ETOH-WTR-2 METHYL PENTANE AZEO DIST COLUMN SIMULATION: UNIFAC
5, 1, 40, 2, 0, 0, 200, 1, 0,
1.0, 0.0, 0.0,
726.9, 0.0, 6.015, 245.0, 290.0, 135.0, 0.10,
40, 0, 98, 0, 169.2, 22.65, 400.0,
37, 0, 96, 0, 191.9, 66.6, 0.0,
239.91, 85.24, 390.85,
93.0, 15.0, 15.0,
```

Table C.8.2 Azeotropic Distillation Column Bottoms Results

System: Ethanol - Water - 2-Methyl Pentane

Models : UNIFAC and Virial (Hayden & O'Connell) Vapor

Variable Process Parameters : Pressure and Boilup ratio

Case No.	Top Stage Pressure (psia)	Boilup Ratio	Bottoms Product Composition (mole%)		
			Ethanol	Water	2-Methyl-C5
4H22	128.0	6.015	98.6416	3.7503E-11	1.3584
4H10	130.0	6.015	98.1550	1.0109E-06	1.8449
4H8	135.0	6.015	96.9976	7.2197E-11	3.0024
4H11	130.0	6.617	98.0819	2.9652E-11	1.9181
4H12	130.0	5.414	98.3805	7.4507E-10	1.6195
4H24	126.0	5.714	99.2261	3.0897E-10	0.7739
4H25	124.0	5.714	99.7446	7.7106E-10	0.2554
4H13	125.0	5.414	98.3900	1.8674E-09	1.6100

Table C.8.3: T and x Profiles in the Azeotropic Column Using UNIFAC Model

Models: UNIFAC for liquid and Virial for vapor phase
System: (1) Ethanol - (2) Water (3) 2-Methyl Pentane
Case #: 4H25

Stage		Liquid Phase Comp. in Mole %		
#	T(F)	(1)	(2)	(3)
40	245.43	28.267	2.914	68.820
38	245.61	27.764	2.789	69.447
36	248.06	47.593	4.458	47.494
34	251.52	50.317	1.341	48.342
32	252.92	51.156	0.346	48.498
30	253.38	51.380	0.851E-1	48.535
28	253.59	51.420	0.420E-1	48.537
26	253.72	51.464	0.503E-2	48.531
24	253.83	51.477	0.122E-2	48.522
22	253.94	51.487	0.296E-3	48.512
20	254.05	51.496	0.719E-4	48.503
18	254.16	51.506	0.175E-4	48.494
16	254.27	51.515	0.424E-5	48.485
14	254.38	51.524	0.103E-5	48.476
12	254.49	51.534	0.248E-6	48.466
10	254.59	51.543	0.606E-7	48.457
8	254.70	51.559	0.154E-7	48.441
6	254.82	51.934	0.398E-8	48.066
4	256.18	65.618	0.145E-8	34.382
2	280.58	95.558	0.120E-8	4.442
R	291.52	99.745	0.771E-9	0.255

C.9 Sample Input and Azeotropic Column Results for Ethanol-Water-1 Hexene System

Table C.9.1 Input for Ethanol-Water-1 Hexene System

```
ETOH-WTR-HEXENE DYHYD: NCASE=5, UNIFAC & VIRIAL VAPOR(EX #4I)
3, 7, 1, 2, 0, 0, 0, 1, 0, 0, 0,
ETOH
0, 46.1, 351.1, 516.2, 63.0, 167.0, 0.248, 58.39, 0.635,
0.0, 0.0, 2.1055, 1.9720, 0.92, 0.0, 0.0, 0.252,
2.25, 1.70, 1.40,
202.1, 351.1,
-0.3499, 9.559E-03, -37.86E-06, 54.59E-09,
2.153, 5.113E-02, -2.004E-05, 0.328E-09,
12.0457, -3667.705, -46.976, 3*0.0,
WATER
0, 18.0, 373.2, 647.6, 217.3, 56.0, 0.348, 18.05, 0.344,
0.0, 0.0, 0.92, 1.40, 1.00, 0.0, 0.0, 0.238,
0.615, 1.84, 1.70,
538.7, 373.2,
0.6741, 2.825E-03, -8.371E-06, 8.601E-09,
7.701, 4.595E-04, 2.521E-06, -0.859E-09,
11.9516, -3984.923, -39.734, 3*0.0,
1-HEXENE
0, 84.162, 336.6, 504.0, 31.3, 350.0, 0.26, 125.05, 0.285,
0.0, 0.0, 4.27, 3.64, 3.64, 0.0, 0.0, 0.2660,
3.647, 0.50, 0.0,
80.32, 336.6,
0.2194, 1.6855E-03, -4.4269E-06, 7.0268E-09,
-0.417, 1.268E-01, -6.933E-5, 1.446E-08,
9.1756, -2654.81, -47.30, 3*0.0,
1.40, 1.55, 0.0,
1.55, 0.0, 0.0,
3*0.0,
 3 ETHANOL
 1 WATER
 3 1-HEXENE

1, 1, 1, 2, 1, 15,
1, 17,
3, 1, 2, 2, 2, 3,
ETOH-WTR-1 HEXENE AZEO DIST COLUMN SIMULATION: UNIFAC
5, 0, 40, 2, 0, 0, 70, 1, 0,
1.0, 0.0, 0.0,
726.9, 0.0, 6.015, 210.0, 255.0, 75.0, 0.10,
40, 0, 98, 0, 169.2, 22.65, 400.0,
37, 0, 96, 0, 191.9, 66.6, 0.0,
```

Table C.9.2 Azeotropic Distillation Column Bottoms Results

System: Ethanol - Water - 1-Hexene

Models : UNIFAC and Virial (Hayden & O'Connell) Vapor

Variable Process Parameters : Pressure and Boilup ratio

Case No.	Top Stage Pressure (psia)	Boilup Ratio	Bottoms Product Composition (mole%)		
			Ethanol	Water	1-Hexene
4I11	71.0	6.015	99.3832	3.9961E-11	0.6168
4I10	72.5	6.015	98.6153	1.1819E-10	1.3847
4I3	75.0	6.015	97.3042	1.5065E-11	2.6958
4I1	80.0	6.015	94.7741	1.3435E-12	5.2259
4I6	75.0	5.414	96.8929	1.1565E-10	3.1071
4I4	75.0	6.316	97.5044	6.2285E-11	2.4956
4I5	75.0	9.023	98.8578	1.4811E-10	1.1422
4I9	75.0	9.924	99.1511	3.7516E-11	0.8489
4I17	75.0	10.226	99.2404	2.1483E-11	0.7596
4I16	74.0	9.924	99.6431	8.2467E-12	0.3569

Table C.9.3: T and x Profiles in the Azeotropic Column Using UNIFAC Model

Models: UNIFAC for liquid phase and Virial for vapor Phase
System: (1) Ethanol - (2) Water - (3) 1-Hexene
Case #: 4I3

Stage #	T(F)	Liquid Phase Compositions in Mole % (1)	(2)	(3)
40	214.68	29.632	3.0201	67.348
39	215.25	29.931	2.7427	67.327
38	215.45	28.566	2.4438	68.990
37	215.57	44.830	5.8608	49.309
36	217.89	47.212	3.2677	49.520
35	219.56	48.623	1.6834	49.694
34	220.59	49.374	0.82778	49.798
33	221.19	49.753	0.39719	49.850
32	221.53	49.940	0.18828	49.871
31	221.74	50.034	0.88734E-01	49.877
30	221.88	50.083	0.41706E-01	49.876
29	221.99	50.110	0.19578E-01	49.870
28	222.09	50.128	0.91855E-02	49.863
26	222.26	50.151	0.20211E-02	49.847
25	222.35	50.160	0.94806E-03	49.839
24	222.43	50.169	0.44474E-03	49.830
23	222.52	50.178	0.20865E-03	49.822
22	222.60	50.186	0.97894E-04	49.814
21	222.68	50.195	0.45934E-04	49.805
20	222.76	50.203	0.21555E-04	49.797
19	222.85	50.212	0.10116E-04	49.788
18	222.93	50.220	0.47481E-05	49.780
17	223.01	50.229	0.22287E-05	49.771
15	223.18	50.245	0.49118E-06	49.755
14	223.26	50.254	0.23061E-06	49.746
13	223.34	50.262	0.10828E-06	49.738
12	223.42	50.270	0.50840E-07	49.730
10	223.59	50.287	0.11202E-07	49.713
9	223.67	50.296	0.52532E-08	49.704
8	223.75	50.304	0.24589E-08	49.696
7	223.83	50.313	0.11464E-08	49.687
6	223.92	50.340	0.53014E-09	49.660
5	224.00	50.728	0.24367E-09	49.272
4	224.20	56.623	0.13063E-09	43.377
3	228.28	79.292	0.94371E-10	20.708
2	246.49	95.051	0.94406E-10	4.9494
1	258.09	99.078	0.17450E-09	0.92180
R	260.95	99.840	0.14769E-09	0.15957

Note: Profiles computed on Vax 11/780 without floating point extender and in single precision mode.

C.10 Sample Input and Azeotropic Column Results for Ethanol-Water-Diethyl Ether System

Table C.10.1 Input for Ethanol-Water-Diethyl Ether System

```
ETOH-WTR-DE-ETHER DEHYD. NCASE=5 WITH UNIFAC & VIRIAL (EX #4J)
3, 7, 1, 2, 0, 0, 0, 1, 0, 0, 0,
ETOH
0, 46.1, 351.1, 516.2, 63.0, 167.0, 0.248, 58.39, 0.635,
0.0, 0.0, 2.1055, 1.9720, 0.92, 0.0, 0.0,0.252,
2.25, 1.70, 1.40,
202.1, 351.1,
-0.8469, 0.1152E-01, -0.3535E-04, 0.4462E-07,
2.153, 5.113E-02, -2.004E-05, 0.328E-09,
12.0457, -3667.705, -46.976, 3*0.0,
WATER
0, 18.0, 373.2, 647.6, 217.3, 56.0, 0.348, 18.05, 0.344,
0.0, 0.0, 0.92, 1.40, 1.00, 0.0, 0.0, 0.238,
0.615, 1.84, 1.70,
538.7, 373.2,
-2.7133, 0.27235E-01, -0.7271E-04, 0.7007E-07,
7.701, 4.595E-04, 2.521E-06, -0.859E-09,
11.9516, -3984.923, -39.734, 3*0.0,
DE-ETHER
0, 74.123, 307.7, 466.7, 35.9, 280.0, 0.262, 103.96, 0.281,
0.0, 0.0, 3.39, 3.02, 3.02, 0.0, 0.0, 0.2650,
3.140, 1.17, 0.0,
86.07, 307.7,
0.46055, -0.2098E-03, 0.29717E-06, .68367E-09,
5.117, 8.022E-02, -2.473E-05, -2.235E-09,
9.4495, -2511.29, -41.95, 3*0.0,
1.40, 1.55, 0.50,
1.55, 1.70, 0.50,
0.50, 0.50, 0.00,
 3 ETHANOL
 1 WATER
 3 DIETHYL ETHER

1, 1, 1, 2, 1, 15,
1, 17,
2, 1, 1, 2, 1, 26,
ETOH-WTR-DIETHYL ETHER AZEO DIST COLUMN SIMULATION: USING UNIFAC
5, 0, 40, 2, 0, 0, 30, 1, 0,
1.0, 0.0, 0.0,
726.9, 0.0, 6.015, 285.0, 245.0, 135.0, 0.10,
40, 0, 98, 0, 169.2, 22.65, 400.0,
37, 0, 96, 0, 191.9, 66.6, 0.0,
```

Table C.10.2 Azeotropic Distillation Column Bottoms Results

System: Ethanol - Water - Diethyl Ether

Models : UNIFAC and Virial (Hayden & O'Connell) vapor

Variable Process Parameters : Pressure and Boilup ratio

Case No.	Top Stage Pressure (psia)	Boilup Ratio	Bottoms Product Composition (mole%)		
			Ethanol	Water	Diethyl ether
4J3 *	14.7	6.015	62.9888	37.0112	1.2689E-14
4J2	40.0	6.015	65.8450	34.1548	9.5114E-13
4J7	85.0	6.015	67.8711	32.1289	5.7101E-18
4J8	110.0	6.015	68.4367	31.5633	2.9766E-14
4J1	135.0	6.015	68.7874	31.2126	5.1550E-18
4J5	250.0	6.015	68.6299	31.3701	3.3514E-15
4J6	135.0	3.080	69.5763	30.4237	2.6247E-13

* Base case

Table C.10.3: Comparison of T and x Profiles in the Azeotropic Column Using NRTL and UNIFAC Models

Models: UNIFAC, NRTL for liquid phase and Virial for vapor Phase
System: (1) Ethanol - (2) Water - (3) Diethyl Ether
Case : 4J1

	NRTL				UNIFAC			
Stg #	T(F)	(1)	(2)	(3)	T(F)	(1)	(2)	(3)
40	260.15	51.21	12.01	36.79	262.25	58.65	11.61	29.75
39	274.40	68.04	18.59	13.37	282.74	73.98	16.65	9.37
38	284.15	74.03	22.08	3.89	291.59	77.95	19.39	2.66
37	287.86	74.79	24.16	1.05	294.43	77.84	21.42	0.73
36	288.81	75.27	24.31	0.42	295.10	78.20	21.50	0.30
35	289.23	75.46	24.38	0.17	295.40	78.35	21.53	0.12
34	289.42	75.53	24.40	0.67E-01	295.56	78.41	21.54	0.48E-01
33	289.53	75.56	24.41	0.26E-01	295.65	78.43	21.55	0.20E-01
32	289.60	75.58	24.41	0.10E-01	295.71	78.44	21.55	0.79E-02
31	289.66	75.58	24.41	0.42E-02	295.77	78.45	21.55	0.32E-02
30	289.72	75.59	24.41	0.17E-02	295.82	78.45	21.55	0.13E-02
29	289.77	75.59	24.41	0.66E-03	295.87	78.45	21.55	0.52E-03
28	289.82	75.59	24.41	0.26E-03	295.92	78.45	21.55	0.21E-03
27	289.86	75.59	24.41	0.10E-03	295.97	78.45	21.55	0.85E-04
25	289.96	75.59	24.41	0.16E-04	296.07	78.45	21.55	0.14E-04
23	290.06	75.59	24.41	0.26E-05	296.17	78.45	21.55	0.23E-05
22	290.11	75.59	24.41	0.10E-05	296.22	78.45	21.55	0.92E-06
20	290.21	75.59	24.41	0.16E-06	296.32	78.45	21.55	0.15E-06
19	290.26	75.59	24.41	0.65E-07	296.36	78.45	21.55	0.61E-07
18	290.30	75.59	24.41	0.26E-07	296.41	78.45	21.55	0.25E-07
17	290.35	75.60	24.40	0.10E-07	296.46	78.45	21.55	0.10E-07
15	290.45	75.61	24.39	0.13E-08	296.56	78.45	21.55	0.17E-08
14	290.50	75.62	24.38	0.36E-09	296.61	78.45	21.55	0.67E-09
13	290.55	75.63	24.37	0.69E-10	296.66	78.44	21.56	0.27E-09
12	290.60	75.66	24.34	0.27E-10	296.71	78.43	21.57	0.11E-09
10	290.71	75.80	24.20	0.50E-11	296.81	78.38	21.62	0.17E-10
9	290.76	75.94	24.06	0.26E-11	296.86	78.34	21.67	0.73E-11
8	290.83	76.19	23.82	0.10E-11	296.92	78.26	21.74	0.29E-11
7	290.91	76.59	23.41	0.45E-12	296.97	78.13	21.87	0.76E-12
6	291.01	77.26	22.74	0.19E-12	297.04	77.92	22.08	0.56E-07
5	291.16	78.33	21.68	0.78E-13	297.11	77.58	22.42	0.56E-11
4	291.39	79.93	20.07	0.32E-13	297.21	77.00	23.00	0.26E-10
3	291.75	82.18	17.82	0.14E-13	297.33	76.03	23.97	0.11E-10
2	292.31	85.04	14.96	0.57E-14	297.53	74.37	25.63	0.42E-11
1	293.11	88.30	11.70	0.23E-14	297.88	71.40	28.60	0.16E-11
R	294.13	91.57	8.430	0.89E-15	298.62	65.79	34.21	0.55E-12

Note: All the compositions are in mole %

C.11 Sample Input and Azeotropic Column Results for Ethanol-Water-2,2-Dimethyl Pentane System

Table C.11.1 Input for Ethanol-Water-2,2-Dimethyl Pentane System

```
ETOH-WTR-DICH3C5 DEHYD. NCASE=5: UNIFAC & VIRIAL (EX #4K)
3, 7, 1, 2, 0, 0, 0, 1, 0, 0, 0,
ETOH
0, 46.1, 351.1, 516.2, 63.0, 167.0, 0.248, 58.39, 0.635,
0.0, 0.0, 2.1055, 1.9720, 0.92, 0.0, 0.0,0.252,
2.25, 1.70, 1.40,
202.1, 351.1,
-0.3499, 9.559E-03, -37.86E-06, 54.59E-09,
2.153, 5.113E-2, -2.004E-5, 0.328E-9,
12.0457, -3667.705, -46.976, 3*0.0,
WATER
0, 18.0, 373.2, 647.6, 217.3, 56.0, 0.348, 18.05, 0.344,
0.0, 0.0, 0.92, 1.40, 1.00, 0.0, 0.0, 0.238,
0.615, 1.84, 1.70,
538.7, 373.2,
0.6741, 2.825E-03, -8.371E-06, 8.601E-09,
7.701, 4.595E-4, 2.521E-6, -0.859E-9,
11.9516, -3984.923, -39.734, 3*0.0,
DICH3C5
0, 100.205, 352.4, 520.4, 27.4, 416.0, 0.267, 148.672, 0.289,
0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.2652,
4.0001, 0.0, 0.0,
69.5574, 352.4,
0.3075, 0.35047E-03, 0.77247E-06, 1.0954E-09,
-11.966, 2.139E-01, -1.519E-04, 4.146E-08,
9.0584, -2740.15, 49.85, 3*0.0,
1.40, 1.55, 0.0,
1.55, 0.0, 0.0,
3*0.0,
 3 ETHANOL
 1 WATER
 3 2,2-DIMETHYL PENTANE

1, 1, 1, 2, 1, 15,
1, 17,
4, 1, 2, 2, 1, 4,
ETOH-WTR-2,2 DIMETHYL PENTANE AZEO COLUMN SIMULATION: UNIFAC
5, 0, 40, 2, 0, 0, 0, 1, 0,
1.0, 0.0, 0.0,
726.9, 0.0, 6.015, 150.0, 175.0, 22.0, 0.10,
40, 0, 98, 0, 169.2, 22.65, 400.0,
37, 0, 96, 0, 191.9, 66.6, 0.0,
```

C.12 Sample Input and Azeotropic Column Results for Ethanol-Water-2,2,3-Trimethyl Butane System

Table C.12.1 Input for Ethanol-Water-2,2,3-Trimethyl Butane System

```
ETOH-WTR-TRICH3C4 DEHYD. NCASE=5: UNIFAC & VIRIAL (EX #4L)
3, 7, 1, 2, 0, 0, 0, 1, 0, 0, 0,
ETOH
0, 46.1, 351.1, 516.2, 63.0, 167.0, 0.248, 58.39, 0.635,
0.0, 0.0, 2.1055, 1.9720, 0.92, 0.0, 0.0, 0.252,
2.25, 1.70, 1.40,
202.1, 351.1,
-0.3499, 9.559E-03, -37.86E-06, 54.59E-09,
2.153, 5.113E-2, -2.004E-5, 0.328E-9,
12.0457, -3667.705, -46.976, 3*0.0,
WATER
0, 18.0, 373.2, 647.6, 217.3, 56.0, 0.348, 18.05, 0.344,
0.0, 0.0, 0.92, 1.40, 1.00, 0.0, 0.0, 0.238,
0.615, 1.84, 1.70,
538.7, 373.2,
0.6741, 2.825E-03, -8.371E-06, 8.601E-09,
7.701, 4.595E-4, 2.521E-6, -0.859E-9,
11.9516, -3984.923, -39.734, 3*0.0,
TRICH3C4
0, 100.205, 354.0, 531.1, 29.2, 398.0, 0.267, 145.225, 0.251,
0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.2685,
3.6960, 0.0, 0.0,
69.048, 354.0,
0.36906, -0.0353E-03, 1.4521E-06, 0.51867E-09,
-5.480, 1.796E-01, -1.056E-04, 2.40E-08,
9.0065, -2764.40, -47.10, 3*0.0,
1.40, 1.55, 0.0,
1.55, 0.0, 0.0,
3*0.0,
 3 ETHANOL
 1 WATER
 3 2,2,3-TRIMETHYL BUTANE

1, 1, 1, 2, 1, 15,
1, 17,
5, 1, 1, 3, 1, 4,
ETOH-WTR-2,2,3 TRIMETHYL BUTANE AZEO DIST COLUMN SIMULATION: USING UNI
5, 0, 40, 2, 0, 0, 0,1, 0,
1.0, 0.0, 0.0,
726.9, 0.0, 6.617, 120.0, 165.0, 10.0, 0.10,
40, 0, 98, 0, 169.2, 22.65, 400.0,
37, 0, 96, 0, 191.9, 66.6, 0.0,
```

Table C.12.2 Azeotropic Distillation Column Bottoms Results

System: Ethanol - Water - 2,2,3-Trimethyl Butane

Models : UNIFAC and Virial (Hayden & O'Connell) Vapor

Variable Process Parameters : Pressure and Boilup ratio

Case No.	TopStage Pressure (psia)	Boilup Ratio	Bottoms Product Composition (mole%)		
			Ethanol	Water	Trimethyl C4
4L3	10.0	6.015	95.8756	3.1308E-09	4.1244
4L1 *	14.7	6.015	79.6356	2.7729E-12	20.3644
4L2	30.0	6.015	52.5954	7.5185E-11	47.4046
4L7	14.7	6.617	80.5392	3.6756E-12	19.4608
4L8	14.7	12.030	84.6264	9.3453E-11	15.3736
4L10	10.0	6.617	96.7827	3.1929E-10	3.2173
4L11	10.0	6.917	97.1660	1.8149E-11	2.8338
4L12	10.0	7.519	97.8175	3.6692E-10	2.1825
4L13	10.0	8.120	98.3465	4.5123E-11	1.6535
4L14	10.0	9.022	98.9765	4.6568E-10	1.0235
4L19	10.0	9.150	99.0554	1.6000E-12	0.9446

* Base case

Table C.12.3: T and x Profiles in the Azeotropic Column Using UNIFAC Model

Models: UNIFAC for liquid phase and Virial for vapor Phase
System: (1) Ethanol - (2) Water - (3) 2,2,3-Trimethyl Butane
Case #: 4L10

Stage #	T(F)	Liquid Phase Compositions in Mole % (1)	(2)	(3)
40	125.03	31.289	3.5335	65.178
39	126.07	32.097	2.9276	64.975
38	126.66	30.531	2.4581	67.011
37	127.21	44.733	5.1204	50.146
36	128.93	46.894	2.8066	50.299
35	130.25	48.170	1.4274	50.403
34	131.21	48.866	0.69481	50.439
33	131.92	49.240	0.33058	50.430
32	132.48	49.450	0.15553	50.395
31	132.98	49.580	0.72795E-01	50.347
30	133.43	49.673	0.33990E-01	50.293
29	133.86	49.747	0.15855E-01	50.237
28	134.29	49.812	0.73930E-02	50.180
26	135.12	49.932	0.16073E-02	50.066
25	135.52	49.990	0.74960E-03	50.009
24	135.93	50.046	0.34964E-03	49.953
23	136.33	50.103	0.16312E-03	49.897
22	136.73	50.158	0.76114E-04	49.842
21	137.12	50.213	0.35524E-04	49.787
20	137.52	50.268	0.16583E-04	49.732
18	138.30	50.376	0.36157E-05	49.624
17	138.68	50.429	0.16888E-05	49.571
16	139.06	50.482	0.78900E-06	49.518
15	139.44	50.535	0.36868E-06	49.465
14	139.82	50.587	0.17231E-06	49.413
13	140.19	50.638	0.80549E-07	49.362
11	140.94	50.741	0.17611E-07	49.259
10	141.30	50.792	0.82366E-08	49.208
9	141.67	50.842	0.38522E-08	49.158
8	142.03	50.892	0.18013E-08	49.108
7	142.39	50.941	0.84178E-09	49.059
6	142.75	50.991	0.39275E-09	49.009
5	143.10	51.040	0.18257E-09	48.960
4	143.46	51.104	0.84226E-10	48.896
3	143.81	51.863	0.39137E-10	48.137
2	144.36	63.372	0.25377E-10	36.628
1	151.05	87.914	0.25953E-10	12.086
R	164.97	97.834	0.24119E-10	2.1663

Note: Profiles computed on Vax 11/780 without floating point extender and in single precision mode

APPENDIX D

OBJECTIVE FUNCTIONS AND SAMPLE INPUT FOR THE PARAMETER ESTIMATION PROGRAM

D.1 Sample Input for the Parameter Estimation Program (MARQDT)

D.2 Objective Functions: Vapor-Liquid Equilibrium Data Regression

D.3 Objective Functions: Liquid-Liquid Equilibrium Data Regression

D.1 Sample Input for the Parameter Estimation Program (MARQDT)

```
ESTIMATION OF MODIFIED UNIQUAC PARAMETERS USING MARQUARDT'S
NON-LINEAR REGRESSION METHOD. PARAMETERS FOR 2-3 PAIR ARE LOCKED.
VAPOR PHASE : VIRIAL EOS (B BY HAYDEN β O'CONNELL)
SYSTEM: 1.(1)ETHANOL-(2)WATER(P=760 MMHG)µ 2.(1)ETHANOL-(3)BENZENE:
   (P=750 MMHG)µ 3.(1)ETHANOL-(2)WATER-(3)BENZENEµ LLEµ T=35 C.
DATA REF.: 1. REIDER R.M.,THOMPSON A.R.,IND.ENG.CHEM.41,2905(1949)
   2. TYRER D., J. CHEM. SOC. (LONDON) 101,1104 (1912).
   3. MORACHEVSKII,AG, ET AL, VESTN LENINGR UNIV KHIM 13,4(1958)117
INITIAL PARAMETERS: RESULTING PARA FROM CASE#41A
ALL THE 6 PARAMETERS FLOATING. ALL TIE LINES ARE USED.(LLEFN=11)

6, 99, 2, 1, 1, 0, 1, 0, 0, 9999.0, 2, 4*0.0,
-5.1189199E+1, -1.0E+4,  1.0E+4,
3.4280649E+2, -1.0E+4,  1.0E+4,
-1.419539E+2,-1.0E+4,  1.0E+4,
9.4838034E+2, -1.0E+4,  1.0E+4,
2.3832808E+2, -1.0E+4,  1.0E+4,
1.4583589E+3, -1.0E+4,  1.0E+4,
2*0.0, 3*-1.0, 2*0.0, 0,
2*1.0E-8, 2.5E-8,
0.0028,  0.9972,  1.E-4,
0.0118,  0.9882,  1.E-4,
0.0137,  0.9863,  1.E-4,
0.0144,  0.9856,  1.E-4,
0.0176,  0.9824,  1.E-4,
0.0222,  0.9778,  1.E-4,
0.0246,  0.9754,  1.E-4,
0.0302,  0.9698,  1.E-4,
0.0331,  0.9669,  1.E-4,
0.0519,  0.9481,  1.E-4,
0.0530,  0.9470,  1.E-4,
0.0625,  0.9375,  1.E-4,
0.0673,  0.9327,  1.E-4,
0.0715,  0.9285,  1.E-4,
0.0871,  0.9129,  1.E-4,
0.1260,  0.8740,  1.E-4,
0.1430,  0.8570,  1.E-4,
0.1720,  0.8280,  1.E-4,
0.2060,  0.7940,  1.E-4,
0.2100,  0.7900,  1.E-4,
0.2550,  0.7450,  1.E-4,
0.2840,  0.7160,  1.E-4,
0.3210,  0.6790,  1.E-4,
0.3240,  0.6760,  1.E-4,
0.3450,  0.6550,  1.E-4,
0.4050,  0.5950,  1.E-4,
0.4300,  0.5700,  1.E-4,
0.4490,  0.5510,  1.E-4,
0.5060,  0.4940,  1.E-4,
0.5450,  0.4550,  1.E-4,
0.6630,  0.3370,  1.E-4,
```

```
0.7350,  0.2650,  1.E-4,
0.8040,  0.1960,  1.E-4,
0.9170,  0.0830,  1.E-4,
0.1585,  0.0,  1.0E-4,
0.2977,  0.0,  1.0E-4,
0.4208,  0.0,  1.0E-4,
0.5367,  0.0,  1.0E-4,
0.6290,  0.0,  1.0E-4,
0.7178,  0.0,  1.0E-4,
0.7982,  0.0,  1.0E-4,
0.8715,  0.0,  1.0E-4,
0.9385,  0.0,  1.0E-4,
0.0140,  0.0040,  1.0E-4,
0.0800,  0.0210,  1.0E-4,
0.1450,  0.0390,  1.0E-4,
0.1450,  0.0390,  1.0E-4,
0.1970,  0.0570,  1.0E-4,
0.2550,  0.0960,  1.0E-4,
0.3200,  0.1720,  1.0E-4,
9999.0,  0.0, 0.0,
 3, 6, 1, 2, 0, 4*0,
11, 4, 0, 3, 0, 10, 21, 11, 0, 3, 2, 0.0, 0.0,
 1, 1, 2, 3, 34, 1, 2, 0,
 2, 1, 2, 3, 9,  1, 0, 3,
 3, 2, 1, 3, 7,  1, 2, 3,
ETOH
0, 46.1, 351.4, 516.2, 63.0, 167.0, 0.248, 58.39, 0.635,
0.0, 0.0, 2.1055, 1.9720, 0.92, 0.0878, 0.0572, 0.252,
2.25, 1.69, 1.40,
202.1, 351.1,
0.58, 3*0.0,
17.52, 3*0.0,
12.0466, -3667.705, -46.976, 3*0.0,
WATER
0, 18.0, 373.1, 647.6, 217.3, 56.0, 0.232, 18.05, 0.344,
0.0, 0.0, 0.92, 1.40, 1.00, 0.0279, 0.0229, 0.238,
0.615, 1.83, 1.70,
538.7, 373.2,
1.0, 3*0.0,
8.17, 3*0.0,
11.9516, -3984.923, -39.734, 3*0.0,
BENZENE
0, 78.1, 353.1, 562.1, 48.3, 259.0, 0.269, 88.26, 0.212,
0.0, 0.0, 3.1878, 2.40, 0.0, 0.0, 0.0, 0.2696,
3.004, 0.0, 0.0,
94.1, 353.3,
0.41, 3*0.0,
19.447, 3*0.0,
9.2082, -2755.644, -53.999, 3*0.0,
1.40, 1.55, 0.0,
1.55, 1.70, 0.0,
0.0,  0.0,  0.0,
10.0, 0.0, 10.0, 0.0, 10.0, 0.0, 10.0, 0.0,
10.0, 0.0, 10.0, 0.0
REG OF 6 PARAMETERS FOR THE PREDICTION OF VLE β LLE AT 35 C
```

```
760.0, 35.0, 65.0, 0.0,
99.30, 96.90, 96.00, 96.00, 95.60, 94.80, 93.80, 93.50, 92.90,
90.50, 90.50, 89.40, 88.40, 88.60, 87.20, 85.40, 84.50, 84.00,
83.40, 83.00, 82.30, 82.00, 81.40, 81.50, 81.20, 80.90, 80.50,
80.20, 80.00, 79.50, 78.80, 78.50, 78.40, 78.30,
69.54, 68.20, 67.76, 67.97, 68.41, 69.00, 70.26, 71.86, 74.40,
0.0320, 0.9680, 0.1130, 0.8870, 0.1570, 0.8430, 0.1350, 0.8650,
0.1560, 0.8440, 0.1860, 0.8140, 0.2120, 0.7880, 0.2310, 0.7690,
0.2480, 0.7520, 0.3180, 0.6820, 0.3140, 0.6860, 0.3390, 0.6610,
0.3700, 0.6300, 0.3620, 0.6380, 0.4060, 0.5940, 0.4680, 0.5320,
0.4870, 0.5130, 0.5050, 0.4950, 0.5300, 0.4700, 0.5270, 0.4730,
0.5520, 0.4480, 0.5670, 0.4330, 0.5860, 0.4140, 0.5860, 0.4140,
0.5910, 0.4090,
0.6140, 0.3860, 0.6260, 0.3740, 0.6330, 0.3670, 0.6610, 0.3390,
0.6730, 0.3270,
0.7330, 0.2670, 0.7760, 0.2240, 0.8150, 0.1850, 0.9060, 0.0940,
0.3531, 0.0, 0.4045, 0.0, 0.4358, 0.0, 0.4662, 0.0, 0.5053, 0.0,
0.5491, 0.0, 0.6063, 0.0, 0.6833, 0.0, 0.7874, 0.0,
0.0560, 0.9430, 0.1540, 0.8430, 0.2410, 0.7440, 0.2410, 0.7440,
0.2980, 0.6690, 0.3480, 0.5880, 0.3860, 0.4900
```

D.2 Objective Functions for Vapor-Liquid Equilibrium Data Regression

The objective functions for the regression of vapor-liquid equilibria are computed for the j th data point and n number of components. The subscript e and c in the following equations denote the experimental and calculated data, and the subscript i represents the component.

Function # 1: The difference of the infinite dilution activity coefficients,

$$Z_j = \frac{1}{n} \sum_{i=1}^{n} |\gamma_{ei}^{\infty} - \gamma_{ci}^{\infty}| \tag{D2.1}$$

Function # 2: The relative difference of the infinite dilution activity coefficients,

$$Z_j = \frac{1}{n} \sum_{i=1}^{n} \frac{|\gamma_{ei}^{\infty} - \gamma_{ci}^{\infty}|}{\gamma_{ei}^{\infty}} \tag{D2.2}$$

Function # 3: The relative difference of the logrithm of infinite dilution activity coefficients,

$$Z_j = \frac{1}{n} \sum_{i=1}^{n} |\mathrm{Ln}\ \gamma_{ei}^{\infty} - \mathrm{Ln}\ \gamma_{ci}^{\infty}| \tag{D2.3}$$

Function#4: The difference of activity coefficients,

$$Z_j = \frac{1}{n} \sum_{i=1}^{n} |\gamma_{ei} - \gamma_{ci}| \tag{D2.4}$$

Function # 5: The relative difference of activity coefficients,

$$Z_j = \frac{1}{n} \sum_{i=1}^{n} \frac{|\gamma_{ei} - \gamma_{ci}|}{\gamma_{ei}} \tag{D2.5}$$

Function # 6: The difference of the logrithm of activity coefficients,

$$z_j = \frac{1}{n} \sum_{i=1}^{n} |\mathrm{Ln}\ \gamma_{ei} - \mathrm{Ln}\ \gamma_{ci}| \qquad \text{(D2.6)}$$

Function # 7: The difference of y's,

$$z_j = \frac{1}{n} \sum_{i=1}^{n} |y_{ei} - y_{ci}| \qquad \text{(D2.7)}$$

Function # 8: The relative difference of y's,

$$z_j = \frac{1}{n} \sum_{i=1}^{n} \frac{|y_{ei} - y_{ci}|}{y_{ei}} \qquad \text{(D2.8)}$$

Function # 9: The difference of the logrithm of y's,

$$z_j = \frac{1}{n} \sum_{i=1}^{n} |\mathrm{Ln}\ y_{ei} - \mathrm{Ln}\ y_{ci}| \qquad \text{(D2.9)}$$

Function # 10: The difference of y's and the relative difference of total P's,

$$z_j = \frac{1}{n} \sum_{i=1}^{n} |y_{ei} - y_{ci}| + \frac{|P_e - P_c|}{P_e} \qquad \text{(D2.10)}$$

Function # 11: The relative difference of y's and the relative difference of total P's,

$$z_j = \frac{1}{n} \sum_{i=1}^{n} \frac{|y_{ei} - y_{ci}|}{y_{ei}} + \frac{|P_e - P_c|}{P_e} \qquad \text{(D2.11)}$$

Function # 12: The difference of the logrithm of y's and the difference of logrithm of total P's,

$$z_j = \frac{1}{n} \sum_{i=1}^{n} |\mathrm{Ln}\ y_{ei} - \mathrm{Ln}\ y_{ci}| + |\mathrm{Ln}\ P_e - \mathrm{Ln}\ P_c| \qquad \text{(D2.12)}$$

Function # 13: The difference of total P's,

$$z_j = | P_e - P_c | \qquad (D2.13)$$

Function#14: The ratio of total P's,

$$z_j = | P_e / P_c | \qquad (D2.14)$$

Function # 15: The relative difference of total P's,

$$z_j = \frac{| P_e - P_c |}{P_e} \qquad (D2.15)$$

Function # 16: The difference of the logrithm of total P's,

$$z_j = | \mathrm{Ln} (P_e / P_c) | \qquad (D2.16)$$

Function # 17: The difference of T's,

$$z_j = | T_e - T_c | \qquad (D2.17)$$

Function#18: The ratio of T's,

$$z_j = | T_e / T_c | \qquad (D2.18)$$

Function # 19: The relative difference of T's,

$$z_j = \frac{| T_e - T_c |}{T_e} \qquad (D2.19)$$

Function # 20: The difference of the logrithm of T's,

$$z_j = | \mathrm{Ln} (T_c / T_e) | \qquad (D2.20)$$

Function # 21: The difference of T's and the difference of y's,

$$z_j = | T_e - T_c | + \frac{1}{n} \sum_{i=1}^{n} | y_{ei} - y_{ci} | \qquad (D2.21)$$

Function # 22: The relative difference of T's and the difference of y's,

$$z_j = \frac{|T_e - T_c|}{T_e} + \frac{1}{n}\sum_{i=1}^{n} |y_{ei} - y_{ci}| \qquad \text{(D2.22)}$$

D.3 Objective Functions: Liquid-Liquid Equilibria Data Regression

The objective functions for liquid-liquid equilibria data regression are computed for the j th data point, n number of components, and two phases denoted by supercript I and II. The subscripts e and c denote the experimental and calculated values, and i denotes the component.

Function # 1: The difference in activities,

$$Z_j = \frac{1}{2n} \sum_{i=1}^{n} |a^{I}_{ci} - a^{II}_{ci}| \qquad \text{(D3.1)}$$

Function # 2: The difference in the logrithm of activities,

$$Z_j = \frac{1}{2n} \sum_{i=1}^{n} |\text{Ln } a^{I}_{ci} - \text{Ln } a^{II}_{ci}| \qquad \text{(D3.2)}$$

Function # 3: The relative difference in activities,

$$Z_j = \frac{1}{2n} \sum_{i=1}^{n} \frac{|a^{I}_{ci} - a^{II}_{ci}|}{a^{I}_{ci} + a^{II}_{ci}} \qquad \text{(D3.3)}$$

Function # 4: The difference in the logrithm of activities, with emphasis on solutes present in the system

$$Z_j = \frac{1}{2n} \sum_{i=1}^{n} |\text{Ln } a^{I}_{ci} - \text{Ln } a^{II}_{ci}| \; +$$

$$\frac{1}{2(n-2)} \sum_{\substack{i=1 \\ i \neq Ie,Ir}}^{n} |\text{Ln } a^{I}_{ci} - \text{Ln } a^{II}_{ci}| \; x^{I}_{ci} x^{II}_{ci} \qquad \text{(D3.4)}$$

where Ie and Ir denotes the rich component in extract and raffinate phases.

Function # 5: The weighted difference in compositions,

$$Z_j = \frac{1}{2n} \sum_{i=1}^{n} w_i^I \, |x_{ei}^I - x_{ci}^I| + w_i^{II} |x_{ei}^{II} - x_{ci}^{II}| \qquad \text{(D3.5)}$$

where the associated weights are computed using W as a constant in the following equations

$$w_i^I = \left|1.0 + W \frac{|x_{ei}^I - x_{ci}^I|}{x_{ei}^I}\right| \text{ and } w_i^{II} = \left|1.0 + W \frac{|x_{ei}^{II} - x_{ci}^{II}|}{x_{ei}^{II}}\right| \qquad \text{(D3.6,7)}$$

Function # 6: The weighted difference in the logarithm of compositions,

$$Z_j = \frac{1}{2n} \sum_{i=1}^{n} w_i^I \, |\text{Ln } x_{ei}^I - \text{Ln } x_{ci}^I| + w_i^{II} |\text{Ln } x_{ei}^{II} - \text{Ln } x_{ci}^{II}| \qquad \text{(D3.8)}$$

Function # 7: The weighted relative difference in compositions,

$$Z_j = \frac{1}{2n} \sum_{i=1}^{n} w_i^I \frac{|x_{ei}^I - x_{ci}^I|}{x_{ei}^I} + w_i^{II} \frac{|x_{ei}^{II} - x_{ci}^{II}|}{x_{ei}^{II}} \qquad \text{(D3.9)}$$

Function # 8: The weighted relative difference in compositions,

$$Z_j = \frac{1}{2n} \sum_{i=1}^{n} w_i^I \frac{|x_{ei}^I - x_{ci}^I|}{x_{ei}^I + x_{ci}^I} + w_i^{II} \frac{|x_{ei}^{II} - x_{ci}^{II}|}{x_{ei}^{II} + x_{ci}^{II}} \qquad \text{(D3.10)}$$

Function # 9: The relative difference in compositions and in the distribution ratios of the solutes,

$$Z_j = \frac{1}{2n} \sum_{i=1}^{n} w_i^I \frac{|x_{ei}^I - x_{ci}^I|}{x_{ei}^I} + w_i^{II} \frac{|x_{ei}^{II} - x_{ci}^{II}|}{x_{ei}^{II}} +$$

$$\sum_{\substack{i=1 \\ i \neq e,Ir}}^{n} \frac{|K_{ei} - K_{ci}|}{K_{ei}} \qquad \text{(D3.11)}$$

Function # 10: The weighted difference inthe logrithm of compositions and in the logrithm of distribution ratios of solutes,

$$Z_j = \frac{1}{2n} \sum_{i=1}^{n} w_i^I \,|\text{Ln } x_{ei}^I - \text{Ln } x_{ci}^I| + w_i^{II} |\text{Ln } x_{ei}^{II} - \text{Ln } x_{ci}^{II}| +$$

$$\frac{1}{2(n-2)} \sum_{\substack{i=1 \\ i \neq e,Ir}}^{n} |\text{Ln } K_{ei} - \text{Ln } K_{ci}| \qquad \text{(D3.12)}$$

Function # 11: The weighted relative difference in the compositions and the relative difference in the distribution ratios of solutes,

$$Z_j = \frac{1}{2n} \sum_{i=1}^{n} w_i^I \frac{|x_{ei}^I - x_{ci}^I|}{x_{ei}^I + x_{ci}^I} + w_i^{II} \frac{|x_{ei}^{II} - x_{ci}^{II}|}{x_{ei}^{II} + x_{ci}^{II}} +$$

$$\frac{1}{2(n-2)} \sum_{\substack{i=1 \\ i \neq e,Ir}}^{n} \frac{|K_{ei} - K_{ci}|}{K_{ei} + K_{ci}} \qquad \text{(D3.13)}$$

Function # 12: The weighted relative difference in the compositions, the relative difference in the distribution ratios of solutes at the infinite dilution, and the interaction parameters,

$$Z_j = \frac{1}{2n} \sum_{i=1}^{n} w_i^{I} \frac{|x_{ei}^{I} - x_{ci}^{I}|}{x_{ei}^{I} + x_{ci}^{I}} + w_i^{II} \frac{|x_{ei}^{II} - x_{ci}^{II}|}{x_{ei}^{II} + x_{ci}^{II}} +$$

$$\frac{1}{2(n-2)} \sum_{\substack{i=1 \\ i \neq Ie, Ir}}^{n} |\mathrm{Ln}\ K_{ei}^{\infty} - \mathrm{Ln}\ K_{ci}^{\infty}| + W_1 \sum_{j=1}^{p} C_j \qquad (D3.14)$$

where W_1 is the another constant weight with p number of interaction parameters.

APPENDIX E

MODIFIED UNIQUAC INTERACTION PARAMETER ESTIMATION RESULTS

E.1 Results of Binary VLE Data Regression

E.1.1 Regression Results of Isobaric Ethanol-Water (VLE) System

E.1.2 Regression Results of Isothermal Ethanol-Water (VLE) System

E.1.3 Regression Results of Isobaric Ethanol-Benzene (VLE) System

E.1.4 Regression Results of Isothermal Ethanol-Benzene (VLE) System

E.2 Results of Binary LLE Data Regression

E.2.1 Regression Results of Benzene-Water (LLE) System at 25 C

E.2.2 Regression Results of Benzene-Water (LLE) System at 25 C

E.2.3 Regression Results of Benzene-Water (LLE) System at 35 C

E.2.4 Regression Results of Benzene-Water (LLE) System at 70 C

E.3 Results of VLE Data Regression

E.3.1 Regression Results of Isobaric Ethanol-Water-Benzene (VLE) System

E.3.2 Regression Results of Combinations of Isobaric Binary and Ternary VLE Systems

E.4 Regressio Results of Ethanol-Water-Benzene (LLE) System

E.5 Results of Simultaneous VLE and LLE Data Regression

E.5.1 Regression Results of Isobaric Binary VLE and Isothermal Ternary LLE Systems

E.5.2 Regression Results of Isothermal Binary VLE and Isothermal Ternary LLE Systems

E.5.3 Regression Results of Isothermal Binary VLE and Isothermal Ternary LLE Systems

E.5.4 Regression Results of Isobaric VLE and LLE, Binary and Ternary Systems

E.1 Results of Binary VLE Data Regression

Table E.1.1: Regression Results of Isobaric Ethanol-Water (VLE) System

System: (1) Ethanol - (2) Water
Gamma Model: Modified UNIQUAC
Phi Model: Virial EOS

Condition: Isobaric, P = 760 mm Hg
Data reference: Reider, R.M.,et.al (1949)
No. of data points = 34

Case No.	VLEFN #	Binary Interaction Parameters, ^oK Intial		Final		$T_{exp}-T_{cal}$ in deg C		$Y_{1exp}-Y_{1cal}$ in mole %		Inf. Dilution Activity Coeff	
		A_{12}	A_{21}	A_{12}	A_{21}	Mean	Max	Mean	Max	(1)	(2)
04A	7	1	1	-89.02	376.71	0.38	0.93	0.534	2.726	5.128	2.329
04B	8	1	1	-70.63	356.65	0.25	0.81	0.623	2.630	5.169	2.405
04C	9	1	1	-67.06	353.68	0.22	0.77	0.655	2.591	5.188	2.422
04D	17	1	1	-67.41	371.92	0.15	0.45	0.897	2.509	5.436	2.465
04E	19	1	1	-68.98	375.07	0.15	0.43	0.902	2.547	5.454	2.462
04F	20	1	1	-68.88	374.90	0.15	0.43	0.903	2.545	5.453	2.462
04G	21	1	1	-50.48	342.07	0.13	0.56	0.883	2.362	5.299	2.508
04H	21	500	500	-54.12	347.85	0.13	0.55	0.879	2.323	6.580	2.490
04I	21	-500	500	-55.88	349.86	0.13	0.55	0.865	2.326	5.319	2.490
04J	21	500	-500	-55.43	349.03	0.13	0.56	0.864	2.334	5.315	2.491

(Cont'd.) Table E.1.1: Regression Results of Isobaric Ethanol-Water (VLE) System

System: (1) Ethanol - (2) Water
Gamma Model: Modified UNIQUAC
Phi Model: Virial EOS

Condition: Isobaric, P = 760 mm Hg
Data reference: Reider, R.M.,et.al (1949)
No. of data points = 34

Case No.	VLEFN #	Binary Interaction Parameters, ^oK Intial A_{12}	Intial A_{21}	Final A_{12}	Final A_{21}	$T_{exp}-T_{cal}$ in deg C Mean	Max	$Y_{1exp}-Y_{1cal}$ in mole % Mean	Max	Inf. Dilution Activity Coeff (1)	(2)
04K	21	-500	-500	-50.82	342.21	0.13	0.57	0.877	2.369	5.295	2.506
04L	21	3000	3000	-361.09	9963.07	3.00	7.10	6.987	21.919	-	1.515
04M	21	-3000	3000	-361.09	9100.83	3.00	7.10	6.987	21.919	-	1.515
04N	21	3000	-3000	8070.10	-206.88	1.48	2.89	3.648	7.192	3.625	-
04O	21	-3000	-3000	-57.02	351.70	0.14	0.55	0.864	2.314	5.326	2.487

Note: '-' shows very high calculated values

Table E.1.2: Regression Results of Isothermal Ethanol-Water (VLE) System

System: (1) Ethanol - (2) Water
Gamma Model: Modified UNIQUAC
Phi Model: Virial EOS

Condition: Isothermal, T = 40 C
Data reference: Mertl, I., et. al. (1972)
No. of data points = 13

Case No.	VLEFN #	Binary Interaction Parameters, °K Intial		Final		$P_{exp}-P_{cal}$ in mm Hg		$Y_{1exp}-Y_{1cal}$ in mole %		Inf. Dilution Activity Coeff	
		A_{12}	A_{21}	A_{12}	A_{21}	Mean	Max	Mean	Max	(1)	(2)
08A*	7	1	1	-41.48	299.42	1.89	8.60	0.529	1.331	5.276	2.520
08B*	8	1	1	-19.36	272.65	1.67	8.69	0.561	1.244	5.239	2.613
08C	9	1	1	-19.16	272.71	1.66	8.72	0.564	1.239	5.243	2.615
08D*	10	1	1	-18.16	219.39	1.85	7.93	0.577	1.561	5.004	2.726
08E	11	1	1	-7.53	253.78	1.74	8.35	0.541	1.289	5.140	2.644
08F*	12	1	1	5.31	238.81	1.72	8.32	0.560	1.433	5.108	2.695
08G*	13	1	1	4.66	238.40	1.74	8.24	0.559	1.412	5.092	2.688
08H*	15	1	1	42.47	185.52	2.09	7.25	0.673	1.805	4.833	2.783
08I	11	1000	1000	8088.41	-237.12	9.32	14.88	5.109	8.243	3.118	-
08J*	10	100	100	12.85	227.37	1.79	8.09	0.570	1.511	5.047	2.713

(Cont'd.) Table E.1.2: Regression Results of Isothermal Ethanol-Water (VLE) System

System: (1) Ethanol - (2) Water
Gamma Model: Modified UNIQUAC
Phi Model: Virial EOS

Condition: Isothermal, T = 40 C
Data reference: Mertl, I., et. al. (1972)
No. of data points = 13

Case No.	VLEFN #	Binary Interaction Parameters, ^{o}K Intial		Final		$P_{exp}-P_{cal}$ in mm Hg		$Y_{1exp}-Y_{1cal}$ in mole %		Inf. Dilution Activity Coeff	
		A_{12}	A_{21}	A_{12}	A_{21}	Mean	Max	Mean	Max	(1)	(2)
08K*	10	-100	100	8.62	233.13	1.76	8.18	0.565	1.461	5.072	2.701
08L*	10	300	300	14.30	225.17	1.81	8.05	0.572	1.524	5.035	2.717
08M*	10	-300	300	8.47	233.41	1.76	8.19	0.564	1.460	5.074	2.700
08N*	9	100	100	-19.12	272.65	1.66	8.72	0.563	1.239	5.243	2.615
08O*	9	-100	100	-19.16	272.72	1.66	8.72	0.564	1.239	5.243	2.615
08P	9	300	300	-19.11	272.65	1.66	8.72	0.563	1.239	5.243	2.615
08Q*	9	-300	300	-19.15	272.70	1.66	8.72	0.564	1.239	5.243	2.615

Note: '-' shows very high calculated values

'*' unconverged cases, values shown were obtained after 99 iterations

Table E.1.3: Regression Results of Isobaric Ethanol-Benzene (VLE) System

System: (1) Ethanol - (2) Benzene
Gamma Model: Modified UNIQUAC
Phi Model: Virial EOS

Condition: Isobaric, P = 750 mm Hg
Data reference: Tyrer D., (1912)
No. of data points = 9

Case No.	VLEFN #	Binary Interaction Parameters, ^{o}K Intial		Final		$T_{exp}-T_{cal}$ in deg C		$Y_{1exp}-Y_{1cal}$ in mole %		Inf. Dilution Activity Coeff	
		A_{12}	A_{21}	A_{12}	A_{21}	Mean	Max	Mean	Max	(1)	(2)
06A	7	1	1	-140.09	955.92	0.33	0.68	0.624	1.869	9.198	4.562
06B	8	1	1	-134.80	942.14	0.44	0.75	0.749	1.490	9.061	4.562
06C	9	1	1	-134.09	940.57	0.46	0.76	0.769	1.438	9.049	4.581
06D	17	1	1	-143.83	915.94	0.11	0.26	0.668	2.491	8.143	4.235
06E	19	1	1	-142.95	910.15	0.12	0.26	0.685	2.458	8.048	4.249
06F	20	1	1	-142.95	910.27	0.12	0.26	0.685	2.457	8.050	4.249
06G	21	1	1	-149.02	953.70	0.10	0.36	0.579	2.672	8.809	4.159
06H	19	3000	3000	-142.93	910.25	0.12	0.26	0.685	2.456	8.050	4.249
06I	19	-3000	3000	-197.77	6917.27	0.48	1.41	2.723	4.487	-	3.474
06J	19	3000	-3000	7791.73	-134.82	2.88	6.33	11.622	17.826	2.014	-

(Cont'd.) Table E.1.3: Regression Results of Isobaric Ethanol-Benzene (VLE) System

System: (1) Ethanol - (2) Benzene
Gamma Model: Modified UNIQUAC
Phi Model: Virial EOS

Condition: Isobaric, P = 750 mm Hg
Data reference: Tyrer D., (1912)
No. of data points = 9

Case No.	VLEFN #	Binary Interaction Parameters, ^{o}K Intial		Final		$T_{exp}-T_{cal}$ in deg C		$Y_{1exp}-Y_{1cal}$ in mole %		Inf. Dilution Activity Coeff	
		A_{12}	A_{21}	A_{12}	A_{21}	Mean	Max	Mean	Max	(1)	(2)
06K	21	500	500	-146.15	931.48	0.11	0.28	0.621	2.578	8.405	4.199
06L	21	500	-500	-151.24	967.80	0.11	0.39	0.563	2.771	9.060	4.121
06M	21	-500	-500	-147.79	943.97	0.10	0.32	0.597	2.632	8.629	4.176
06N	21	1000	1000	-151.47	961.51	0.11	0.39	0.507	2.594	8.636	4.132
06O	21	-1000	1000	-197.31	7151.03	0.48	1.43	2.708	4.450	-	3.478
06P	21	1000	-1000	8027.14	-133.09	2.87	6.42	11.634	17.795	2.026	-
06Q	21	-1000	-1000	-148.36	947.94	0.10	0.34	0.591	2.654	8.700	4.168

Note: '-' shows very high calculated values

Table E.1.4: Regression Results of Isothermal Ethanol-Benzene (VLE) System

System: (1) Ethanol - (2) Benzene
Gamma Model: Modified UNIQUAC
Phi Model: Virial EOS

Condition: Isothermal, T = 40 C
Data reference: Udovenko, V.V.,et. al. (1952)
No. of data points = 11

Case No.	VLEFN #	Binary Interaction Parameters, ^{o}K Intial A_{12}	Intial A_{21}	Final A_{12}	Final A_{21}	$P_{exp}-P_{cal}$ in mm Hg Mean	$P_{exp}-P_{cal}$ in mm Hg Max	$Y_{1exp}-Y_{1cal}$ in mole % Mean	$Y_{1exp}-Y_{1cal}$ in mole % Max	Inf. Dilution Activity Coeff (1)	Inf. Dilution Activity Coeff (2)
09A	7	1	1	-119.31	1026.46	1.55	3.25	0.358	0.819	15.371	4.973
09B	8	1	1	-115.27	1017.19	2.34	4.70	0.394	1.065	15.218	5.115
09C	9	1	1	-114.68	1015.79	2.46	4.90	0.406	1.128	15.194	5.136
09D	10	1	1	-121.87	1017.74	0.88	2.02	0.404	2.020	14.817	4.863
09E*	11	1	1	-119.68	1019.94	1.28	2.94	0.371	0.854	15.031	4.948
09F	12	1	1	-119.07	1017.84	1.37	3.15	0.376	0.825	15.002	4.969
09G	13	1	1	-124.01	1027.14	0.84	1.88	0.436	1.066	15.092	4.798
09H	15	1	1	-124.12	1025.88	0.83	1.89	0.442	1.075	15.028	4.792
09I	16	1	1	-124.07	1025.62	0.83	1.89	0.441	1.073	15.020	4.793

Note: '*' shows unconverged case after 99 iterations

E.2 Results of Binary LLE Data Regression

Table E.2.1: Regression Results of Benzene-Water (LLE) System at 25 C

System: (1) Benzene - (2) Water
Gamma Model: Modified UNIQUAC

Condition: Isothermal, T = 25 C
Data reference: Polak, J. (1973)
No. of data points = 1

Case No.	LLEFN #	Binary Interaction Parameters, ^oK Intial		Final		Phase Rich in (1) Mean % Rel. x Diff.		Phase Rich in (2) Mean % Rel. x Diff.*	
		A_{12}	A_{21}	A_{12}	A_{21}	(1)	(2)	(1)	(2)
22A	5	1	1	1.00	1.00	3.4890E+1	0.1500E+5	0.6800E+5	0.2833E+2
22B	6	1	1	1412.98	352.59	0.4780E-3	0.2098E+0	0.2448E+0	0.1010E-3
22C	8	1	1	400.43	420.88	6.1820E+0	0.2729E+4	0.1880E-1	0.5960E-5
22D	10	1	1	1417.58	350.84	0.2500E-2	1.1060E+0	1.1610E+0	0.4830E-3
22E	11	1	1	1407.65	354.46	0.4030E-2	1.7800E+0	1.7200E+0	0.7160E-3
22F	5	500	500	1301.05	6917.60	0.3112E-2	1.3740E+0	1.0000E+2	0.4160E-1
22G	6	500	500	1410.01	353.60	0.2372E-2	1.0470E+0	1.0490E+0	0.4353E-3
22H	7	500	500	1302.20	7755.97	0.2230E-2	0.9839E+0	1.0000E+2	0.4160E-1
22I	8	500	500	1407.05	353.87	0.4670E-2	2.0620E+0	1.2460E+0	0.5190E-3
22J	10	500	500	1417.69	350.77	0.2560E-2	1.1310E+0	1.2170E+0	0.5070E-3
22K	11	500	500	306.67	457.69	8.3200E+0	3.6740E+3	8.1210E+0	0.3381E-2

(Cont'd.) Table E.2.1: Regression Results of Benzene-Water (LLE) System at 25 C

System: (1) Benzene - (2) Water
Gamma Model: Modified UNIQUAC

Condition: Isothermal, T = 25 C
Data reference: Polak, J. (1973)
No. of data points = 1

Case No.	LLEFN #	Binary Interaction Parameters, ^oK Intial		Final		Phase Rich in (1) Mean % Rel. x Diff.		Phase Rich in (2) Mean % Rel. x Diff.*	
		A_{12}	A_{21}	A_{12}	A_{21}	(1)	(2)	(1)	(2)
22L	6	-500	-500	5951.19	-175.90	4.0810E+0	1.8020E+3	0.1632E+5	6.7870E+0
22M	9	-500	-500	4503.43	-446.75	4.9980E+1	0.2207E+5	1.0000E+2	1.0000E+2
22N	10	-500	-500	5775.94	-295.68	4.9980E+1	0.2207E+5	1.0000E+2	1.0000E+2
22O	11	-500	-500	6130.14	-522.00	4.4630E+1	0.1970E+5	0.9210E+5	3.8310E+1
22P	5	1000	1000	1300.62	8164.75	0.3400E-2	1.5210E+0	1.0000E+2	0.4160E-1
22Q	6	1000	1000	1416.14	351.35	0.1560E-2	0.6920E+0	0.7474E+0	0.3100E-3
22R	7	1000	1000	1305.08	5182.22	0.2400E-4	0.1020E-1	1.0000E+2	0.4160E-1
22S	8	1000	1000	1416.87	350.41	0.1800E-2	0.8170E+0	1.5190E+0	0.6320E-3
22T	10	1000	1000	1416.17	351.37	0.1595E-2	0.7025E+0	0.7315E+0	0.3000E-3
22U	11	1000	1000	1414.66	347.81	0.5735E-3	0.2543E+0	3.7090E+0	0.1544E-2
22V	5	2000	2000	1441.03	348.80	0.1890E-1	8.3530E+0	2.7090E+0	0.1120E-2

(Cont'd.) Table E.2.1: Regression Results of Benzene-Water (LLE) System at 25 C

System: (1) Benzene - (2) Water
Gamma Model: Modified UNIQUAC

Condition: Isothermal, T = 25 C
Data reference: Polak, J. (1973)
No. of data points = 1

Case No.	LLEFN #	Binary Interaction Parameters, ^{o}K Intial		Final		Phase Rich in (1) Mean % Rel. x Diff.		Phase Rich in (2) Mean % Rel. x Diff.*	
		A_{12}	A_{21}	A_{12}	A_{21}	(1)	(2)	(1)	(2)
22W	6	2000	2000	-284.78	1275.24	4.8310E+1	0.2133E+5	2.7200E+0	0.1133E-2
22X	7	2000	2000	1424.75	351.14	0.7916E-2	3.4940E+0	0.8636E+0	0.3578E-3
22Y	8	2000	2000	1413.50	352.45	0.1255E-3	0.5621E-1	0.1337E+0	0.5963E-4
22Z	11	2000	2000	1408.06	353.72	0.3920E-2	1.7350E+0	1.1290E+0	0.4711E-3
22AA	5	3000	3000	1436.31	358.12	0.1806E-1	7.9710E+0	4.7780E+0	0.1990E-2
22BB	6	3000	3000	1413.35	352.46	0.2390E-3	0.1053E+0	0.1422E+0	0.5960E-4
22CC	7	3000	3000	1413.93	351.73	0.0000E+0	0.1750E-3	0.4472E+0	0.1850E-3
22DD	6	1500	500	1415.42	351.61	0.1093E-2	0.4829E+0	0.5397E+0	0.2266E-3
22EE	8	1500	500	1409.36	353.95	0.2856E-2	1.2620E+0	1.3230E+0	0.5546E-3

* $(x_{iexp}-x_{ical})/x_{iexp}*100$

Table E.2.2: Regression Results of Benzene-Water (LLE) System at 25 C

System: (1) Benzene - (2) Water
Gamma Model: Modified UNIQUAC

Condition: Isothermal, T = 25 C
Data reference: Sorenson, et. al. (1979)
No. of data points = 1

Case No.	LLEFN #	Binary Interaction Parameters, ^oK Intial		Final		Phase Rich in (1) Mean % Rel. x Diff.		Phase Rich in (2) Mean % Rel. x Diff.*	
		A_{12}	A_{21}	A_{12}	A_{21}	(1)	(2)	(1)	(2)
23A	8	1	1	392.17	424.59	6.2720E+0	2.0840E+3	1.2680E+0	0.5130E-3
23B	8	100	100	1332.69	354.44	0.4215E-2	1.4000E+0	1.4830E+0	0.6023E-3
23C	8	200	200	1335.51	354.21	0.6920E-2	2.3000E+0	1.6500E+0	0.6620e-3
23D	8	200	-200	1216.70	5192.00	0.4053e-2	1.3470E+0	1.0000E+2	0.4052E-1
23E	8	-200	-200	-145.93	-286.40	4.9330E+1	0.1640E+5	0.1215E+6	4.9220E+1
23F	8	300	300	1325.14	355.17	0.3120E-2	1.0380E+0	0.9519E+0	0.3816E-3
23G	8	500	500	221.37	482.87	1.0960E+1	3.6420E+3	0.3900E-2	0.0000E+0
23H	8	-500	500	-287.84	1150.50	4.9980E+1	0.1160E+5	1.3400E+0	0.5420E-3
23I	8	500	200	1327.85	356.37	0.7770E-4	0.2530E-4	0.5461E-1	0.2385E-4
23J	8	1000	1000	1326.61	356.80	0.1022E-2	0.3393E+0	0.4006E+0	0.1610E-3
23K	8	1000	200	1326.94	356.69	0.7234E-3	0.2398E+0	0.3124E+0	0.1312E-3
23L	8	3000	3000	1217.13	9032.94	0.3610E-2	1.1980E+0	1.0000E+2	0.4050E-1

* $(x_{iexp}-x_{ical})/x_{iexp}*100$

Table E.2.3: Regression Results of Benzene-Water (LLE) System at 35 C

System: (1) Benzene - (2) Water
Gamma Model: Modified UNIQUAC

Condition: Isothermal, T = 35 C
Data reference: Sorensen, et. al. (1979)
No. of data points = 1

Case No.	LLEFN #	Binary Interaction Parameters, ^{o}K Intial		Final		Phase Rich in (1) Mean % Rel. x Diff.		Phase Rich in (2) Mean % Rel. x Diff.*	
		A_{12}	A_{21}	A_{12}	A_{21}	(1)	(2)	(1)	(2)
25A	8	1	1	0.99	0.99	1.6840E+1	1.1172E+3	1.1670E+5	4.9280E+1
25B	8	100	100	904.77	373.41	0.5348E-1	3.7210E+0	0.9800E+0	0.4114E-3
25C	8	200	200	897.73	373.18	0.2097E-1	1.4590E+0	1.4340E+0	0.6023E-3
25D	8	300	300	892.72	375.24	0.1112E-2	0.7727E-1	0.1579E-2	0.0000E+0
25E	8	400	400	892.57	374.99	0.6046E-5	0.6572E-5	0.2021E+0	0.8348E-4
25F	8	500	500	1165.01	365.16	0.8382E+0	5.8320E+1	0.7952E+0	0.3339E-3
25G	8	1000	1000	890.94	374.51	0.8501E-2	0.5916E+0	0.6518E+0	0.2743E-3
25H	8	2000	2000	894.29	374.53	0.7249E-2	0.5044E+0	0.5023E+0	0.2087E-3

* $(x_{iexp}-x_{ical})/x_{iexp}*100$

Table E.2.4: Regression Results of Benzene-Water (LLE) System at 70 C

System: (1) Benzene - (2) Water
Gamma Model: Modified UNIQUAC

Condition: Isothermal, T = 70 C
Data reference: Sorensen, et. al. (1979)
No. of data points = 1

Case No.	LLEFN #	Binary Interaction Parameters, °K Intial		Final		Phase Rich in (1) Mean % Rel. x Diff.		Phase Rich in (2) Mean % Rel. x Diff.*	
		A_{12}	A_{21}	A_{12}	A_{21}	(1)	(2)	(1)	(2)
24A	8	1	1	1072.25	359.35	0.1566E-1	1.3000E+0	1.3650E+0	0.8410E-3
24B	8	100	100	1074.55	360.63	0.5550E-2	0.4607E+0	0.3802E+0	0.2326E-3
24C	8	200	200	1076.58	360.33	0.1140E-2	0.9480E-1	0.5373E+0	0.3280E-3
24D	8	300	300	1072.31	362.37	0.1084E-1	0.9001E+0	0.7914E+0	0.4891E-3
24E	8	400	400	1073.22	362.25	0.7806E-2	0.6484E+0	0.7283E+0	0.4533E-3
24F	8	500	500	1078.14	360.12	0.6316E-2	0.5242E+0	0.6443E+0	0.3936E-3
24G	8	1000	1000	1073.41	362.17	0.7239E-2	0.6011E+0	0.6796E+0	0.4175E-3
24H	8	2000	2000	1868.37	-162.42	0.1780E-1	1.4780E+0	5.9800E+3	3.6800E+0

* $(x_{iexp}-x_{ical})/x_{iexp}*100$

Table E.3.1: Regression Results of Ethanol-Water-Benzene (VLE) System

System: (1) Etoh - (2) Water (3) Bz
Gamma Model: Modified UNIQUAC
Phi Model: Virial EOS

Condition: Isobaric, P = 760 mmHg
Data Reference: Hands, C.H.G., et. al. (1945)
Data set: Ethanol-Water-Benzene (VLE, 760 mmHg)

Case #	VLEFN #	Final Binary Interaction Parameters in deg K						Mean & (Max) T and y's		
		A_{12}	A_{21}	A_{13}	A_{31}	A_{23}	A_{32}	dev$ in T deg C	dev$ in mole% y1	y2
03A*	21	-180.69	7787.48	-156.49	8696.35	701.73	-16.91	0.28 (0.91)	2.101 (7.140)	3.324 (6.054)
03B#	21	-177.19	8470.27	-158.48	8365.53	632.96	4.80	0.29 (0.83)	1.953 (6.790)	3.296 (6.001)
03C+	21	-131.51	1134.12	-179.08	7385.74	311.18	220.55	0.33 (0.83)	1.242 (3.601)	2.597 (5.234)
03X+	21	-57.02	351.70	-151.47	961.51	375.24	892.72	4.65 (11.58)	7.007 (14.127)	5.370 (5.234)

Initial Binary Interaction Parameters in deg K

*	1.0	1.0	1.0	1.0	1.0	1.0
#	-57.02	351.70	-151.47	961.51	1.0	1.0
+	-57.02	351.70	-151.47	961.51	375.24	892.72

$ dev in T = $(T_{exp}-T_{cal})$ and dev in y_i = $(y_{iexp}-y_{ical})$*100

Table E.3.2A: Regression Results of Combinations of Isobaric Binary and Ternary VLE System

System: (1) Etoh - (2) Water - (3) Bz
Gamma Model: Modified UNIQUAC
Phi Model: Virial EOS

Condition: Isobaric, P = 760 mm Hg
Data Sets and References:

(a)	Etoh-Water,	Reider, R.M., et. al. (1949)
(b)	Etoh-Bz,	Tyrer, D., (1912)
(c)	Etoh-Wtr-Bz,	Hands, C.H.G., et. al. (1945)

Case #	VLEFN #	Final Binary Interaction Parameters in deg K						Data Sets used in the Regression
		A_{12}	A_{21}	A_{13}	A_{31}	A_{23}	A_{32}	
70A	21	-42.16	330.98	-160.45	1219.45	481.52	153.10	a + b + c
71A	21	-123.81	1132.14	-189.03	7798.44	283.95	264.94	b + c
72A	21	-127.85	969.31	-147.10	1010.11	380.62	159.99	b(x4) + c
73A	21	-48.89	342.70	-147.13	1008.58	464.06	156.05	a + b(x4) + c
74A	21	-56.14	350.85	-146.65	982.05	243.88	745.91	a + b + c (partial)

Table E.3.2B: Regression Results of Combinations of Isobaric Binary and Ternary VLE System

System: (1) Etoh - (2) Water - (3) Bz
Gamma Model: Modified UNIQUAC
Phi Model: Virial EOS

Condition: Isobaric, P = 760 mm Hg
Data Sets and References:
(a) Etoh-Water, Reider, R.M., et. al. (1949)
(b) Etoh-Bz, Tyrer, D., (1912)
(c) Etoh-Wtr-Bz, Hands, C.H.G., et. al. (1945)

Case #	VLEFN #	Mean & (Max) Abs (Te-Tc) deg C			Mean & (Max) Absolute diff in mole %				Data Sets used in the Regression
					y_1			y_2	
		System			System			System	
		(a)	(b)	(c)	(a)	(b)	(c)	(c)	
70A	21	0.14 (0.56)	0.45 (1.45)	0.55 (1.51)	0.920 (2.398)	1.391 (2.067)	1.620 (5.150)	1.881 (4.854)	a + b + c
71A	21	-	0.48 (1.47)	0.33 (0.83)	-	2.316 (3.679)	1.218 (3.944)	2.596 (5.307)	b + c
72A	21	-	0.12 (0.59)	0.49 (1.16)	-	0.594 (1.812)	1.818 (4.464)	2.300 (4.880)	b(x4) + c
73A	21	0.14 (0.51)	0.12 (0.58)	0.62 (1.53)	0.931 (2.362)	0.586 (1.823)	1.819 (5.163)	1.820 (4.490)	a + b(x4) + c
74A	21	0.14 (0.54)	0.12 (0.41)	0.14 (0.38)	0.874 (2.308)	0.572 (1.945)	0.274 (0.524)	0.610 (1.160)	a + b + c(partial)

Table E.4: Regression Results of Ethanol-Water-Benzene (LLE) System

System: (1) Etoh - (2) Water - (3) Bz
Gamma Model: Modified UNIQUAC

Condition: Isothermal, T = 35 C
Data Reference: Moracheskii, A.G., et. al. (1958)
Data sets: Ethanol-Water-Benzene (LLE, 35 C)

Case #	No. of Tie Lines	LLEFN #	W	Final Binary Interaction Parameters in deg K					
				A_{12}	A_{21}	A_{13}	A_{31}	A_{23}	A_{32}
21B	All	11	0	-348.16	-626.36	-287.33	26.31	466.73	8667.88
21C	All	11	0	-39.12	343.62	-148.67	1302.72	381.49	790.14
21X	All	11	0	-19.16	272.65	-121.87	1017.74	375.24	892.72
				Initial Binary Interaction Parameters in deg K					
21A*	All	11	0	1.0	1.0	1.0	1.0	1.0	1.0
21B	All	11	0	1.0	1.0	1.0	1.0	375.24	892.72
21C	All	11	0	-19.16	272.65	-121.87	1017.74	375.24	892.72

* unconverged case

(Cont'd.) Table E.4: Regression Results of Ethanol-Water-Benzene (LLE) System

System: (1) Etoh - (2) Water - (3) Bz
Gamma Model: Modified UNIQUAC

Condition: Isothermal, T = 35 C
Data Reference: Moracheskii, A.G., et. al. (1958)
Data sets: Ethanol-Water-Benzene (LLE, 35 C)

Case #	No. of Tie Lines	LLEFN #	W	Diff. of compositions in mole %, Mean & (Max)							Mean diff of d. ratio (1)
				Phase Rich in (3)			Phase Rich in (2)			overall	
				(1)	(2)	(3)	(1)	(2)	(3)		
21B	All	11	0	0.6929	0.6338	0.5186	0.7065	0.9825	0.4487	0.6638	0.0502
				(1.102)	(1.484)	(1.081)	(1.011)	(1.777)	(1.947)	(1.947)	(0.0939)
21C	All	11	0	1.7550	3.6050	4.7180	1.0470	2.2950	1.2480	2.4447	0.0904
				(3.225)	(15.530)	(18.760)	(2.784)	(7.314)	(4.530)	(18.760)	(0.1613)
21X	All	11	0								

$ Difference = $(x_{iexp}-x_{ical})/x_{iexp}*100$

Table E.5.1A: Regression Results of Isobaric Binary VLE and Isothermal Ternary LLE System

System: (1) Etoh - (2) Water - (3) Bz
Gamma Model: Modified UNIQUAC
Phi Model: Virial EOS

Condition: Isobaric for VLE, P = 760 mm Hg
Isothermal for LLE, T = 35 C
Data Sets and References:
(a) Etoh-Water, Reider, R.M., et. al. (1949)
(b) Etoh-Bz, Tyrer, D., (1912)
(c) Etoh-Wtr-Bz, Morachevskii, A.G., et.al.(1958)

Case #	No. of Tie Lines	LLEFN #	W	Final Binary Interaction Parameters in deg K					
				A_{12}	A_{21}	A_{13}	A_{31}	A_{23}	A_{32}
40A	1	8	10	-50.30	341.47	-143.79	962.94	219.52	1248.05
40B	1	8	50	-46.98	336.04	-133.65	890.55	187.00	1249.35
41A	All	8	0	-51.19	342.81	-141.95	948.38	238.32	1458.36
41B	All	8	150	-159.10	501.06	-179.65	1204.55	279.61	1934.31
41C	All	8	200	-164.77	502.68	-146.15	947.65	282.79	1722.61
41D	All	8	250	-212.13	616.88	-184.15	1147.76	355.88	2225.09
41E	All	8	300	-259.37	704.22	-202.77	1240.01	367.14	1657.59
42A	1	11	0	-50.95	342.11	-143.50	961.14	192.06	1256.00
42C	1	11	100	-45.57	334.04	-134.87	899.00	174.23	1678.78

(Cont'd.) Table E.5.1A: Regression Results of Isobaric Binary VLE and Isothermal Ternary LLE System

System: (1) Etoh - (2) Water - (3) Bz
Gamma Model: Modified UNIQUAC
Phi Model: Virial EOS

Condition: Isobaric for VLE, P = 760 mm Hg
Isothermal for LLE, T = 35 C
Data Sets and References:
(a) Etoh-Water, Reider, R.M., et. al. (1949)
(b) Etoh-Bz, Tyrer, D., (1912)
(c) Etoh-Wtr-Bz, Morachevskii, A.G., et.al.(1958)

Case #	No. of Tie Lines	LLEFN #	W	Final Binary Interaction Parameters in deg K					
				A_{12}	A_{21}	A_{13}	A_{31}	A_{23}	A_{32}
42D	1	11	150	-48.23	338.05	-143.07	962.15	195.60	1357.21
43B	All	11	50	-43.01	328.01	-147.89	1083.40	265.68	1694.69
43C	All	11	100	-64.63	354.35	-145.42	1089.17	268.50	1628.50
43D	All	11	150	-135.43	412.51	-179.60	1231.84	320.27	1502.13
43E	All	11	65	-50.23	330.29	-150.49	1065.60	270.51	1675.13
43F	All	11	80	-90.02	408.10	-155.39	1151.31	278.00	1969.57

Table E.5.1B: Regression Results of Isobaric Binary VLE and Isothermal Ternary LLE System

System: (1) Etoh - (2) Water - (3) Bz
Gamma Model: Modified UNIQUAC
Phi Model: Virial EOS

Condition: Isobaric for VLE, P = 760 mm Hg
Isothermal for LLE, T = 35 C
Data Sets and References:
(a) Etoh-Water, Reider, R.M., et. al. (1949)
(b) Etoh-Bz, Tyrer, D., (1912)
(c) Etoh-Wtr-Bz, Morachevskii, A.G., et.al.(1958)

Case #	No. of Tie Lines	VLEFN #	LLEFN #	W	Mean & (Max) Abs (Te-Tc) deg C			Mean & (Max) Absolute diff in mole %			
								y_1			y_2
					System			System			System
					(a)	(b)	(c)	(a)	(b)	(c)	(c)
40A	1	21	8	10	0.13 (0.57)	0.11 (0.37)	2.47 (6.84)	0.879 (2.373)	0.600 (1.817)	4.215 (8.889)	3.301 (6.314)
40B	1	21	8	50	0.14 (0.59)	0.12 (0.31)	1.91 (5.59)	0.879 (2.414)	0.719 (1.459)	3.331 (7.418)	2.736 (5.397)
41A	All	21	8	0	0.13 (0.57)	0.10 (0.32)	3.51 (8.04)	0.877 (2.365)	0.613 (1.755)	5.007 (10.183)	3.917 (7.313)
41B	All	21	8	150	0.61 (1.16)	0.54 (0.81)	2.73 (8.05)	0.978 (2.188)	1.452 (3.763)	6.743 (12.545)	3.592 (7.023)
41C	All	21	8	200	0.70 (1.29)	0.20 (0.39)	3.24 (9.26)	1.006 (2.363)	0.560 (2.132)	7.015 (13.772)	4.222 (8.068)
41D	All	21	8	250	0.90 (1.75)	0.76 (1.07)	3.69 (10.31)	1.571 (2.890)	1.634 (4.325)	8.760 (16.259)	4.535 (8.751)

(Cont'd.) Table E.5.1B: Regression Results of Isobaric Binary VLE and Isothermal Ternary LLE System

System: (1) Etoh - (2) Water - (3) Bz
Gamma Model: Modified UNIQUAC
Phi Model: Virial EOS

Condition: Isobaric for VLE, P = 760 mm Hg
Isothermal for LLE, T = 35 C
Data Sets and References:
(a) Etoh-Water, Reider, R.M., et. al. (1949)
(b) Etoh-Bz, Tyrer, D., (1912)
(c) Etoh-Wtr-Bz, Morachevskii, A.G., et.al.(1958)

Case #	No. of Tie Lines	VLEFN #	LLEFN #	W	Mean & (Max) Abs (Te-Tc) deg C			Mean & (Max) Absolute diff in mole %			
					System			y_1 System			y_2 System
					(a)	(b)	(c)	(a)	(b)	(c)	(c)
41E	All	21	8	300	1.39 (2.58)	1.18 (1.59)	3.19 (10.31)	2.126 (4.803)	2.485 (11.302)	9.194 (17.209)	3.942 (7.825)
42A	1	21	11	0	0.13 (0.57)	0.11 (0.36)	1.91 (5.61)	0.873 (2.376)	0.602 (1.804)	3.428 (7.535)	2.700 (5.280)
42C	1	21	11	100	0.14 (0.59)	0.12 (0.30)	1.86 (5.42)	0.884 (2.423)	0.695 (1.499)	3.288 (7.242)	2.710 (5.380)
42D	1	21	11	150	0.14 (0.58)	0.10 (0.39)	2.08 (5.97)	0.879 (2.399)	0.607 (1.758)	3.666 (7.866)	2.904 (5.565)
43B	All	21	11	50	0.15 (0.64)	0.33 (1.01)	3.84 (9.52)	0.857 (2.505)	0.902 (1.486)	6.029 (11.665)	4.601 (8.551)
43C	All	21	11	100	0.18 (0.69)	0.44 (1.13)	3.87 (9.66)	0.716 (2.492)	0.997 (1.569)	6.285 (12.150)	4.597 (8.616)

(Cont'd.) Table E.5.1B: Regression Results of Isobaric Binary VLE and Isothermal Ternary LLE System

System: (1) Etoh - (2) Water - (3) Bz
Gamma Model: Modified UNIQUAC
Phi Model: Virial EOS

Condition: Isobaric for VLE, P = 760 mm Hg
Isothermal for LLE, T = 35 C
Data Sets and References:
(a) Etoh-Water, Reider, R.M., et. al. (1949)
(b) Etoh-Bz, Tyrer, D., (1912)
(c) Etoh-Wtr-Bz, Morachevskii, A.G., et.al.(1958)

Case #	No. of Tie Lines	VLEFN #	LLEFN #	W	Mean & (Max) Abs (Te-Tc) deg C			Mean & (Max) Absolute diff in mole %			
					System			y_1 System			y_2 System
					(a)	(b)	(c)	(a)	(b)	(c)	(c)
43D	All	21	11	150	0.94 (1.63)	0.50 (0.77)	3.41 (9.54)	1.134 (3.480)	1.094 (3.675)	7.528 (14.018)	4.451 (8.514)
43E	All	21	11	65	0.20 (0.77)	0.19 (0.82)	3.75 (9.48)	0.724 (2.670)	0.754 (1.809)	6.076 (11.868)	4.590 (8.520)
43F	All	21	11	80	0.18 (0.40)	0.30 (1.10)	3.84 (9.71)	0.842 (2.600)	1.036 (1.860)	6.466 (12.466)	4.510 (8.510)

Table E.5.1C: Regression Results of Isobaric Binary VLE and Isothermal Ternary LLE System

System: (1) Etoh - (2) Water - (3) Bz
Gamma Model: Modified UNIQUAC
Phi Model: Virial EOS

Condition: Isobaric for VLE, P = 760 mm Hg
Isothermal for LLE, T = 35 C
Data Sets and References:
(a) Etoh-Water, Reider, R.M., et. al. (1949)
(b) Etoh-Bz, Tyrer, D., (1912)
(c) Etoh-Wtr-Bz, Morachevskii, A.G., et.al.(1958)

Case #	No. of Tie Lines	VLE FN #	LLE FN #	W	Diff. of compositions in mole %, Mean & (Max)							Mean diff of d. ratio (1)
					Phase Rich in (3)			Phase Rich in (2)			overall	
					(1)	(2)	(3)	(1)	(2)	(3)		
40A	1	21	8	10	0.2415 (2.171)	0.2717 (8.027)	0.4078 (7.619)	1.4760 (1.922)	3.2310 (8.147)	1.8790 (7.753)	1.2512 (8.147)	0.1495 (0.355)
40B	1	21	8	50	1.4650 (1.997)	2.1620 (8.626)	3.4370 (10.310)	1.2820 (1.836)	2.5410 (5.654)	1.8130 (6.739)	2.1167 (10.310)	0.1584 (0.442)
41A	All	21	8	0	0.2086 (1.884)	0.3266 (9.108)	0.4013 (9.512)	1.2860 (1.752)	3.1150 (7.782)	1.9820 (7.989)	1.2199 (9.512)	0.1389 (0.366)
41B	All	21	8	150	1.1742 (3.121)	1.2435 (5.656)	2.4315 (7.857)	1.4211 (2.813)	2.6621 (6.474)	1.3456 (3.662)	1.7130 (7.857)	0.1122 (0.162)
41C*	All	21	8	200	2.5800 (4.173)	1.5247 (4.459)	3.3365 (8.632)	1.4605 (2.801)	0.6075 (1.165)	0.8530 (2.739)	1.7270 (8.632)	0.2813 (0.350)
41D*	All	21	8	250	0.4840 (0.843)	0.8089 (2.376)	0.7910 (1.534)	0.3764 (0.789)	1.4632 (4.203)	1.1347 (3.618)	0.8430 (4.203)	0.0587 (0.210)

* One tie line eliminated for the mean computation

(Cont'd.) Table E.5.1C: Regression Results of Isobaric Binary VLE and Isothermal Ternary LLE System

System: (1) Etoh - (2) Water - (3) Bz
Gamma Model: Modified UNIQUAC
Phi Model: Virial EOS

Condition: Isobaric for VLE, P = 760 mm Hg
Isothermal for LLE, T = 35 C
Data Sets and References:
(a) Etoh-Water, Reider, R.M., et. al. (1949)
(b) Etoh-Bz, Tyrer, D., (1912)
(c) Etoh-Wtr-Bz, Morachevskii, A.G., et.al.(1958)

Case #	No. of Tie Lines	VLE FN #	LLE FN #	W	Diff. of compositions in mole %, Mean & (Max)							Mean diff of d. ratio (1)
					Phase Rich in (3)			Phase Rich in (2)			overall	
					(1)	(2)	(3)	(1)	(2)	(3)		
41E	All	21	8	300	0.8880	1.2520	1.5226	0.6886	2.7195	2.1365	1.5345	0.0649
					(1.726)	(5.686)	(4.877)	(1.299)	(7.997)	(7.454)	(7.997)	(0.115)
42A	1	21	11	0	1.5344	1.9456	2.6689	1.4021	3.4120	2.1551	2.1864	0.1495
					(2.171)	(8.027)	(7.619)	(1.922)	(8.147)	(7.753)	(8.147)	(0.355)
42C	1	21	11	100	1.4190	2.2070	3.1960	1.2550	2.4510	1.7550	2.0470	0.1527
					(1.910)	(8.905)	(10.580)	(1.788)	(5.559)	(6.561)	(10.580)	(0.425)
42D	1	21	11	150	1.5235	1.8627	2.6105	1.3295	3.1228	1.9799	2.0715	0.1439
					(2.053)	(7.879)	(7.664)	(1.873)	(7.540)	(7.281)	(7.879)	(0.392)
43B	All	21	11	50	1.1840	2.4745	2.3690	0.9198	2.0993	1.6927	1.7893	0.0839
					(2.499)	(8.218)	(10.720)	(1.245)	(4.957)	(4.246)	(10.720)	(0.184)
43C	All	21	11	100	0.8251	1.9099	2.7350	0.6472	1.1864	0.9337	1.3729	0.0432
					(2.474)	(4.106)	(6.282)	(2.048)	(2.734)	(3.330)	(6.282)	(0.170)

(Cont'd.) Table E.5.1C: Regression Results of Isobaric Binary VLE and Isothermal Ternary LLE System

System: (1) Etoh - (2) Water - (3) Bz
Gamma Model: Modified UNIQUAC
Phi Model: Virial EOS

Condition: Isobaric for VLE, P = 760 mm Hg
Isothermal for LLE, T = 35 C
Data Sets and References:
(a) Etoh-Water, Reider, R.M., et. al. (1949)
(b) Etoh-Bz, Tyrer, D., (1912)
(c) Etoh-Wtr-Bz, Morachevskii, A.G., et.al.(1958)

Case #	No. of Tie Lines	VLE FN #	LLE FN #	W	Diff. of compositions in mole %, Mean & (Max)							Mean diff of d. ratio
					Phase Rich in (3)			Phase Rich in (2)			overall	
					(1)	(2)	(3)	(1)	(2)	(3)		(1)
43D	All	21	11	150	1.7606 (3.328)	1.8361 (8.167)	2.8257 (11.500)	1.6272 (3.339)	2.9347 (6.869)	2.4314 (8.258)	2.2359 (11.500)	0.1074 (0.173)
43E	All	21	11	65	1.4500 (3.452)	2.7380 (12.020)	2.6860 (15.470)	1.4780 (4.134)	2.4940 (5.361)	1.0930 (3.787)	1.9890 (15.470)	0.1102 (0.204)
43F	All	21	11	80	0.9884 (2.795)	1.6800 (4.853)	1.6590 (7.648)	0.8907 (2.403)	1.9010 (4.592)	1.0650 (3.635)	1.3640 (7.648)	0.1102 (0.204)

Table E.5.2A: Regression Results of Isothermal Binary VLE and Isothermal Ternary LLE System

System: (1) Etoh - (2) Water - (3) Bz
Gamma Model: Modified UNIQUAC
Phi Model: Virial EOS

Condition: Isothermal for VLE, T = 40 C
Isothermal for LLE, T = 35 C
Data Sets and References:
(a) Etoh-Water, Mertl, I., et. al. (1972)
(b) Etoh-Bz, Udovenko, V.V., et. al. (1952)
(c) Etoh-Wtr-Bz, Morachevskii, A.G., et.al. (1958)

Case #	No. of Tie Lines	VLEFN #	LLEFN #	W	Final Binary Interactive Parameters in deg K					
					A_{12}	A_{21}	A_{13}	A_{31}	A_{23}	A_{32}
Intial Parameters Values -->					-19.16	272.71	-121.87	1017.74	375.24	892.72
46A	1	9	8	0	-14.65	261.45	-118.86	1027.32	253.41	869.74
46B	1	9	8	20	-10.02	267.40	-121.69	1008.99	236.90	923.43
46C	1	9	8	40	-9.28	264.59	-123.28	1010.45	236.78	927.39
46D	1	9	8	60	-9.32	266.97	-122.64	1006.63	235.77	920.25
47A	All	9	8	0	12.56	234.56	-140.78	1064.35	181.17	1764.09
47B	All	9	8	15	-203.21	370.34	-193.92	1060.12	348.59	1531.91
47C	All	9	8	30	-238.23	860.90	-226.60	1312.64	427.70	1470.93
47D	All	9	8	45	-362.17	452.02	-220.37	830.11	391.76	8990.45

(Cont'd.) Table E.5.2A: Regression Results of Isothermal Binary VLE and Isothermal Ternary LLE System

System: (1) Etoh - (2) Water - (3) Bz
Gamma Model: Modified UNIQUAC
Phi Model: Virial EOS

Condition: Isothermal for VLE, T = 40 C
Isothermal for LLE, T = 35 C
Data Sets and References:
(a) Etoh-Water, Mertl, I., et. al. (1972)
(b) Etoh-Bz, Udovenko, V.V., et. al. (1952)
(c) Etoh-Wtr-Bz, Morachevskii, A.G., et.al. (1958)

Case #	No. of Tie Lines	VLEFN #	LLEFN #	W	Final Binary Interactive Parameters in deg K					
					A_{12}	A_{21}	A_{13}	A_{31}	A_{23}	A_{32}
48A	1	9	11	0	-12.50	265.18	-121.02	1018.14	245.56	901.67
48B	1	9	11	20	-8.79	269.86	-123.73	1002.89	230.06	949.93
48C	1	9	11	40	-5.64	269.61	-122.71	993.79	227.13	955.77
48D	1	9	11	60	-3.68	265.30	-123.14	995.53	227.51	938.56
49A	All	9	11	0	1.05	199.09	-154.76	1239.53	305.94	1045.77
49B	All	9	11	15	-253.48	256.63	-218.88	902.48	363.12	1679.80
49C	All	9	11	30	-368.27	350.72	-226.16	772.02	393.94	9796.87
49D	All	9	11	45	-421.05	321.88	-231.69	696.84	424.62	2170.84

Table E.5.2B: Regression Results of Isothermal Binary VLE and Isothermal Ternary LLE System

System: (1) Etoh - (2) Water - (3) Bz
Gamma Model: Modified UNIQUAC
Phi Model: Virial EOS

Condition: Isothermal for VLE, T = 40 C
Isothermal for LLE, T = 35 C
Data Sets and References:
(a) Etoh-Water, Mertl, I., et. al. (1972)
(b) Etoh-Bz, Udovenko, V.V., et. al. (1952)
(c) Etoh-Wtr-Bz, Morachevskii, A.G., et.al. (1958)

Case #	No. of Tie Lines	VLEFN #	LLEFN #	W	Mean & (Max) Abs (Pe-Pc) in mmHg			Mean & (Max) Absolute diff in mole % y1			y2
					System		@	System		*	System
					(a)	(b)	(c)	(a)	(b)	(c)	(c) *
46A	1	9	8	0	26.74 (30.46)	44.20 (51.14)	3.41 (8.46)	0.667 (1.403)	1.026 (1.635)	5.386 (10.667)	4.009 (7.917)
46B	1	9	8	20	26.17 (30.21)	45.38 (52.38)	3.14 (7.87)	0.835 (1.506)	1.013 (1.663)	4.813 (9.753)	3.760 (7.393)
46C	1	9	8	40	26.24 (30.22)	45.72 (52.71)	3.09 (7.80)	0.812 (1.502)	1.004 (1.772)	4.760 (9.720)	3.736 (7.344)
46D	1	9	8	60	26.14 (30.21)	45.67 (52.68)	3.08 (7.74)	0.843 (1.522)	1.008 (1.733)	4.721 (9.616)	3.705 (7.294)

@ Predicted ternary VLE, diff. in T's (deg C) VLEFN # 21

* Predicted ternary VLE, VLEFN # 21

(Cont'd.) Table E.5.2B: Regression Results of Isothermal Binary VLE and Isothermal Ternary LLE System

System: (1) Etoh - (2) Water - (3) Bz
Gamma Model: Modified UNIQUAC
Phi Model: Virial EOS

Condition: Isothermal for VLE, T = 40 C
Isothermal for LLE, T = 35 C

Data Sets and References:
(a) Etoh-Water, Mertl, I., et. al. (1972)
(b) Etoh-Bz, Udovenko, V.V., et. al. (1952)
(c) Etoh-Wtr-Bz, Morachevskii, A.G., et.al. (1958)

Case #	No. of Tie Lines	VLEFN #	LLEFN #	W	Mean & (Max) Abs (Pe-Pc) in mmHg			Mean & (Max) Absolute diff in mole % y1			y2
					System (a)	(b)	(c) @	System (a)	(b)	(c) *	System (c) *
47A	All	9	8	0	26.12 (30.10)	48.48 (55.25)	2.29 (6.09)	0.823 (1.801)	1.386 (2.941)	3.760 (7.692)	3.178 (6.208)
47B	All	9	8	15	35.99 (41.36)	60.68 (72.51)	2.94 (8.64)	5.328 (9.447)	4.635 (7.193)	8.867 (17.228)	4.338 (8.254)
47C	All	9	8	30	37.88 (45.29)	64.05 (79.71)	3.63 (9.69)	6.893 (12.577)	5.971 (10.085)	9.238 (16.666)	3.885 (7.646)
47D	All	9	8	45	44.29 (54.10)	71.90 (87.05)	3.33 (6.23)	11.421 (22.022)	7.389 (11.913)	10.480 (21.815)	4.266 (7.268)
48A	1	9	11	0	26.43 (30.26)	44.97 (51.93)	3.28 (8.18)	0.758 (1.419)	1.016 (1.602)	5.089 (10.226)	3.896 (7.667)

@ Predicted ternary VLE, diff. in T's (deg C) VLEFN # 21

* Predicted ternary VLE, VLEFN # 21

(Cont'd.) Table E.5.2B: Regression Results of Isothermal Binary VLE and Isothermal Ternary LLE System

System: (1) Etoh - (2) Water - (3) Bz
Gamma Model: Modified UNIQUAC
Phi Model: Virial EOS

Condition: Isothermal for VLE, T = 40 C
Isothermal for LLE, T = 35 C

Data Sets and References:
(a) Etoh-Water, Mertl, I., et. al. (1972)
(b) Etoh-Bz, Udovenko, V.V., et. al. (1952)
(c) Etoh-Wtr-Bz, Morachevskii, A.G., et.al. (1958)

Case #	No. of Tie Lines	VLEFN #	LLEFN #	W	Mean & (Max) Abs (Pe-Pc) in mmHg			Mean & (Max) Absolute diff in mole % y1			y2
						System	*		System	*	System
					(a)	(b)	(c)	(a)	(b)	(c)	(c) *
48B	1	9	11	20	25.99 (30.18)	46.04 (53.06)	3.01 (7.58)	0.891 (1.676)	1.002 (1.816)	4.554 (9.358)	3.641 (7.143)
48C	1	9	11	40	25.78 (30.14)	46.05 (53.12)	3.00 (7.52)	0.950 (1.863)	1.006 (1.762)	4.474 (9.180)	3.620 (7.091)
48D	1	9	11	60	25.84 (30.14)	46.11 (53.16)	2.95 (7.43)	0.929 (1.767)	1.004 (1.788)	4.432 (9.110)	3.577 (7.032)
49A	All	9	11	0	28.43 (31.29)	48.43 (56.39)	3.79 (9.83)	1.265 (2.086)	2.110 (3.950)	6.503 (12.997)	4.783 (9.154)
49B	All	9	11	15	41.88 (50.40)	68.59 (84.29)	3.04 (6.36)	9.556 (18.222)	6.852 (11.096)	9.862 (20.107)	3.961 (7.074)

@ Predicted ternary VLE, diff. in T's (deg C) VLEFN # 21

* Predicted ternary VLE, VLEFN # 21

(Cont'd.) Table E.5.2B: Regression Results of Isothermal Binary VLE and Isothermal Ternary LLE System

System: (1) Etoh - (2) Water - (3) Bz
Gamma Model: Modified UNIQUAC
Phi Model: Virial EOS

Condition: Isothermal for VLE, T = 40 C
Isothermal for LLE, T = 35 C

Data Sets and References:

(a)	Etoh-Water,	Mertl, I., et. al. (1972)
(b)	Etoh-Bz,	Udovenko, V.V., et. al. (1952)
(c)	Etoh-Wtr-Bz,	Morachevskii, A.G., et.al. (1958)

Case #	No. of Tie Lines	VLEFN #	LLEFN #	W	Mean & (Max) Abs (Pe-Pc) in mmHg			Mean & (Max) Absolute diff in mole %			
								y1			y2
					(a)	System (b)	@ (c)	(a)	System (b)	* (c)	System (c) *
49C	All	9	11	30	46.13 (57.04)	74.80 (90.90)	3.54 (5.45)	12.866 (25.172)	8.137 (13.168)	10.807 (22.929)	4.381 (7.078)
49D	All	9	11	45	49.05 (61.75)	78.37 (95.66)	4.01 (6.37)	15.174 (30.079)	9.061 (14.710)	11.621 (25.332)	4.943 (7.734)

@ Predicted ternary VLE, diff. in T's (deg C) VLEFN # 21

* Predicted ternary VLE, VLEFN # 21

Table E.5.2C: Regression Results of Isothermal Binary VLE and Isothermal Ternary LLE System

System: (1) Etoh - (2) Water - (3) Bz
Gamma Model: Modified UNIQUAC
Phi Model: Virial EOS

Condition: Isothermal for VLE, T = 40 C
Isothermal for LLE, T = 35 C

Data Sets and References:

(a)	Etoh-Water,	Mertl, I., et. al. (1972)
(b)	Etoh-Bz,	Udovenko, V.V., et. al. (1952)
(c)	Etoh-Wtr-Bz,	Morachevskii, A.G., et.al. (1958)

Case #	No. of Tie Lines	LLEFN #	W	Diff. of Compositions in mole %, Mean & (Max)							Mean diff. of d. ratio (1)
				Phase Rich in (3)			Phase Rich in (2)			Overall	
				(1)	(2)	(3)	(1)	(2)	(3)		
46A	1	8	0	4.068	3.150	6.902	2.664	1.600	1.674	3.243	0.1897
				(9.541)	(10.950)	(20.490)	(5.014)	(2.470)	(6.499)	(20.490)	(0.3141)
46B	1	8	20	3.037	2.973	5.880	2.040	1.226	1.698	2.809	0.1524
				(7.697)	(10.610)	(18.310)	(4.242)	(2.280)	(6.522)	(18.310)	(0.2617)
46C	1	8	40	0.709	5.194	0.121	0.060	0.051	7.898	2.339	0.1432
				(2.441)	(15.760)	(0.493)	(0.097)	(0.237)	(16.560)	(16.560)	(0.2424)
46D	1	8	60	2.720	2.897	5.495	1.873	1.187	1.721	2.649	0.1413
				(6.790)	(10.270)	(17.060)	(3.888)	(2.740)	(6.627)	(17.060)	(0.2357)
47A	All	8	0	0.290	2.602	2.892	0.206	1.924	1.848	1.627	0.0338
				(0.573)	(8.818)	(9.303)	(0.562)	(6.820)	(6.999)	(9.303)	(0.1416)
47B	All	8	15	0.997	2.055	2.842	0.847	1.962	2.049	1.792	0.0684
				(2.649)	(8.750)	(11.400)	(2.306)	(4.982)	(7.288)	(11.400)	(0.1257)

(Cont'd.) Table E.5.2C: Regression Results of Isothermal Binary VLE and Isothermal Ternary LLE System

System: (1) Etoh - (2) Water - (3) Bz
Gamma Model: Modified UNIQUAC
Phi Model: Virial EOS

Condition: Isothermal for VLE, T = 40 C
Isothermal for LLE, T = 35 C

Data Sets and References:
(a) Etoh-Water, Mertl, I., et. al. (1972)
(b) Etoh-Bz, Udovenko, V.V., et. al. (1952)
(c) Etoh-Wtr-Bz, Morachevskii, A.G., et.al. (1958)

Case #	No. of Tie Lines	LLEFN #	W	Diff. of Compositions in mole %, Mean & (Max)							Mean diff. of d. ratio (1)
				Phase Rich in (3)			Phase Rich in (2)			Overall	
				(1)	(2)	(3)	(1)	(2)	(3)		
47C	All	8	30	1.378 (2.295)	0.917 (3.815)	1.572 (2.675)	1.087 (1.933)	3.209 (9.666)	2.209 (8.037)	1.729 (9.666)	0.0819 (0.1903)
47D	All	8	45	0.540 (1.139)	1.007 (4.528)	1.216 (4.478)	0.534 (0.997)	1.963 (6.456)	1.787 (6.712)	1.175 (6.712)	0.0470 (0.1010)
48A	1	11	0	3.424 (8.301)	3.038 (10.730)	6.257 (19.030)	2.287 (4.517)	1.383 (2.041)	1.701 (6.557)	3.015 (19.030)	0.1668 (0.2794)
48B	1	11	20	2.459 (6.476)	2.851 (10.290)	5.259 (16.770)	1.687 (3.712)	1.051 (2.884)	1.723 (6.596)	2.505 (16.770)	0.1307 (0.2258)
48C	1	11	40	2.356 (6.393)	2.853 (10.310)	5.198 (16.710)	1.611 (3.669)	0.987 (2.943)	1.730 (6.612)	2.456 (16.700)	0.1268 (0.2232)
48D	1	11	60	2.274 (6.180)	2.828 (10.140)	5.054 (16.320)	1.575 (3.587)	0.979 (3.020)	1.730 (6.607)	2.407 (16.320)	0.1237 (0.2178)

(Cont'd.) Table E.5.2C: Regression Results of Isothermal Binary VLE and Isothermal Ternary LLE System

System: (1) Etoh - (2) Water - (3) Bz
Gamma Model: Modified UNIQUAC
Phi Model: Virial EOS

Condition: Isothermal for VLE, T = 40 C
Isothermal for LLE, T = 35 C
Data Sets and References:
(a) Etoh-Water, Mertl, I., et. al. (1972)
(b) Etoh-Bz, Udovenko, V.V., et. al. (1952)
(c) Etoh-Wtr-Bz, Morachevskii, A.G., et.al. (1958)

Case #	No. of Tie Lines	LLEFN #	W	Diff. of Compositions in mole %, Mean & (Max)							Mean diff. of d. ratio (1)
				Phase Rich in (3)			Phase Rich in (2)			Overall	
				(1)	(2)	(3)	(1)	(2)	(3)		
49A	All	11	0	0.767	2.189	2.593	0.651	2.795	2.327	1.887	0.0512
				(1.852)	(8.079)	(7.639)	(1.590)	(8.753)	(8.394)	(8.753)	(0.1576)
49B	All	11	15	1.021	0.868	1.611	0.750	1.167	1.134	1.092	0.0629
				(2.844)	(3.612)	(6.456)	(1.907)	(3.396)	(2.867)	(6.456)	(0.1092)
49C	All	11	30	0.547	0.908	1.119	0.450	1.969	1.748	1.123	0.0421
				(1.165)	(3.962)	(3.676)	(1.021)	(6.521)	(6.624)	(6.624)	(0.1032)
49D	All	11	45	0.716	2.250	2.593	1.162	1.025	1.055	1.467	0.0462
				(1.463)	(11.200)	(12.260)	(3.752)	(2.302)	(2.590)	(12.260)	(0.1278)

Table E.5.3A: Regression Results of Isothermal Binary VLE and Isothermal Ternary LLE System

System: (1) Etoh - (2) Water - (3) Bz
Gamma Model: Modified UNIQUAC
Phi Model: Virial EOS

Condition: Isothermal for VLE, T = 40 C
Isothermal for LLE, T = 35 C
Data Sets and References:
(a) Etoh-Water, Mertl, I., et. al. (1972)
(b) Etoh-Bz, Udovenko, V.V., et. al. (1952)
(c) Etoh-Wtr-Bz, Morachevskii, A.G., et.al. (1958)

Case #	No. of Tie Lines	VLEFN #	LLEFN #	W	Final Binary Interactive Parameters in deg K					
					A_{12}	A_{21}	A_{13}	A_{31}	A_{23}	A_{32}
Intial Parameter Values -->					18.16	219.39	-121.87	1017.74	375.24	892.72
50B	1	10	8	20	150.94	365.52	-72.36	6423.39	209.42	889.32
50C	1	10	8	40	50.77	296.82	-119.27	3122.24	312.99	851.72
50D	1	10	8	60	21.94	274.98	-133.97	2181.95	340.74	856.50
51A	All	10	8	0	399.00	182.49	-48.90	1472.68	310.99	643.42
51B	All	10	8	5	33.62	217.62	-128.24	1152.36	292.35	1239.39
51C	All	10	8	15	-202.22	542.62	-179.49	1245.44	330.84	1419.99
52A	1	10	11	0	252.23	290.48	-59.15	1561.12	183.26	846.08
52B	1	10	11	10	162.21	342.57	-75.27	6622.45	295.70	808.80

(Cont'd.) Table E.5.3A: Regression Results of Isothermal Binary VLE and Isothermal Ternary LLE System

System: (1) Etoh - (2) Water - (3) Bz
Gamma Model: Modified UNIQUAC
Phi Model: Virial EOS

Condition: Isothermal for VLE, T = 40 C
Isothermal for LLE, T = 35 C
Data Sets and References:
(a) Etoh-Water, Mertl, I., et. al. (1972)
(b) Etoh-Bz, Udovenko, V.V., et. al. (1952)
(c) Etoh-Wtr-Bz, Morachevskii, A.G., et.al. (1958)

Case #	No. of Tie Lines	VLEFN #	LLEFN #	W	Final Binary Interactive Parameters in deg K					
					A_{12}	A_{21}	A_{13}	A_{31}	A_{23}	A_{32}
Intial Parameter Values -->					18.16	219.39	-121.87	1017.74	375.24	892.72
52C	1	10	11	20	90.81	329.87	-101.47	4172.23	304.01	845.95
52D	1	10	11	30	94.34	415.93	-88.49	9652.48	185.14	1063.56
53A	All	10	11	0	39.83	242.50	-135.57	1293.69	363.53	864.81
53B	All	10	11	4	3.14	267.03	-146.53	1226.86	298.02	1241.79
53C	All	10	11	6	35.21	190.83	-150.56	1282.01	320.56	1228.66
53D	All	10	11	8	-138.67	348.84	-176.43	1113.23	306.11	1512.86

Table E.5.3B: Regression Results of Isothermal Binary VLE and Isothermal Ternary LLE System

System: (1) Etoh - (2) Water - (3) Bz
Gamma Model: Modified UNIQUAC
Phi Model: Virial EOS

Condition: Isothermal for VLE, T = 40 C
Isothermal for LLE, T = 35 C
Data Sets and References:
(a) Etoh-Water, Mertl, I., et. al. (1972)
(b) Etoh-Bz, Udovenko, V.V., et. al. (1952)
(c) Etoh-Wtr-Bz, Morachevskii, A.G., et.al. (1958)

Case #	No. of Tie Lines	VLEFN #	LLEFN #	W	Mean & (Max) Abs (Pe-Pc) in mmHg			Mean & (Max) Absolute diff in mole % y1			y2
						System	@		System	*	System *
					(a)	(b)	(c)	(a)	(b)	(c)	(c)
50B	1	10	8	20	11.55 (26.51)	21.66 (29.55)	6.40 (10.55)	7.445 (14.690)	5.605 (16.235)	3.913 (10.469)	5.382 (10.187)
50C	1	10	8	40	20.70 (29.07)	33.76 (40.67)	6.13 (12.40)	3.155 (6.582)	3.398 (12.427)	6.851 (11.968)	5.588 (10.895)
50D	1	10	8	60	23.68 (29.69)	37.89 (44.91)	5.77 (12.42)	1.818 (3.825)	2.851 (11.127)	7.343 (13.363)	5.566 (10.925)
51A	All	10	8	0	8.37 (22.15)	17.44 (27.14)	8.70 (14.45)	8.185 (12.466)	6.329 (14.134)	6.178 (13.111)	7.920 (13.918)
51B	All	10	8	5	25.55 (29.92)	43.52 (50.10)	5.12 (11.59)	1.004 (2.178)	1.377 (2.194)	7.052 (13.144)	5.621 (10.407)

@ Predicted ternary VLE results, diff. in T's (deg C) and VLEFN # 21
* Predicted ternary VLE results, VLEFN # 21

(Cont'd.) Table E.5.3B: Regression Results of Isothermal Binary VLE and Isothermal Ternary LLE System

System: (1) Etoh - (2) Water - (3) Bz
Gamma Model: Modified UNIQUAC
Phi Model: Virial EOS

Condition: Isothermal for VLE, T = 40 C
Isothermal for LLE, T = 35 C

Data Sets and References:
(a) Etoh-Water, Mertl, I., et. al. (1972)
(b) Etoh-Bz, Udovenko, V.V., et. al. (1952)
(c) Etoh-Wtr-Bz, Morachevskii, A.G., et.al. (1958)

Case #	No. of Tie Lines	VLEFN #	LLEFN #	W	Mean & (Max) Abs (Pe-Pc) in mmHg			Mean & (Max) Absolute diff in mole % y1			y2
					(a)	System (b)	@ (c)	(a)	System (b)	* (c)	System * (c)
51C	All	10	8	15	32.04 (37.35)	54.21 (64.73)	3.31 (9.59)	2.831 (5.330)	3.365 (5.748)	8.296 (15.559)	4.266 (8.361)
52A	1	10	11	0	9.14 (24.67)	19.46 (28.61)	6.48 (10.07)	8.296 (14.649)	5.886 (14.631)	3.443 (11.905)	5.835 (10.506)
52B	1	10	11	10	11.78 (26.43)	22.41 (30.28)	8.30 (14.53)	7.295 (14.074)	5.440 (15.991)	6.656 (10.659)	7.160 (12.946)
52C	1	10	11	20	16.46 (28.09)	28.92 (36.40)	7.08 (13.35)	5.068 (10.303)	4.161 (13.902)	6.774 (11.113)	6.265 (11.767)
52D	1	10	11	30	13.27 (27.45)	25.50 (33.33)	5.83 (9.86)	6.834 (14.554)	4.735 (14.956)	4.026 (8.840)	4.944 (9.250)
53A	All	10	11	0	23.98 (29.64)	42.90 (49.32)	5.85 (12.89)	1.690 (3.166)	1.709 (4.706)	7.431 (13.967)	5.922 (11.425)

@ Predicted ternary VLE results, diff. in T's (deg C) and VLEFN # 21
* Predicted ternary VLE results, VLEFN # 21

(Cont'd.) Table E.5.3B: Regression Results of Isothermal Binary VLE and Isothermal Ternary LLE System

System: (1) Etoh - (2) Water - (3) Bz
Gamma Model: Modified UNIQUAC
Phi Model: Virial EOS

Condition: Isothermal for VLE, T = 40 C
Isothermal for LLE, T = 35 C
Data Sets and References:
(a) Etoh-Water, Mertl, I., et. al. (1972)
(b) Etoh-Bz, Udovenko, V.V., et. al. (1952)
(c) Etoh-Wtr-Bz, Morachevskii, A.G., et.al. (1958)

Case #	No. of Tie Lines	VLEFN #	LLEFN #	W	Mean & (Max) Abs (Pe-Pc) in mmHg			Mean & (Max) Absolute diff in mole % y1			y2
					(a)	System (b)	@ (c)	(a)	System (b)	* (c)	System * (c)
53B	All	10	11	4	25.30 (30.03)	46.64 (53.75)	4.65 (10.86)	1.113 (2.281)	1.732 (3.353)	6.629 (12.536)	5.204 (9.747)
53C	All	10	11	6	26.72 (30.10)	46.78 (54.41)	4.85 (11.48)	0.707 (1.901)	1.993 (3.677)	7.197 (13.698)	5.591 (10.399)
53D	All	10	11	8	32.15 (36.40)	55.71 (65.72)	2.87 (8.75)	2.873 (4.680)	3.404 (5.490)	7.539 (14.449)	4.261 (8.109)

@ Predicted ternary VLE results, diff. in T's (deg C) and VLEFN # 21
* Predicted ternary VLE results, VLEFN # 21

Table E.5.3C: Regression Results of Isothermal Binary VLE and Isothermal Ternary LLE System

System: (1) Etoh - (2) Water - (3) Bz
Gamma Model: Modified UNIQUAC
Phi Model: Virial EOS

Condition: Isothermal for VLE, T = 40 C
Isothermal for LLE, T = 35 C
Data Sets and References:
(a) Etoh-Water, Mertl, I., et. al. (1972)
(b) Etoh-Bz, Udovenko, V.V., et. al. (1952)
(c) Etoh-Wtr-Bz, Morachevskii, A.G., et.al. (1958)

Case #	No. of Tie Lines	VLE FN #	LLE FN #	W	Diff. of compositions in mole %, Mean & (Max)							Mean diff of d. ratio (2)
					Phase Rich in (3) (1)	Phase Rich in (3) (2)	Phase Rich in (3) (3)	Phase Rich in (2) (1)	Phase Rich in (2) (2)	Phase Rich in (2) (3)	Overall	
50B	1	21	8	20	7.8460 (21.600)	4.0190 (13.630)	11.2700 (35.220)	4.0370 (8.363)	2.6560 (5.380)	1.6170 (6.295)	5.2402 (35.220)	0.2962 (0.608)
50C	1	21	8	40	1.6540 (3.260)	2.6090 (9.378)	3.6550 (11.180)	1.4720 (2.849)	2.7260 (7.338)	2.4600 (8.729)	2.4293 (11.180)	0.1210 (0.250)
50D	1	21	8	60	1.2860 (3.404)	2.2630 (8.271)	2.5990 (7.576)	1.1370 (2.954)	3.4340 (9.763)	2.5930 (9.230)	2.2187 (9.763)	0.1038 (0.269)
51A	All	21	8	0	0.7183 (1.351)	3.4200 (9.232)	2.9600 (8.979)	0.6465 (1.497)	3.3530 (10.090)	2.9040 (9.938)	2.3336 (10.090)	0.0456 (0.126)
51B	All	21	8	5	2.6510 (4.328)	4.3430 (15.270)	6.9940 (18.470)	1.5400 (2.836)	1.3970 (2.964)	1.3370 (3.308)	3.0437 (15.270)	0.1282 (0.170)
51C	All	21	8	15	1.3740 (2.543)	1.4400 (3.802)	2.8130 (6.345)	1.1670 (2.153)	1.3790 (2.551)	0.8302 (3.124)	1.5005 (6.345)	0.0866 (0.148)

(Cont'd.) Table E.5.3C: Regression Results of Isothermal Binary VLE and Isothermal Ternary LLE System

System: (1) Etoh - (2) Water - (3) Bz
Gamma Model: Modified UNIQUAC
Phi Model: Virial EOS

Condition: Isobaric for VLE, P = 760 mm Hg
Isothermal for LLE, T = 35 C
Data Sets and References:
(a) Etoh-Water, Reider, R.M., et. al. (1949)
(b) Etoh-Bz, Tyrer, D., (1912)
(c) Etoh-Wtr-Bz, Morachevskii, A.G., et.al.(1958)

Case #	No. of Tie Lines	VLE FN #	LLE FN #	W	Diff. of compositions in mole %, Mean & (Max)							Mean diff of d. ratio
					Phase Rich in (3)			Phase Rich in (2)			overall	
					(1)	(2)	(3)	(1)	(2)	(3)		(1)
52A	1	21	11	0	5.5020 (18.050)	3.7960 (12.820)	8.6500 (30.870)	2.9460 (7.627)	1.5000 (3.694)	1.7240 (6.423)	4.0197 (30.870)	0.2016 (0.527)
52B	1	21	11	10	4.9890 (16.460)	3.7400 (12.890)	8.0440 (29.350)	2.9680 (7.691)	0.8454 (1.887)	2.2990 (7.805)	3.8142 (29.350)	0.2067 (0.493)
52C	1	21	11	20	2.0980 (7.157)	3.0660 (11.240)	4.5570 (18.400)	1.5880 (4.319)	2.0470 (3.876)	2.4740 (8.194)	2.6383 (18.400)	0.1235 (0.250)
52D	1	21	11	30	5.5600 (18.490)	3.8610 (13.860)	9.0160 (32.350)	2.7040 (7.218)	1.4600 (4.175)	1.5050 (5.683)	4.0177 (32.350)	0.2105 (0.534)
53A	All	21	11	0	1.1740 (2.678)	2.2090 (7.835)	2.3990 (10.510)	0.9214 (1.862)	2.1370 (5.912)	1.3280 (4.424)	1.6947 (10.510)	0.0659 (0.115)
53B	All	21	11	4	1.3400 (2.949)	2.3560 (7.792)	1.4270 (4.843)	1.2340 (2.887)	3.8270 (12.000)	2.6100 (9.110)	2.1323 (12.000)	0.0808 (0.150)

(Cont'd.) Table E.5.3C: Regression Results of Isothermal Binary VLE and Isothermal Ternary LLE System

System: (1) Etoh - (2) Water - (3) Bz
Gamma Model: Modified UNIQUAC
Phi Model: Virial EOS

Condition: Isobaric for VLE, P = 760 mm Hg
Isothermal for LLE, T = 35 C
Data Sets and References:
(a) Etoh-Water, Reider, R.M., et. al. (1949)
(b) Etoh-Bz, Tyrer, D., (1912)
(c) Etoh-Wtr-Bz, Morachevskii, A.G., et.al.(1958)

Case #	No. of Tie Lines	VLE FN #	LLE FN #	W	Diff. of compositions in mole %, Mean & (Max)							Mean diff of d. ratio
					Phase Rich in (3)			Phase Rich in (2)			overall	
					(1)	(2)	(3)	(1)	(2)	(3)		(1)
53C	All	21	11	6	1.4240 (3.424)	3.7910 (15.380)	4.5180 (18.810)	2.6300 (11.520)	4.7280 (18.500)	2.2320 (6.988)	3.2205 (18.810)	0.0423 (0.132)
53D	All	21	11	8	0.7330 (1.529)	1.6100 (5.017)	2.0500 (6.546)	0.4157 (0.7756	1.6220 (3.905)	1.2990 (3.357)	1.2883 (6.546)	0.0495 (0.090)

Table E.5.4A: Regression Results of Isobaric Binary VLE and LLE, Binary and Ternary System

System: (1) Etoh - (2) Wtr - (3) Bz
Model: Modified UNIQUAC
Phi Model: Virial EOS

Condition: Isobaric for VLE, P = 760 mm Hg
Isothermal for LLE, T = 35 C

Data Sets and References:

(a)	Etoh-Water,	Reider, R.M., et. al. (1949)
(b)	Etoh-Bz,	Tyrer, D., (1912)
(c)	Etoh-Wtr-Bz,	Hands, C.H.G., et. al. (1945)
(d)	Water-Benzene	Sorensen, et. al. (1979)
(e)	Etoh-Wtr-Bz,	Morachevskii, A.G., et.al. (1958)

Case #	No. of Tie Lines	VLEFN #	LLEFN #	W	Final Binary Interaction Parameters in deg K A_{12}	A_{21}	A_{13}	A_{31}	A_{23}	A_{32}	Data Sets used in the Regression
Initial set of parameters					-57.02	351.00	-151.47	961.51	375.24	892.72	
60A	All	21	11	0	-58.67	359.24	-157.21	1067.48	111.17	1068.43	a+b+c+e
60C	All	21	11	50	-125.84	405.90	-189.76	1128.92	211.00	1826.72	a+b+c+e
60D	All	21	11	100	-144.86	396.09	-192.86	1128.22	251.49	2211.54	a+b+c+e
61A	All	21	11	0	-106.69	997.55	-223.20	9215.29	100.21	1058.46	c+d
63A	All	21	11	0	-50.30	344.71	-172.04	1223.01	119.96	1038.39	a+b+c+d
66A	All	21	11	0	-164.16	7816.18	-186.60	2414.43	198.90	418.09	c+e

Table E.5.4B: Regression Results of Isobaric Binary VLE and LLE, Binary and Ternary System

System: (1) Etoh - (2) Wtr - (3) Bz
Model: Modified UNIQUAC
Phi Model: Virial EOS

Condition: Isobaric for VLE, P = 760 mm Hg
Isothermal for LLE, T = 35 C

Data Sets and References:
(a) Etoh-Water, Reider, R.M., et. al. (1949)
(b) Etoh-Bz, Tyrer, D., (1912)
(c) Etoh-Wtr-Bz, Hands, C.H.G., et. al. (1945)
(d) Water-Benzene Sorensen, et. al. (1979)
(e) Etoh-Wtr-Bz, Morachevskii, A.G., et.al. (1958)

Case #	No. of Tie Lines	VLEFN #	LLEFN #	W	Mean & (Max) Abs ($T_{exp}-T_{cal}$) C			Mean & (Max) Absolute diff in mole % y_1			y_2
					System (a)	System (b)	System (c)	System (a)	System (b)	System (c)	System (c)
60A	All	21	11	0	0.15 (0.45)	0.20 (0.61)	0.54 (2.05)	0.933 (2.497)	0.759 (2.394)	0.939 (4.133)	0.973 (3.895)
60C	All	21	11	50	0.81 (1.44)	1.00 (1.30)	1.31 (4.58)	0.908 (3.291)	1.911 (4.843)	4.654 (9.360)	2.123 (4.331)
60D	All	21	11	100	1.31 (2.17)	1.11 (1.42)	1.80 (5.92)	1.820 (4.220)	2.057 (5.089)	6.010 (11.610)	2.851 (5.536)
61A	All	21	11	0	- -	- -	0.29 (0.82)	- -	- -	2.288 (4.899)	2.404 (5.314)
63A	All	21	11	0	0.14 (0.51)	0.33 (0.82)	0.52 (2.00)	0.927 (2.367)	1.224 (3.064)	1.120 (4.117)	0.948 (3.835)
66A	All	21	11	0	- -	- -	0.35 (0.91)	- -	- -	1.348 (5.045)	2.764 (5.947)

Note: '-' mean not applicable

Table E.5.4B: Regression Results of Isobaric Binary VLE and LLE, Binary and Ternary System

System: (1) Etoh - (2) Wtr - (3) Bz
Model: Modified UNIQUAC
Phi Model: Virial EOS

Condition: Isobaric for VLE, P = 760 mm Hg
Isothermal for LLE, T = 35 C

Data Sets and References:
(a) Etoh-Water, Reider, R.M., et. al. (1949)
(b) Etoh-Bz, Tyrer, D., (1912)
(c) Etoh-Wtr-Bz, Hands, C.H.G., et. al. (1945)
(d) Water-Benzene Sorensen, et. al. (1979)
(e) Etoh-Wtr-Bz, Morachevskii, A.G., et.al. (1958)

Case #	No. of Tie Lines	VLE FN #	LLE FN #	W	Diff. of compositions in mole %, Mean & (Max)							Mean diff of d.ratio (1)
					Phase Rich in (3)			Phase Rich in (2)			over -all	
					(1)	(2)	(3)	(1)	(2)	(3)		
60A	All	21	11	0	3.4620	2.2520	5.5880	3.5080	4.5430	1.7240	3.5128	0.2744
60C	All	21	11	50	3.5830	2.0000	5.5830	3.6050	4.4130	1.0590	3.3738	0.2828
60D	All	21	11	100	2.8780	1.9750	4.8270	2.8560	4.6500	1.9330	3.1865	0.2058
61A	All	21	11	0	9.2610 (13.190)	7.6650 (15.900)	16.9300 (21.360)	22.7100 (38.600)	26.0000 (49.000)	3.7800 (12.400)	14.3910 (49.000)	9.1800 (10.940)
63A	All	21	11	0	4.7000 (7.299)	3.1500 (5.028)	7.8510 (12.130)	5.8640 (9.682)	7.6230 (17.750)	2.3350 (8.146)	5.2538 (17.750)	0.4102 (0.573)
66A	All	21	11	0	8.0440 (11.260)	13.6900 (15.890)	21.7300 (26.010)	17.8400 (32.340)	19.6100 (38.390)	1.8210 (6.057)	13.7892 (38.390)	20.1300 (40.770)

APPENDIX F

ETHANOL-WATER-BENZENE PROCESS PLANT SIMULATION RESULTS

F.1 Simulated Process Without Ethanol Concentrator (Case A)

F.2 Simulated Process Including Ethanol Concentrator (Case B)

```
 *** ***  PROSIM FLOW SHEET SIMULATION  *** ***
                  VERSION ONE
                  MARCH  1985

CASE # A: SIMULATION OF AZEO DIST PROCESS PLANT; VLE NRTL & LLE NRTL & IDEAL

NUMBER OF COMPONENTS =  3

VAPOR-LIQUID EQUILIBRIUM DATA CODES:

   LIQUID =   4
   VAPOR =    0
   ENTHALPY = 2


DEFINED CODE VALUES:

   PRINT/DEBUG =              0
   VLE DATA    =              0

   NCIM #      =              0

   FEED VAPORIZATION =        0
   # OF PROCESS ALTERNATES =  0


DEFINED CODES AND VALUES:

   NO. OF LIQ PHASES =      1
   # PARAMETER SETS =       2




NOTE: ALL FLOWS ARE PER UNIT TIME, AND ENERGY
      VALUES ARE IN UNITS OF K-BTU PER UNIT TIME.
```

```
NOTE: THE EQUATIONS FOR ENTHALPY AND VAPOR       PRESSURE ARE:

  (1)  ENTHALPY DATA
       HEAT OF VAPORIZATION ... cal per gm
       REFERENCE TEMPERATURE ... Deg K

  (2)  SPECIFIC HEAT CONSTANTS       LIQUID
          C1=a, C2=b, .... , C4=d
          cal per gram  vs  Deg K
          Cp = a + bT + cT^2 + dT^3

  (3)  SPECIFIC HEAT CONSTANTS       VAPOR
          C1=a, C2=b, .... , C4=d
          cal per g-mole  vs  Deg K
          Cp = a + bT + cT^2 + dT^3

  (4)  VAPOR PRESSURE CONSTANTS
          C1, C2, ... , C6
          C1=a, C2=b, .... , C6=f
          Atm  versus  Deg K
          ln(P) = a + b/(c + T) + d*ln(T) + e*T + f*T^2

        9         9         4        16         1

BEGIN NETWORK READ
   4      MIXR      M-2    15   16  -32    0    0    0    0
   6      ACTL      CT-1   17   14  -18  -19    0    0    0
   7      DVDR      DV-1   34  -16  -23    0    0    0    0
  10      SMIX      M-3    18   23  -15  -30    0    0    0
  11      BCTL      DS-3   30  -21    0    0    0    0    0
  12      DIST      D-3    21  -22  -31    0    0    0    0
  15      HTCL      H-3    32  -17    0    0    0    0    0
  16      MIXR      M-4    33   22  -34    0    0    0    0
  17      CNTL      CT-2   19   35  -36  -33    0    0    0
NETWORK COMPLETE
          4          17
          6           3
          7          24
         10           1
         11          26
         12          25
         15           2
         16          11
         17           3

BEGIN EQUIPMENT DATA READ
        0         0         0         0         0         0         0
        0         0         0         0         0         0         0
        0         0         0         0         0         0         0
        0         0         0         0         0         0         0
        0         0         0         0         0         0         0
        0         0         0         0         0         0         0
        0         0
```

```
  4.0000        0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+0C
 0.00000E+00    0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00
 0.00000E+00    0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+0C
 0.00000E+00    C.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+0C
 0.00000E+00

  6.0000         80.000       0.00000E+00    3.0000         1.0000        1.0000
  150.00         175.00        14.696        14.696       0.00000E+00   0.00000E+00
  2.0000         80.000        77.000       0.00000E+00   0.00000E+00    310.64
 0.00000E+00    0.10000E-02   0.00000E+00    75.000         1.0000        10.000
 0.00000E+00

  7.0000        0.00000E+00    1.0000       0.00000E+00   0.00000E+00   0.00000E+0C
 0.00000E+00    0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00
 0.00000E+00    0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+0C
 0.00000E+00    0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+0C
 0.00000E+00

  10.000         95.000        14.696       0.00000E+00    13.000       0.00000E+00
 0.00000E+00    0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00
 0.00000E+00    0.00000E+00   C.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00
 0.00000E+00    0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00
 0.00000E+00

  11.000         12.000       0.00000E+00    1.0000        14.000        -19.000
 0.00000E+00    0.00000E+00    1.0000        2.0000       0.00000E+00   0.00000E+00
 0.00000E+00    0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00
 0.00000E+00    0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00
 0.00000E+00

  12.000         9.0000       0.00000E+00    3.0000         1.0000        1.0000
  150.00         175.00        1.0000        1.0000       0.00000E+00   0.00000E+00
  1.0000         9.0000       0.00000E+00   0.00000E+00   0.00000E+00    5.4470
 0.00000E+00    0.10000E-02   0.00000E+00    75.000         1.0000        10.000
 0.00000E+00

  15.000        C.00000E+00    95.000       0.00000E+00   0.00000E+00   0.00000E+00
 0.00000E+00    0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00
 0.00000E+00    0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00
 0.00000E+00    C.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+0C
 0.00000E+00

  16.000        0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+0C
 0.00000E+00    0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00
 0.00000E+00    0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+0C
 0.00000E+00    0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+0C
 0.00000E+00

  17.000         1.0000        3.0000       0.00000E+00   0.00000E+00    2.0000
 0.00000E+00    0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+0C
 0.00000E+00    C.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+0C
 0.00000E+00    0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+0C
 0.00000E+00
EQUIPMENT DATA COMPLETE

BEGIN STREAM EXTENSIVE LIST READ
        16          17          18          19          22          23          31          32
        33          34          36           0           0           0           0           C
         0           0           0           0           0           0           0           C
         0           0           0           0           0           0           0           C
```

```
        0          0          0          0          0          0          0          0
        0          0          0          0          0          0          0          0
        0          0          0          0          0          0          0          0
        0          0          0          0          0          0          0          0
        0          0          0          0          0          0          0          0
        0          0          0          0          0          0          0          0
        0          0          0          0          0          0          0          0
        0          0          0          0          0          0          0          0
        0          0          0          0

   14.000      0.00000E+00   115.15       95.368       19.783       0.00000E+00
  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
  0.00000E+00

   15.000      0.00000E+00   279.77       78.647       33.000        168.13
  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
  0.00000E+00

   30.000      0.00000E+00   37.153       13.282       20.702        3.1694
  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
  0.00000E+00

   35.000      0.00000E+00  0.81058      0.00000E+00  0.00000E+00  0.81058
  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
  0.00000E+00
STREAM EXTENSIVE LIST COMPLETE

BEGIN STREAM INTENSIVE LIST READ
        0          0          0          0          0          0          0          0
        0          0          0          0          0          0          0          0
        0          0          0          0          0          0          0          0
        0          0          0          0          0          0          0          0
        0          0          0          0          0          0          0          0
        0          0          0          0          0          0          0          0
        0          0          0          0          0          0          0          0
        0          0          0          0          0          0          0          0
        0          0          0          0          0          0          0          0
        0          0          0          0          0          0          0          0
        0          0          0          0          0          0          0          0
        0          0          0          0          0          0          0          0
        0          0          0          0

   14.000       1.0000      0.00000E+00   95.000       14.696       0.00000E+00
  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00   1.0000

   15.000      0.00000E+00  0.00000E+00   95.000       14.696       0.00000E+00
  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00   1.0000

   16.000      0.00000E+00   1.0000       175.00       14.696       0.00000E+00
  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00   1.0000

   17.000      0.00000E+00  0.00000E+00   100.00       14.696       0.00000E+00
  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00   1.0000

   18.000      0.00000E+00   1.0000       150.00       14.696       0.00000E+00
  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00   1.0000

   19.000      0.00000E+00  0.00000E+00   175.00       14.696       0.00000E+00
  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00   1.0000
```

```
   21.000        0.00000E+00   0.00000E+00    95.000        14.696          0.00000E+00
 0.00000E+00     0.00000E+00   0.00000E+00   0.00000E+00    1.0000

   22.000        0.00000E+00    1.0000        150.00        14.696          0.00000E+00
 0.00000E+00     0.00000E+00   0.00000E+00   0.00000E+00    1.0000

   23.000        0.00000E+00    1.0000        150.00        14.696          0.00000E+00
 0.00000E+00     0.00000E+00   0.00000E+00   0.00000E+00    1.0000

   30.000        0.00000E+00   0.00000E+00    95.000        14.696          0.00000E+00
 0.00000E+00     0.00000E+00   0.00000E+00   0.00000E+00    1.0000

   31.000         2.0000       0.00000E+00    160.00        14.696          0.00000E+00
 0.00000E+00     0.00000E+00   0.00000E+00   0.00000E+00    1.0000

   32.000        0.00000E+00   0.00000E+00    120.00        14.696          0.00000E+00
 0.00000E+00     0.00000E+00   0.00000E+00   0.00000E+00    1.0000

   33.000        0.00000E+00   0.00000E+00    95.000        14.696          0.00000E+00
 0.00000E+00     0.00000E+00   0.00000E+00   0.00000E+00    1.0000

   34.000        0.00000E+00   0.00000E+00    125.00        14.696          0.00000E+00
 0.00000E+00     0.00000E+00   0.00000E+00   0.00000E+00    1.0000

   35.000         1.0000       0.00000E+00    95.000        14.696          0.00000E+00
 0.00000E+00     0.00000E+00   0.00000E+00   0.00000E+00    1.0000

   36.000         2.0000       0.00000E+00    175.00        14.696          0.00000E+00
 0.00000E+00     0.00000E+00   0.00000E+00   0.00000E+00    1.0000
STREAM INTENSIVE LIST COMPLETE

BEGIN CALCULATION DATA READ
        20           1           1
 0.20000E-01

         4          15           6          11          12          17          16           7
        10           0           0           0           0           0           0           0
         0           0           0           0           0           0           0           0
         0           0           0           0           0           0           0           0
         0           0           0           0           0           0           0           0
         0           0           0           0           0           0           0           0
         0           0

        15          30           0           0           0           0           0           0
         0           0

        15          30           0           0           0           0           0           0
         0           0
CALCULATION DATA COMPLETE
```

```
CASE # A: SIMULATION OF AZEO DIST PROCESS PLANT; VLE NRTL & LLE NRTL & IDEAL

                 'PROCESS VECTORS'

...... EQUIPMENT ......                STREAM NUMBERS
NUMBER  SUBROUTINE NAME

   4       MIXR     M-2          15    16   -32     0
   6       ACTL     CT-1         17    14   -18   -19
   7       DVDR     DV-1         34   -16   -23     0
  10       SMIX     M-3          18    23   -15   -30
  11       BCTL     DS-3         30   -21     0     0
  12       DIST     D-3          21   -22   -31     0
  15       HTCL     H-3          32   -17     0     0
  16       MIXR     M-4          33    22   -34     0
  17       CNTL     CT-2         19    35   -36   -33


ASE # A: SIMULATION OF AZEO DIST PROCESS PLANT; VLE NRTL & LLE NRTL & IDEAL

                      'STREAM CONNECTIONS'

                     STREAM    EQUIPMENT
                             FROM    TO

                       14       0      6
                       15      10      4
                       16       7      4
                       17      15      6
                       18       6     10
                       19       6     17
                       21      11     12
                       22      12     16
                       23       7     10
                       30      10     11
                       31      12      0
                       32       4     15
                       33      17     16
                       34      16      7
                       35       0     17
                       36      17      0
```

```
CASE # A: SIMULATION OF AZEO DIST PROCESS PLANT; VLE NRTL & LLE NRTL & IDEAL

           'OTHER SYSTEM VARIABLES'

NUMBER OF COMPONENTS                           3

COMPONENT NUMBERS USED                     0,  0,  0,

RECYCLE EQUIPMENT LIST                     4, 15,  6, 11, 12, 17, 16,  7, 10,

STREAMS USED IN CONVERGENCE ROUTINE      15,30,

PREFERRED CUT STREAM LIST                15,30,

TOLERANCE, 'DERROR'                       0.0200

MAX. LOOPS IN RECYCLE CALC.                   20
```

```
'INPUT DATA'


CASE # A: SIMULATION OF AZEO DIST PROCESS PLANT; VLE NRTL & LLE NRTL & IDEAL

STREAM NUMBER            14            15            16            17

EQUIP CONXION      FR  0 TO  6   FR 10 TO  4   FR  7 TO  4   FR 15 TO  6   FR
VAPOR FRACTION         0.0000        0.0000        1.0000        0.0000
TEMPERATURE, F        95.0000       95.0000      175.0000      100.0000
PRESSURE, PSIA        14.6960       14.6960       14.6960       14.6960
ENTHALPY, K-BTU     -238.6199     -669.0634        0.0000        0.0000
L/H LIQUID FRAC        1.0000        1.0000        1.0000        1.0000

                                COMPOSITION, LB-MOLES/UNIT TIME

ETOH                 95.36771      78.64739       0.00000       0.00000
WATER                19.78290      32.99990       0.00000       0.00000
BENZENE               0.00000     168.12753       0.00000       0.00000

         TOTAL      115.15060     279.77484       0.00000       0.00000



STREAM NUMBER            18            19            22            23

EQUIP CONXION      FR  6 TO 10   FR  6 TO 17   FR 12 TO 16   FR  7 TO 10   FR
VAPOR FRACTION         1.0000        0.0000        1.0000        1.0000
TEMPERATURE, F       150.0000      175.0000      150.0000      150.0000
PRESSURE, PSIA        14.6960       14.6960       14.6960       14.6960
ENTHALPY, K-BTU        0.0000        0.0000        0.0000        0.0000
L/H LIQUID FRAC        1.0000        1.0000        1.0000        1.0000

                                COMPOSITION, LB-MOLES/UNIT TIME

ETOH                  0.00000       0.00000       0.00000       0.00000
WATER                 0.00000       0.00000       0.00000       0.00000
BENZENE               0.00000       0.00000       0.00000       0.00000

         TOTAL        0.00000       0.00000       0.00000       0.00000
```

```
STREAM NUMBER            30              31              32              33

EQUIP CONXION     FR 10 TO 11    FR 12 TO  0    FR  4 TO 15    FR 17 TO 16    FR
VAPOR FRACTION         0.0000          0.0000          0.0000          0.0000
TEMPERATURE, F        95.0000        160.0000        120.0000         95.0000
PRESSURE, PSIA        14.6960         14.6960         14.6960         14.6960
ENTHALPY, K-BTU      -79.2641          0.0000          0.0000          0.0000
L/H LIQUID FRAC        1.0000          1.0000          1.0000          1.0000

                                  COMPOSITION, LB-MOLES/UNIT TIME

ETOH                 13.28196         0.00000         0.00000         0.00000
WATER                20.70165         0.00000         0.00000         0.00000
BENZENE               3.16941         0.00000         0.00000         0.00000

         TOTAL       37.15302         0.00000         0.00000         0.00000



STREAM NUMBER            34              35              36

EQUIP CONXION     FR 16 TO  7    FR  0 TO 17    FR 17 TO  0    FR
VAPOR FRACTION         0.0000          0.0000          0.0000
TEMPERATURE, F       125.0000         95.0000        175.0000
PRESSURE, PSIA        14.6960         14.6960         14.6960
ENTHALPY, K-BTU        0.0000         -2.1075          0.0000
L/H LIQUID FRAC        1.0000          1.0000          1.0000

                                  COMPOSITION, LB-MOLES/UNIT TIME

ETOH                  0.00000         0.00000         0.00000
WATER                 0.00000         0.00000         0.00000
BENZENE               0.00000         0.81058         0.00000

         TOTAL        0.00000         0.81058         0.00000



*****BEGIN TRIAL AND ERROR RECYCLE CALCULATIONS WITH EQUIPMENT LIST..
      4, 15,  6, 11, 12, 17, 16,  7, 10,

  ***  SUBSET LOOP COMPLETE  ***
```

```
FINAL RESULTS

CASE # A: SIMULATION OF AZEO DIST PROCESS PLANT; VLE NRTL & LLE NRTL & IDEAL

STREAM NUMBER           14             15             16             17

EQUIP CONXION     FR  0 TO  6   FR 10 TO  4   FR  7 TO  4   FR 15 TO  6   FR
VAPOR FRACTION        0.0000        0.0000        0.9098        0.0000
TEMPERATURE, F       95.0000       95.0000       45.7580       95.0000
PRESSURE, PSIA       14.6960       14.6960        1.0000       14.6960
ENTHALPY, K-BTU    -238.6199     -669.5720        0.0000     -668.7388
L/H LIQUID FRAC       1.0000        1.0000        1.0000        1.0000

                              COMPOSITION, LB-MOLES/UNIT TIME

ETOH                95.36771      78.76645       0.00000      78.57763
WATER               19.78290      33.08500       0.00000      32.94643
BENZENE              0.00000     168.15891       0.00000     168.11349

         TOTAL     115.15060     280.01035       0.00000     279.63757



STREAM NUMBER           18             19             22             23

EQUIP CONXION     FR  6 TO 10   FR  6 TO 17   FR 12 TO 16   FR  7 TO 10   FR
VAPOR FRACTION        1.0000        0.0000        1.0000        0.9098
TEMPERATURE, F      149.1139      171.6422       52.4409       45.7580
PRESSURE, PSIA       14.6960       14.6960        1.0000        1.0000
ENTHALPY, K-BTU     4497.7769       -1.5666       69.4771       67.3723
L/H LIQUID FRAC       1.0000        1.0000        1.0000        1.0000

                              COMPOSITION, LB-MOLES/UNIT TIME

ETOH                90.60188      83.34265       1.35585       1.35585
WATER               52.72929       0.00000       0.93700       0.93700
BENZENE            167.30380       0.80902       3.18826       3.99728

         TOTAL     310.63498      84.15167       5.48111       6.29012
```

```
STREAM NUMBER             30            31            32            33

EQUIP CONXION       FR 10 TO 11   FR 12 TO  0   FR  4 TO 15   FR 17 TO 16   FR
VAPOR FRACTION          0.0000        0.0000        0.0000        0.0000
TEMPERATURE, F         95.0000       75.8444       94.9984       95.0000
PRESSURE, PSIA         14.6960        1.0000       14.6960       14.6960
ENTHALPY, K-BTU       -78.7528      -79.4617     -668.7445       -2.1034
L/H LIQUID FRAC         1.0000        1.0000        1.0000        1.0000

                                  COMPOSITION, LB-MOLES/UNIT TIME

ETOH                  13.19192      11.97723      78.57763       0.00000
WATER                 20.58685      19.83069      32.94643       0.00000
BENZENE                3.13598       0.00002     168.11349       0.80902

         TOTAL        36.91476      31.80794     279.63757       0.80902



STREAM NUMBER             34            35            36

EQUIP CONXION       FR 16 TO  7   FR  0 TO 17   FR 17 TO  0   FR
VAPOR FRACTION          0.9098        0.0000        0.0000
TEMPERATURE, F         45.7580       95.0000      171.6422
PRESSURE, PSIA          1.0000       14.6960       14.6960
ENTHALPY, K-BTU        67.3723       -2.1034       -1.5666
L/H LIQUID FRAC         1.0000        1.0000        1.0000

                                  COMPOSITION, LB-MOLES/UNIT TIME

ETOH                   1.35585       0.00000      83.34265
WATER                  0.93700       0.00000       0.00000
BENZENE                3.99728       0.80902       0.80902

         TOTAL         6.29012       0.80902      84.15167


CASE # A: SIMULATION OF AZEO DIST PROCESS PLANT; VLE NRTL & LLE NRTL & IDEAL

SUMMARY OF ENERGY REQUIREMENTS:

UNIT NUMBER =  15
HEAT AND COOL
HEAT TRANSFERED IN M-BTU =        0.006
```

```
 *** ***  PROSIM FLOW SHEET SIMULATION  *** ***
                 VERSION ONE
                 MARCH  1985

CASE # B: SIMULATION OF AZEO DIST PROCESS PLANT; VLE NRTL & LLE NRTL & IDEAL

NUMBER OF COMPONENTS =  3

VAPOR-LIQUID EQUILIBRIUM DATA CODES:

    LIQUID =    4
    VAPOR =     0
    ENTHALPY = 2


DEFINED CODE VALUES:

    PRINT/DEBUG =                0
    VLE DATA    =                0

    NCIM #      =                0

    FEED VAPORIZATION =          0
    # OF PROCESS ALTERNATES =    0


DEFINED CODES AND VALUES:

    NO. OF LIQ PHASES =         1
    # PARAMETER SETS =          2




NOTE: ALL FLOWS ARE PER UNIT TIME, AND ENERGY
      VALUES ARE IN UNITS OF K-BTU PER UNIT TIME.
```

```
NOTE: THE EQUATIONS FOR ENTHALPY AND VAPOR       PRESSURE ARE:

   (1)   ENTHALPY DATA
         HEAT OF VAPORIZATION ... cal per gm
         REFERENCE TEMPERATURE ... Deg K

   (2)   SPECIFIC HEAT CONSTANTS       LIQUID
            C1=a, C2=b, .... , C4=d
            cal per gram  vs  Deg K
            Cp = a + bT + cT^2 + dT^3

   (3)   SPECIFIC HEAT CONSTANTS       VAPOR
            C1=a, C2=b, .... , C4=d
            cal per g-mole  vs  Deg K
            Cp = a + bT + cT^2 + dT^3

   (4)   VAPOR PRESSURE CONSTANTS
            C1, C2, ... , C6
            C1=a, C2=b, .... , C6=f
            Atm  versus  Deg K
            ln(P) = a + b/(c + T) + d*ln(T) + e*T + f*T^2

         11         11         5         19         1

BEGIN NETWORK READ
    1       DIST      D-1     10    31   -11   -12     0     0     0
    3       HTCL      H-1     11   -14     0     0     0     0     0
    4       MIXR      M-2     15    16   -32     0     0     0     0
    6       ACTL      CT-1    17    14   -18   -19     0     0     0
    7       DVDR      DV-1    34   -16   -23     0     0     0     0
   10       SMIX      M-3     18    23   -15   -30     0     0     0
   11       DCTL      DS-3    30   -21     0     0     0     0     0
   12       DIST      D-3     21   -22   -31     0     0     0     0
   15       HTCL      H-3     32   -17     0     0     0     0     0
   16       MIXR      M-4     33    22   -34     0     0     0     0
   17       CNTL      CT-2    19    35   -36   -33     0     0     0
NETWORK COMPLETE
            1          17
            3           2
            4          11
            6           3
            7          24
           10           1
           11          26
           12          23
           15           2
           16          11
           17           3

BEGIN EQUIPMENT DATA READ
         0         0         0         0         0         0         0
         0         0         0         0         0         0         0
         0         0         0         0         0         0         0
         0         0         0         0         0         0         0
         0         0         0         0         0         0         0
         0         0         0         0         0         0         0
```

```
       0          0

   1.0000       26.000       12.000        3.0000       1.0000       1.0000
   150.00       211.00       14.696        14.696      0.00000E+00  0.00000E+00
   2.0000       13.000       26.000       0.00000E+00  0.00000E+00  0.00000E+00
   115.15       3.0000      -1.0000        75.000      0.00000E+00  0.00000E+00
  0.00000E+00

   3.0000      0.00000E+00   95.000       0.00000E+00  0.00000E+00  0.00000E+00
  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
  0.00000E+00

   4.0000      0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
  0.00000E+00

   6.0000       80.000      0.00000E+00   3.0000       1.0000       1.0000
   150.00       175.00       14.696       14.696      0.00000E+00  0.00000E+00
   2.0000       80.000       77.000      0.00000E+00  0.00000E+00   310.70
  0.00000E+00  0.10000E-02  0.00000E+00   75.000       1.0000       15.000
  0.00000E+00

   7.0000      0.00000E+00   1.0000      0.00000E+00  0.00000E+00  0.00000E+00
  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
  0.00000E+00

   10.000       95.000       14.696      0.00000E+00   13.000      0.00000E+00
  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
  0.00000E+00

   11.000       12.000      0.00000E+00   1.0000      0.23320      0.18390
  0.58290      0.37883      0.62117      0.00000E+00  0.00000E+00  0.00000E+00
  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
  0.00000E+00

   12.000       9.0000      0.00000E+00   3.0000       1.0000       1.0000
   140.00       165.00       4.8000       4.8000      0.00000E+00  0.00000E+00
   1.0000       9.0000      0.00000E+00  0.00000E+00  0.00000E+00   5.4380
  0.00000E+00  0.10000E-02  0.00000E+00   50.000      0.00000E+00  0.00000E+00
  0.00000E+00

   15.000      0.00000E+00   95.000      0.00000E+00  0.00000E+00  0.00000E+00
  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
  0.00000E+00

   16.000      0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
```

```
   0.00000E+00

    17.000       1.0000       3.0000      0.00000E+00  0.00000E+00   2.0000
   0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
   0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
   0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
   0.00000E+00
 EQUIPMENT DATA COMPLETE

 BEGIN STREAM EXTENSIVE LIST READ
        11          12          16          17          18          19          21          22
        23          31          32          33          34          36           0           0
         0           0           0           0           0           0           0           0
         0           0           0           0           0           0           0           0
         0           0           0           0           0           0           0           0
         0           0           0           0           0           0           0           0
         0           0           0           0           0           0           0           0
         0           0           0           0           0           0           0           0
         0           0           0           0           0           0           0           0
         0           0           0           0           0           0           0           0
         0           0           0           0           0           0           0           0
         0           0           0           0           0           0           0           0
         0           0           0           0

    10.000      0.00000E+00   2611.7       83.432       2528.2      0.00000E+00
   0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
   0.00000E+00

    14.000      0.00000E+00   115.15       95.450       19.700      0.00000E+00
   0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
   0.00000E+00

    15.000      0.00000E+00   279.76       78.643       32.995       168.13
   0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
   0.00000E+00

    30.000      0.00000E+00   37.148       13.281       20.698       3.1700
   0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
   0.00000E+00

    35.000      0.00000E+00  0.78430      0.00000E+00  0.00000E+00  0.78430
   0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
   0.00000E+00
 STREAM EXTENSIVE LIST COMPLETE

 BEGIN STREAM INTENSIVE LIST READ
         0           0           0           0           0           0           0           0
         0           0           0           0           0           0           0           0
         0           0           0           0           0           0           0           0
         0           0           0           0           0           0           0           0
         0           0           0           0           0           0           0           0
         0           0           0           0           0           0           0           0
         0           0           0           0           0           0           0           0
         0           0           0           0           0           0           0           0
         0           0           0           0           0           0           0           0
         0           0           0           0           0           0           0           0
         0           0           0           0           0           0           0           0
         0           0           0           0           0           0           0           0
         0           0           0           0
```

```
   10.000       1.0000       0.00000E+00   184.00       14.696        0.00000E+00
 0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00   1.0000

   11.000      0.00000E+00  0.00000E+00   160.00       14.696        0.00000E+00
 0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00   1.0000

   12.000       2.0000      0.00000E+00   210.00       14.696        0.00000E+00
 0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00   1.0000

   14.000      0.00000E+00  0.00000E+00   95.000       14.696        0.00000E+00
 0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00   1.0000

   15.000      0.00000E+00  0.00000E+00   95.000       14.696        0.00000E+00
 0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00   1.0000

   16.000      0.00000E+00   1.0000       175.00       14.696        0.00000E+00
 0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00   1.0000

   17.000      0.00000E+00  0.00000E+00   100.00       14.696        0.00000E+00
 0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00   1.0000

   18.000      0.00000E+00   1.0000       150.00       14.696        0.00000E+00
 0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00   1.0000

   19.000      0.00000E+00  0.00000E+00   175.00       14.696        0.00000E+00
 0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00   1.0000

   21.000      0.00000E+00  0.00000E+00   95.000       14.696        0.00000E+00
 0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00   1.0000

   22.000      0.00000E+00   1.0000       150.00       14.696        0.00000E+00
 0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00   1.0000

   23.000      0.00000E+00   1.0000       150.00       14.696        0.00000E+00
 0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00   1.0000

   30.000      0.00000E+00  0.00000E+00   95.000       14.696        0.00000E+00
 0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00   1.0000

   31.000      0.00000E+00  0.00000E+00   160.00       14.696        0.00000E+00
 0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00   1.0000

   32.000      0.00000E+00  0.00000E+00   120.00       14.696        0.00000E+00
 0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00   1.0000

   33.000      0.00000E+00  0.00000E+00   95.000       14.696        0.00000E+00
 0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00   1.0000

   34.000      0.00000E+00  0.00000E+00   125.00       14.696        0.00000E+00
 0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00   1.0000

   35.000       1.0000      0.00000E+00   95.000       14.696        0.00000E+00
 0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00   1.0000

   36.000       2.0000      0.00000E+00   175.00       14.696        0.00000E+00
 0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00   1.0000
STREAM INTENSIVE LIST COMPLETE

BEGIN CALCULATION DATA READ
      20         1         1
```

```
   0.10000E-01

         4        15         6        11        12         1         3        17
        16         7        10         0         0         0         0         0
         0         0         0         0         0         0         0         C
         0         0         0         0         0         0         0         C
         0         0         0         0         0         0         0         C
         0         0         0         0         0         0         0         C
         0         0

        14        15        30         0         0         0         0         C
         0         0

        14        15        30         0         0         0         0         C
         0         0
CALCULATION DATA COMPLETE
```

```
CASE # 8: SIMULATION OF AZEO DIST PROCESS PLANT; VLE NRTL & LLE NRTL & IDEAL

                    'PROCESS VECTORS'

...... EQUIPMENT ......                 STREAM NUMBERS
NUMBER  SUBROUTINE NAME

   1        DIST     D-1             10   31  -11  -12
   3        HTCL     H-1             11  -14    0    0
   4        MIXR     M-2             15   16  -32    0
   6        ACTL     CT-1            17   14  -18  -19
   7        DVDR     DV-1            34  -16  -23    0
  10        SMIX     M-3             18   23  -15  -30
  11        DCTL     DS-3            30  -21    0    0
  12        DIST     D-3             21  -22  -31    0
  15        HTCL     H-3             32  -17    0    0
  16        MIXR     M-4             33   22  -34    0
  17        CNTL     CT-2            19   35  -36  -33
```

```
CASE # 8: SIMULATION OF AZEO DIST PROCESS PLANT; VLE NRTL & LLE NRTL & IDEAL

                        'STREAM CONNECTIONS'

                      STREAM     EQUIPMENT
                               FROM    TO

                        10       0      1
                        11       1      3
                        12       1      0
                        14       3      6
                        15      10      4
                        16       7      4
                        17      15      6
                        18       6     10
                        19       6     17
                        21      11     12
                        22      12     16
                        23       7     10
                        30      10     11
                        31      12      1
                        32       4     15
                        33      17     16
                        34      16      7
                        35       0     17
                        36      17      0
```

```
CASE # B: SIMULATION OF AZEO DIST PROCESS PLANT; VLE NRTL & LLE NRTL & IDEAL

           'OTHER SYSTEM VARIABLES'

NUMBER OF COMPONENTS                          3

COMPONENT NUMBERS USED                    0,  0,  0,

RECYCLE EQUIPMENT LIST                    4, 15,  6, 11, 12,  1,  3, 17, 16,
                                         10,

STREAMS USED IN CONVERGENCE ROUTINE     14,15,30,

PREFERRED CUT STREAM LIST               14,15,30,

TOLERANCE, 'DERROR'                      0.0100

MAX. LOOPS IN RECYCLE CALC.                  20
```

```
'INPUT DATA'

CASE # B: SIMULATION OF AZEO DIST PROCESS PLANT; VLE NRTL & LLE NRTL & IDEAL

STREAM NUMBER             10              11              12              14

EQUIP CONXION       FR  0 TO  1    FR  1 TO  3    FR  1 TO  0    FR  3 TO  6    FR
VAPOR FRACTION          0.0000          0.0000          0.0000          0.0000
TEMPERATURE, F        184.0000        160.0000        210.0000         95.0000
PRESSURE, PSIA         14.6960         14.6960         14.6960         14.6960
ENTHALPY, K-BTU     -1250.2102          0.0000          0.0000       -238.5989
L/H LIQUID FRAC         1.0000          1.0000          1.0000          1.0000

                                 COMPOSITION, LB-MOLES/UNIT TIME

ETOH                  83.43170         0.00000         0.00000        95.45022
WATER               2528.23047         0.00000         0.00000        19.70037
BENZENE                0.00000         0.00000         0.00000         0.00000

        TOTAL       2611.66187         0.00000         0.00000       115.15060



STREAM NUMBER             15              16              17              18

EQUIP CONXION       FR 10 TO  4    FR  7 TO  4    FR 15 TO  6    FR  6 TO 10    FR
VAPOR FRACTION          0.0000          1.0000          0.0000          1.0000
TEMPERATURE, F         95.0000        175.0000        100.0000        150.0000
PRESSURE, PSIA         14.6960         14.6960         14.6960         14.6960
ENTHALPY, K-BTU      -669.0345          0.0000          0.0000          0.0000
L/H LIQUID FRAC         1.0000          1.0000          1.0000          1.0000

                                 COMPOSITION, LB-MOLES/UNIT TIME

ETOH                  78.64269         0.00000         0.00000         0.00000
WATER                 32.99490         0.00000         0.00000         0.00000
BENZENE              168.12608         0.00000         0.00000         0.00000

        TOTAL        279.76370         0.00000         0.00000         0.00000
```

```
STREAM NUMBER          19            21            22            23

EQUIP CONXION     FR  6 TO 17   FR 11 TO 12   FR 12 TO 16   FR  7 TO 10    FR
VAPOR FRACTION        0.0000        0.0000        1.0000        1.0000
TEMPERATURE, F      175.0000       95.0000      150.0000      150.0000
PRESSURE, PSIA       14.6960       14.6960       14.6960       14.6960
ENTHALPY, K-BTU       0.0000        0.0000        0.0000        0.0000
L/H LIQUID FRAC       1.0000        1.0000        1.0000        1.0000

                               COMPOSITION, LB-MOLES/UNIT TIME

ETOH                 0.00000       0.00000       0.00000       0.00000
WATER                0.00000       0.00000       0.00000       0.00000
BENZENE              0.00000       0.00000       0.00000       0.00000

         TOTAL       0.00000       0.00000       0.00000       0.00000



STREAM NUMBER          30            31            32            33

EQUIP CONXION     FR 10 TO 11   FR 12 TO  1   FR  4 TO 15   FR 17 TO 16    FR
VAPOR FRACTION        0.0000        0.0000        0.0000        0.0000
TEMPERATURE, F       95.0000      160.0000      120.0000       95.0000
PRESSURE, PSIA       14.6960       14.6960       14.6960       14.6960
ENTHALPY, K-BTU     -79.2555        0.0000        0.0000        0.0000
L/H LIQUID FRAC       1.0000        1.0000        1.0000        1.0000

                               COMPOSITION, LB-MOLES/UNIT TIME

ETOH                13.28082       0.00000       0.00000       0.00000
WATER               20.69753       0.00000       0.00000       0.00000
BENZENE              3.17000       0.00000       0.00000       0.00000

         TOTAL      37.14835       0.00000       0.00000       0.00000
```

```
STREAM NUMBER              34             35             36

EQUIP CONXION     FR 16 TO  7   FR  0 TO 17   FR 17 TO  0   FR
VAPOR FRACTION         0.0000         0.0000         0.0000
TEMPERATURE, F       125.0000        95.0000       175.0000
PRESSURE, PSIA        14.6960        14.6960        14.6960
ENTHALPY, K-BTU        0.0000        -2.0391         0.0000
L/H LIQUID FRAC        1.0000         1.0000         1.0000

                                COMPOSITION, LB-MOLES/UNIT TIME

ETOH                  0.00000        0.00000        0.00000
WATER                 0.00000        0.00000        0.00000
BENZENE               0.00000        0.78430        0.00000

         TOTAL        0.00000        0.78430        0.00000


  ***  SUBSET LOOP COMPLETE  ***
```

```
FINAL RESULTS

CASE # 8: SIMULATION OF AZEO DIST PROCESS PLANT; VLE NRTL & LLE NRTL & IDEAL

STREAM NUMBER            10            11            12            14

EQUIP CONXION      FR  0 TO  1   FR  1 TO  3   FR  1 TO  0   FR  3 TO  6   FR
VAPOR FRACTION          0.0000        0.0000        0.0000        0.0000
TEMPERATURE, F        184.0000      153.8289      211.9922       95.0000
PRESSURE, PSIA         14.6960       14.6960       14.6960       14.6960
ENTHALPY, K-BTU     -1250.2102      -67.7280       -3.6281     -238.5979
L/H LIQUID FRAC         1.0000        1.0000        1.0000        1.0000

                              COMPOSITION, LB-MOLES/UNIT TIME

ETOH                  83.43170      95.45193       0.00037      95.45193
WATER               2528.23047      19.69789    2528.23340      19.69789
BENZENE                0.00000       0.00008       0.00000       0.00008

          TOTAL     2611.66187     115.14990    2528.23364     115.14990



STREAM NUMBER            15            16            17            18

EQUIP CONXION      FR 10 TO  4   FR  7 TO  4   FR 15 TO  6   FR  6 TO 10   FR
VAPOR FRACTION          0.0000        0.8775        0.0000        1.0000
TEMPERATURE, F         95.0000       99.6651       95.0000      149.1172
PRESSURE, PSIA         14.6960        4.8000       14.6960       14.6960
ENTHALPY, K-BTU      -668.9789        0.0000     -669.0304     4498.3696
L/H LIQUID FRAC         1.0000        1.0000        1.0000        1.0000

                              COMPOSITION, LB-MOLES/UNIT TIME

ETOH                  78.62567       0.00000      78.63961      90.65314
WATER                 32.98320       0.00000      32.99416      52.69683
BENZENE              168.12511       0.00000     168.12692     167.32634

          TOTAL      279.73398       0.00000     279.76068     310.67633
```

```
STREAM NUMBER          19            21            22            23

EQUIP CONXION    FR  6 TO 17   FR 11 TO 12   FR 12 TO 16   FR  7 TO 10   FR
VAPOR FRACTION        0.0000        0.0000        1.0000        0.8775
TEMPERATURE, F      171.6569       95.0000      101.9489       99.6651
PRESSURE, PSIA       14.6960       14.6960        4.8000        4.8000
ENTHALPY, K-BTU      -1.5339      -79.2645       73.4274       71.3476
L/H LIQUID FRAC       1.0000        1.0000        1.0000        1.0000

                           COMPOSITION, LB-MOLES/UNIT TIME

ETOH                83.43219      13.28153       1.26078       1.26078
WATER                0.00000      20.70020       0.99885       0.99885
BENZENE              0.79995       3.16979       3.16971       3.96967

         TOTAL      84.23215      37.15152       5.42935       6.22930



STREAM NUMBER          30            31            32            33

EQUIP CONXION    FR 10 TO 11   FR 12 TO  1   FR  4 TO 15   FR 17 TO 16   FR
VAPOR FRACTION        0.0000        0.0000        0.0000        0.0000
TEMPERATURE, F       95.0000      129.9099       94.9976       95.0000
PRESSURE, PSIA       14.6960        4.8000       14.6960       14.6960
ENTHALPY, K-BTU     -79.3082      -42.7308     -669.0167       -2.0798
L/H LIQUID FRAC       1.0000        1.0000        1.0000        1.0000

                           COMPOSITION, LB-MOLES/UNIT TIME

ETOH                13.28933      12.02075      78.63961       0.00000
WATER               20.70906      19.70135      32.99416       0.00000
BENZENE              3.17323       0.00008     168.12692       0.79995

         TOTAL      37.17162      31.72217     279.76068       0.79995
```

```
STREAM NUMBER            34              35              36

EQUIP CONXION     FR 16 TO  7    FR  0 TO 17    FR 17 TO  0    FR
VAPOR FRACTION          0.8775          0.0000          0.0000
TEMPERATURE, F         99.6651         95.0000        171.6569
PRESSURE, PSIA          4.8000         14.6960         14.6960
ENTHALPY, K-BTU        71.3476         -2.0798         -1.5339
L/H LIQUID FRAC         1.0000          1.0000          1.0000

                                  COMPOSITION, LB-MOLES/UNIT TIME

ETOH                   1.26078         0.00000        83.43219
WATER                  0.99885         0.00000         0.00000
BENZENE                3.96967         0.79995         0.79995

         TOTAL         6.22930         0.79995        84.23215


CASE # B: SIMULATION OF AZEO DIST PROCESS PLANT; VLE NRTL & LLE NRTL & IDEAL

SUMMARY OF ENERGY REQUIREMENTS:

UNIT NUMBER =   3
HEAT AND COOL
HEAT TRANSFERED IN M-BTU =     170.870

UNIT NUMBER =  15
HEAT AND COOL
HEAT TRANSFERED IN M-BTU =       0.014
```

APPENDIX G

COMPUTER PROGRAMS

G.1 Process Simulation Program and Affiliated Subprograms

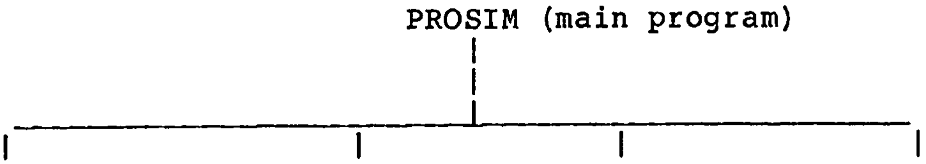
G.2 Absorption/Distillation Program and Affiliated Subprograms

G.3 Three Phase Flash Program and Affiliated Subprograms

G.4 Non-linear Regression Program and Affiliated Subprograms

The computer listing of the selected subprograms, flaged by '*', is included in this Appendix because of the voluminous code. The listing of program(s) will be furnished upon request to the interested individual or company.

G.1 Process Simulation Program and Affiliated Subprograms



PROSIM1
(file)

ABSR
ADBF*
BZTL*
CNTL*
CTRL
DCTL*
DIST
DREAD
DVDR
EPRINT
EQUIP
HTCL
HYTR
MIXR
PUMP
RCYCLE
RESULT
SCAN
SPLT
TEST
TRANSX
VALV
ZEROX

ACTL*
BCTL*
CLEAN
COMP
DCHECK
DENETS
DPRINT
DSPT*
ECTL*
EQCALL
GSXP
HXER
INIT
OVHD
RCTL*
REAC
SBOX*
SMIX*
SUBSET
TRANSF
TPRINT
ZERO
ADD1

PROSIM2
(file)

ABSR1
ABSR2
DIST1
DIST2
MATRIX
CORECT
GAUSL
KCOLMN
KFAC
TESTCL
SUMUP

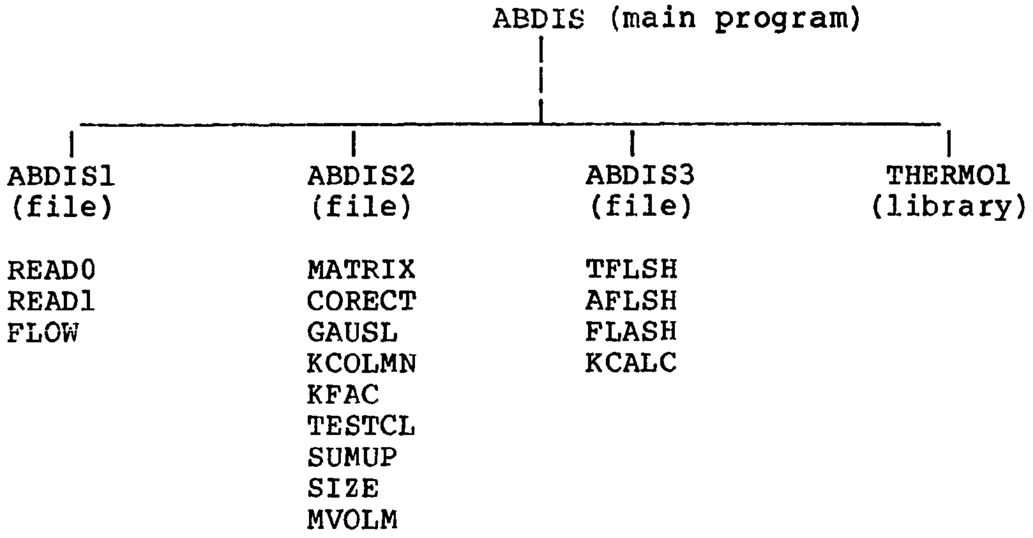
PROSIM3
(file)

ANYONE
INTLIZ
DEWT1
DEWP
BUBT1
BUBT2
BUBP
TWOLIQ*
FLSH1*
FLSH2*
AFLSH2*
KCALC2*
PRINT2*
PRCHK

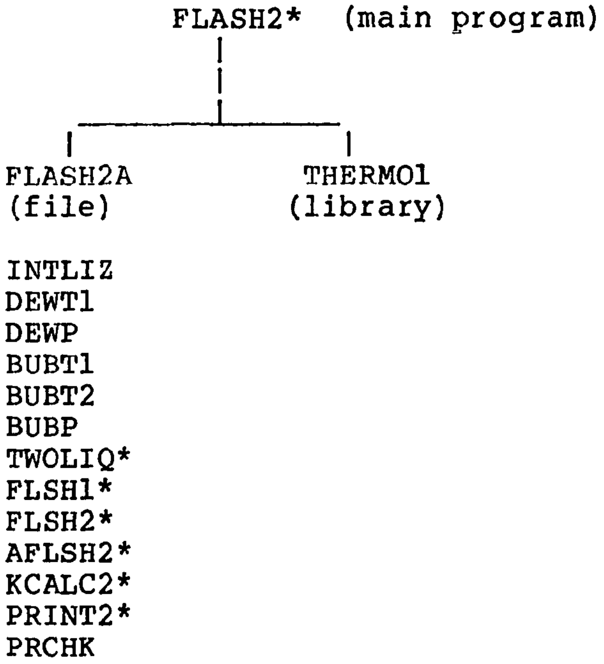
THERMO1
(library)

START*
CDATA*
RUNFAC*
SWITCH*
WEG
LIQH
VAPH
FUGCY
XSHVAP
ACTVY
XSHLQ
VIRFG1*
ZVIR1*
BCALC*
SVIR*
VIRFG2
ZVIR2
RKFUG
ZRK
ZCUBIC
SRKFUG
ZSRK
ONEDIM
VLAAR
XHVLR
MARGL
XHMARG
WILSN
XHWIL
RENON
XHREN
UNQAC1
XHUNQ1
UNQAC2*
XHUNQ2*
UNIFAC*

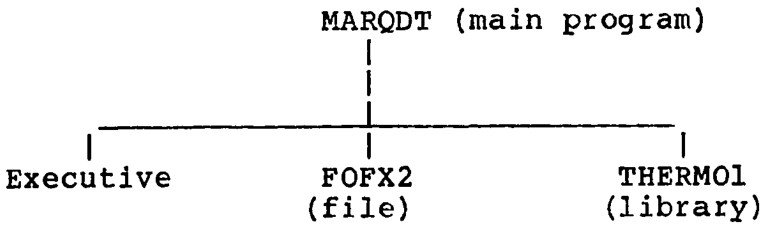
G.2 Absorption/Distillation Program and Affiliated Subprograms



G.3 Three Phase Flash Program and Affiliated Subprograms



G.4 Non-linear Regression Program and Affiliated Subprograms



FOFX*
INTLIZ*
BUBP
BUBPT1
TWOLIQ*
FXVLE*
FX2LIQ*
INFY*
KCALC2*
PRINT2*
PRINT3*
TALLY1*

```
      PROGRAM    PROSIM
C
C     VERSION #    .... MARCH 1985
C
C     THE FOLLOWING ARE THE MAIN PROGRAM FILE AND OTHER SUPPLEMENTARY
C     FILES:
C     (A) PROSIM1.FOR
C     (B) PROSIM2.FOR
C     (C) PROSIM3.FOR
C     (D) THERMO1.FOR
C     (E) THERMO2.FOR
C     (F) THERMO3.FOR
C     (G) DATABANK.UNI  (ONLY WITH UNIFAC ACTIVITY COEFFICIENT MODEL)
C
C     MODULES DELCP, GSXP AND COMP USE ONLY R-K EOS.
C
      COMMON  /CONTL/  NIN,NOUT,NOCOMP,NE,NEN,KUNITS
      COMMON  /EQPA/   B(1252)
      COMMON  /EQPB/   CF(150)
      COMMON  /MTST/   H(300)
      COMMON  /STMA/   J(2403)
      COMMON  /STRMIN/ K(128)
      COMMON  /STMOUT/ LL(128)
      COMMON  /SYSAA/  M(70)
      COMMON  /SYSA/   N(801)
      COMMON  /SYSB/   IIO(127)
      COMMON  /SYSC/   PP(5)
      COMMON  /SYSD/   QF(154)
      COMMON  /BLANK/  NCR, NPRT, KEEPIT(22)
      COMMON  /CMPRO/  NK, NCM1, NCP1, IDLL, IDLV, IDH, LDBUG, ISW,
     *                 NDIM, ZNAME(2,10), L(10), NTCOMP(10), NLIQ, IPSET
      COMMON  /CLMN/   TIGER(22)
      COMMON  /ZDATA/  CAT(1107)
      COMMON  /STRM/   DOG(82)
      COMMON  /TWOLQ/  DUMB1(71)
      COMMON  /ZFEEDZ/ AAAA(15)
C
D     WRITE (6,9999)
 9999 FORMAT(' ',30X,'PROGRAM PROSIM')
C
C     SYSTEM LIMITS
C       10 COMPONENTS
C       50 STREAMS
C       100 NODES(PIECES OF EQUIPMENT)
C
      NCR=5
      NPRT=6
C
C     KODE =  0 REQUIRES AN INITIALIZATION OF ALL VARIABLES
C     KODE = -1 IMPLIES A VARIATION OF THE PREVIOUS CASE
C     KODE =  1 PROBLEM DATA HAS ERROR - TERMINATE PROGRAM
C
C     DEC Error-Set Routines Activitated
C          Errset 72 = Floating Point Overflow
C          Errset 73 = Divide Check
C          Errset 74 = Floating Point Underflow
C          Errset 77 = Subscript Out Of Range
C
      CALL ERRSET (72, .TRUE., .TRUE., .FALSE., .FALSE., 999)
      CALL ERRSET (73, .TRUE., .TRUE., .FALSE., .FALSE., 999)
```

```
C
C     THIS BLOCK (ACTL) SIMULATES THE DISTILLATE RATE
C     OF AN AZEOTROPIC DISTILLATION COLUMN
C     BASED ON THE COMPUTED BOTTOMS PRODUCT COMPOSITION
C
C     *  NEW ESTIMATE OF THE DISTILLATE RATE USING SECANT METHOD
C        (IN CASE OF WET ALCOHOL PRODUCT)
C
C     *  NEW ESTIMATE OF THE DISTILLATE RATE BY HEURISTIC METHOD
C        (IN CASE OF DRY AND IMPURE ALCOHOL)
C
      COMMON  /BLANK/  NCR, NPRT, KEEPIT(22)
      COMMON  /CMPRO/  NK, NCM1, NCP1, IDLL, IDLV, IDH, LDBUG, ISW,
     *                 NDIM, ZNAME(2,10), L(10), NTCOMP(10), NLIQ, IPSET
      COMMON  /CONTL/  NIN,NOUT,NOCOMP,NE,NEN,KUNITS
      COMMON  /SYSC/   LA,LB,LC,LOOP,LOOPS
      COMMON  /SYSD/   KEFLAG(50),KSFLAG(100),KTRACE,DERROR,NPFREQ,
     *                 IPUNCH
      COMMON  /EQPA/   EQPAR(25,50),NEMAX,MAXEQP
      COMMON  /STRMIN/ SINUM(4),SIFLAG(4),SIVPFR(4),SITEMP(4),SIPRES(4),
     *                 SIENTH(4),SIVISC(4),SITHK(4),SIZ(4),SIS(4),
     *                 SIFRAL(4),SIMOLE(4),SICOMP(10,4),SIKV(10,4)
      COMMON  /STMOUT/ SONUM(4),SOFLAG(4),SOVPFR(4),SOTEMP(4),SOPRES(4),
     *                 SOENTH(4),SOVISC(4),SOTHK(4),SOZ(4),SOS(4),
     *                 SOFRAL(4),SOMOLE(4),SOCOMP(10,4),SOKV(10,4)
      REAL             SIDUM(4,12),SODUM(4,12),COMIN(10),ZF(10),XF(10)
      REAL             XBT(3), XBTSV(3)
      INTEGER          ISAVE(10)
      EQUIVALENCE      (SIDUM(1,1),SINUM(1)),(SODUM(1,1),SONUM(1))
      REAL             XBSET(3)/0.99, 5.0E-3, 0.01/
      REAL             XB(3)/0.99, 1.E-4, 0.01/
      REAL             XD(3)/0.28, 0.18, 0.54/
C
C          EQPAR(1,NE) = EQUIPMENT NUMBER
C          EQPAR(2,NE) = NUMBER OF STAGES IN STRIPPING SECTION
C          EQPAR(3,NE) = NUMBER OF STAGES IN RECTIFYING SECTION
C          EQPAR(4,NE) = TYPE OF UNIT
C          EQPAR(5,NE) = STAGE EFFICIENCY STRIPPING SECTION ... FRACTION
C          EQPAR(6,NE) = STAGE EFFICIENCY RECTIFYING SECTION ... FRACTION
C          EQPAR(7,NE) = TOP STAGE TEMPERATURE (DEG K)
C          EQPAR(8,NE) = BOTTOM STAGE TEMPERATURE (DEG K)
C          EQPAR(9,NE) = TOP STAGE PRESSURE (ATM)
C          EQPAR(10,NE) = BOTTOM STAGE PRESSURE (ATM)
C          EQPAR(11,NE) = TEMPERATURE TOLLERANCE (DEFAULT = 0.01)
C          EQPAR(12,NE) = FLOW TOLLERANCE (DEFAULT = 0.0005)
C          EQPAR(13,NE) = NUMBER OF FEEDS
C          EQPAR(14,NE) = STAGE NUMBER FOR THE 1ST FEED
C          EQPAR(15,NE) = STAGE NUMBER FOR THE 2ND FEED
C          EQPAR(16,NE) = STAGE NUMBER FOR THE 3RD FEED
C          EQPAR(17,NE) = STAGE NUMBER FOR THE 4TH FEED
C          EQPAR(18,NE) = SPECIFIED DISTILLATE VAPOR RATE, DESTV
C          EQPAR(19,NE) = SPECIFIED DISTILLATE LIQUID RATE, DESTL
C          EQPAR(20,NE) = REFLUX RATIO OR BOILUP RATIO
C          EQPAR(21,NE) = DISTILLATE CODE (IDCODE)
C                          -1 : SUBCOOLED LIQUID
C                           0 : VAPOR/LIQUID DISTILLATE
C                          +1 : LIQUID AT BUBBLE POINT
C          EQPAR(22,NE) = ITRMAX (MAXIMUM VALUE FOR ITERATIONS)
C          EQPAR(23,NE) = DISTILLATE VAPOR/(V+L) FRACTION
C          EQPAR(24,NE) = MAX ITERATION FOR ACTL BLOCK
```

```
C
C          INPUT VALUES    NCASE         DESCRIPTION
C               3            3      DISTILLATION COLUMN (RR SPECIFIED)
C               4            4      DISTILLATION COLUMN (BOILUP SPECIFIED)
C               5            5      SELF REFLUXING COLUMN (BOILUP SPECIFIED)
C               6            6      SELF REBOILING COLUMN (RR SPECIFIED)
C
C     IOK=0 SUCCESSFUL CALCULATIONS
C     IOK=1 EXCESS BENZENE IN THE BTMS (ACTION INC DIST RATE)
C     IOK=1 EXCESS WATER IN THE BTMS (ACTION DEC DIST RATE)
C
C     DO LOOP ON SODUM=SIDUM
C
      IF (LDBUG .GE. 1) WRITE (6,9999)
 9999 FORMAT(' ',30X,'SUBROUTINE ACTL')
C
C     IF (LDBUG .GE. 1) THEN
C        WRITE (NPRT,4)
C   4    FORMAT (/' PARAMETERS IN SUB. ACTL ARE:'/)
C        WRITE (NPRT,*) (C(J),J=1,12)
C        WRITE (NPRT,*) (ALPHA(J),J=1,6)
C     END IF
      IOK=0
      KNT=0
      DRATE=0
      ISW=0
      SUM1=0.0
      SUM2=0.0
C
      DO 30 I=1,NOCOMP
      XF(I)=0.0
      ZF(I)=0.0
   30 COMIN(I)=0.0
      DO 50 I=1,NOCOMP
      DO 50 J=1,NIN
      COMIN(I)=COMIN(I)+SICOMP(I,J)
   50 SOCOMP(I,J)=SICOMP(I,J)
C
C     DO 60 J=3,12
C     DO 60 I=1,NIN
C  60 SODUM(I,J)=SIDUM(I,J)
C
      DRATE=0.0
      FRATE=0.0
      DO 100 J=1,NIN
C     SOMOLE(J)=SIMOLE(J)
  100 FRATE=FRATE+SIMOLE(J)
C
      DO 150 I=1,NOCOMP
  150 XF(I)=COMIN(I)/FRATE
C
C     LOOP FOR NEW ESTIMATION OF DISTILLATE RATE BY CHANGING
C     XD(2) BECAUSE XB(2)=0.0, OTHERWISE SET NEW VALUES OF
C     OTHER XB'S AND XD'S
C     EQPAR(18,NE)/EQPAR(19,NE) INTITIALLY CARRIES FIRST GUESS
C
      KUNITS=EQPAR(25,NE)+0.1
      IF (KUNITS .EQ. 0) THEN
         DRATE=EQPAR(18,NE)+EQPAR(19,NE)
      ELSE
```

```
         DRATE=(EQPAR(18,NE)+EQPAR(19,NE))*453.59
      END IF
      KMAX=EQPAR(24,NE)+0.1
      DRSV=0.95*DRATE
      FXNSV=0.95*XB(2)-XBSET(2)
  155 CONTINUE
      SUM1=0.0
      SUM2=0.0
      SUM3=0.0
      DO 160 I=1,NOCOMP
      SUM1=SUM1+XF(I)
      SUM2=SUM2+XD(I)
      SUM3=SUM3+XB(I)
  160 CONTINUE
      DO 170 I=1,NOCOMP
      XF(I)=XF(I)/SUM1
      XD(I)=XD(I)/SUM2
      XB(I)=XB(I)/SUM3
  170 CONTINUE
C
      IF (LDBUG .GE. 1) THEN
         WRITE (NPRT,240)
  240    FORMAT (' SUB ACTL:FEED, DIST AND BTMS COMPOSITIONS '/)
         WRITE (NPRT,*) (XF(J),J=1,NOCOMP),(XD(J),J=1,NOCOMP),
     *   (XB(J),J=1,NOCOMP)
         WRITE (NPRT,*)
         WRITE (NPRT,250) DRATE, FRATE
  250    FORMAT (' CHECK IN ACTL: DRATE & FRATE ',2E20.8)
      END IF
C
  290 IF (FRATE-DRATE) 300,300,350
  300 DRATE=0.9*FRATE
      GO TO 290
C     WRITE (NPRT,310)
C 310 FORMAT ('0PROGRAM STOPPED ... DISTILLATE RATE TOO HIGH. READ
C    * PROPER VALUES OF XD & XB ARRAYS IN DCTL BLOCK ')
C     CALL EXIT
C     RETURN
C
  350 IF (EQPAR(21,NE)) 400,420,400
  400 EQPAR(18,NE)=0.0
      EQPAR(19,NE)=DRATE
      GO TO 500
  420 EQPAR(18,NE)=DRATE*EQPAR(23,NE)
      EQPAR(19,NE)=DRATE*(1.0-EQPAR(23,NE))
  500 IF (LDBUG .GE. 1) THEN
         WRITE (NPRT,550) EQPAR(18,NE),EQPAR(19,NE)
         WRITE (NPRT,*)
      END IF
  550 FORMAT (/' SUB CSPT: DESTV = ',E13.5,' & DESTL = ',E13.5)
C
      KUNITS=EQPAR(25,NE)+0.1
      IF (KUNITS .EQ. 0) GO TO 555
      EQPAR (18,NE)=EQPAR(18,NE)/453.59
      EQPAR (19,NE)=EQPAR(19,NE)/453.59
  555 CONTINUE
C
      CALL DIST
C     IF (KNT .GT. 0) CALL ZDIST
      WRITE (NPRT,578)
```

```
  578 FORMAT (' SUB ACTL STMT#578: RETURNED FROM DIST')
C
C     CHECK WHETHER THE BTMS COMPOSITION IS CORRECT
C     SOCOMP(I,2)
      DO 600 I=1,NOCOMP
  600 XBT(I)=SOCOMP(I,2)/SOMOLE(2)
C     DESIRED CONDITIONS
      IF (XBT(1) .GE. XBSET(1) .AND.
     %    XBT(2) .LE. XBSET(2) .AND.
     %    XBT(3) .LE. XBSET(3) .AND.
     %    XBT(2) .LE. XBT(3))  GO TO 700
C
C     LESS ETOH & MORE BZ IN BTMS
      IF (XBT(1) .LT. XBSET(1)) THEN
         IF (XBT(3) .GT. XBSET(3)) IOK=1
         IF (XBT(3) .GT. 0.02) IOK=10
         IF (XBT(3) .GT. 0.04) IOK=11
         IF (XBT(3) .GT. 0.10) IOK=12
      END IF
      IF (IOK .NE. 0) GO TO 605
C     LESS ETOH & MORE WATER IN BTMS
      IF (XBT(1) .LT. XBSET(1) .AND.
     %    XBT(2) .GT. XBSET(2)) IOK=2
C
C     LESS ETOH, MORE WATER & MORE BZ IN BTMS
      IF (IOK .NE. 0) GO TO 605
      IF (XBT(1) .LT. XBSET(1) .AND.
     %    XBT(2) .GT. XBSET(2) .AND.
     %    XBT(3) .LT. XBSET(3)) IOK=3
      IF (IOK .EQ. 0) GO TO 700
C
C     SECANT METHOD FOR NEW VALUE OF DRATE
  605 CONTINUE
      SUMA=0.0
      DO 610 I=1,NOCOMP
  610 SUMA=SUMA+XBT(I)
      DO 612 I=1,NOCOMP
  612 XBT(I)=XBT(I)/SUMA
      FXN=XBT(2)-XBSET(2)
      IF (IOK .EQ. 2 .OR. IOK .EQ. 3) THEN
         DELTA=-FXN*(DRATE-DRSV)/(FXN-FXNSV)
      END IF
      IF (IOK .EQ. 1) DELTA=0.0005*DRATE
      IF (IOK .EQ. 10) DELTA=0.01*DRATE
      IF (IOK .EQ. 11) DELTA=0.025*DRATE
      IF (IOK .EQ. 12) DELTA=0.05*DRATE
C
      FXNSV=FXN
      DRSV=DRATE
      DRATE=DRATE+DELTA
      KNT=KNT+1
      WRITE (NPRT,625) LOOP, KNT, IOK
  625 FORMAT (' IN ACTL: LOOP =',I3,' KNT =',I3,' IOK=',I3)
      IF (KNT .LE. KMAX) GO TO 155
      WRITE (NPRT,690)
  690 FORMAT (' ACTL CALCULATIONS INCOMPLETE/UNSATISFACTORY ')
      CALL EXIT
C
  700 WRITE (NPRT,710)
  710 FORMAT (' ACTL SUCCESSFULLY COMPLETED')
```

```
      RETURN
      END
      SUBROUTINE ADBF
C
C     THIS MODULE HAS BEEN EXPANDED TO TAKE CARE OF 13
C     DIFFERENT CASES BY CALLING SUBPROGRAM ANYONE, A GENERALIZED
C     FLASH ALGORITHM
C
      COMMON  /BLANK/  NCR, NPRT, KEEPIT(22)
      COMMON  /CONTL/  NIN,NOUT,NOCOMP,NE,NEN,KUNITS
      COMMON  /CMPRO/  NK, NCM1, NCP1, IDLL, IDLV, IDH, LDBUG, ISW,
     *                 NDIM, ZNAME(2,10), L(10), NTCOMP(10), NLIQ, IPSET
      COMMON  /SYSB/   KRET(66),KCNT,KDUM(4),IROMAN(56)
      COMMON  /SYSD/   KEFLAG(50),KSFLAG(100),KTRACE,DERROR,NPFREQ,
     *                 IPUNCH
      COMMON  /EQPA/   EQPAR(25,50),NEMAX,MAXEQP
      COMMON  /STRMIN/ SINUM(4),SIFLAG(4),SIVPFR(4),SITEMP(4),SIPRES(4),
     *                 SIENTH(4),SIVISC(4),SITHK(4),SIZ(4),SIS(4),
     *                 SIFRAL(4),SIMOLE(4),SICOMP(10,4),SIKV(10,4)
      COMMON  /STMOUT/ SONUM(4),SOFLAG(4),SOVPFR(4),SOTEMP(4),SOPRES(4),
     *                 SOENTH(4),SOVISC(4),SOTHK(4),SOZ(4),SOS(4),
     *                 SOFRAL(4),SOMOLE(4),SOCOMP(10,4),SOKV(10,4)
      COMMON  /STRM/   T, P, Z(10), Y(10), X(10), FRACV, ZVAP,
     *                 EK(10), VP(10), FUG(10), GAM(10), SVAP,
     *                 HOFZ, HVAP, HLIQ, DHV, XSH, NOBUB, NODEW
      COMMON  /TWOLQ/  X1(10), X2(10), DUMB1(40), DHL(2), HIDLL(2),
     +                 HREALL(2), FRACL, DUMB2(4)
      COMMON  /ZFEEDZ/ PF, TF, FEED(10), AAAA(3)
C
C         EQPAR(1,NE) = EQUIPMENT NUMBER
C         EQPAR(2,NE) = MODE OF FLASH CALCULATION
C
D     WRITE (6,9999)
 9999 FORMAT(' ',30X,'SUBROUTINE ADBF')
      IF (EQPAR(2,NE).LE.0.0 .OR. EQPAR(2,NE).GT.13.0) EQPAR(2,NE)=8.0
      MODE=EQPAR(2,NE)+0.1
C
C     NOUT=1 FOR MODE # 5 AND PRESET IN THE CALLING PROGRAM
C     NOUT=2 FOR MODE # 1, 3, 6, 11, 13
C     NOUT=3 FOR MODE # 2, 4, 7, 8, 9, 10, 12
C
C
C     OPTIONS AVAILABLE FOR TOTAL # OF OUTPUT STREAMS FROM THE
C     EQUIPMENT MODULE "ADBF" ARE: 1, 2 OR 3.
C
C     MODE=NTYPE
C
C       NTYPE    DESCRIPTION
C
C          1     DEW POINT TEMPERATURE
C          2     BUBBLE POINT TEMPERATURE (1/2 LIQ)
C          3     ALL VAPOR ENTHALPY WITH PRIOR DEW POINT
C          4     ALL LIQUID ENTHALPY WITH PRIOR BUBBLE POINT (1/2 LIQ)
C          5     ALL VAPOR ENTHALPY
C          6     ALL LIQUID ENTHALPY (1/2 LIQ)
C          7     ISOTHERMAL FLASH (1/2 LIQ)
C          8     ISOTHERMAL FLASH ... NO DEW/BUBBLE POINT (1/2 LIQ)
C          9     ADIABATIC FLASH (1/2 LIQ)
C         10     ADIABATIC FLASH ... NO DEW/BUBBLE POINT (1/2 LIQ)
C         11     DEW POINT PRESSURE
```

```
C         12     BUBBLE POINT PRESSURE (1/2 LIQUID)
C         13     LIQ - LIQ SEPERATION BELOW BUBBLE POINT (2 LIQ)
C
C     ONLY MODE=8, 10, 13 HAVE BEEN COMPLETELY ESTABLISHED
C
C
C
      SVNOUT=NOUT
      IF (NOUT .EQ. 1) GO TO 3
      NOUT=3
      IF (MODE .EQ. 5) NOUT=1
      IF (MODE .EQ. 6) NOUT=2
      IF (MODE .EQ. 1  .OR. MODE .EQ.  3) NOUT=2
      IF (MODE .EQ. 11 .OR. MODE .EQ. 13) NOUT=2
C
    3 P=SIPRES(1)
      T=SITEMP(1)
      DO 5 I=1,NOUT
      SIPRES(I)=P
      SOPRES(I)=P
      SITEMP(I)=T
    5 SOTEMP(I)=T
C
      HOFZ=SIENTH(1)/SIMOLE(1)
      FRACV=SIVPFR(1)
      FRACL=SIFRAL(1)
      DO 10 I=1,NOCOMP
   10 FEED(I)=SICOMP(I,1)
C
      IF (LDBUG .GE. 1) THEN
         WRITE (NPRT,12)
         WRITE (NPRT,*)  FRACV,FRACL,T,P,HOFZ,(FEED(J),J=1,NOCOMP)
   12    FORMAT (/' SUB ADBF AT FTN#12: FRACV/ FRACL / T / P /
     * HOFZ / FEED /'/)
      END IF
C
      CALL ANYONE (MODE)
C
      SIVPFR(1)=FRACV
      SIFRAL(1)=FRACL
      SIENTH(1)=(HVAP*FRACV+HREALL(1)*(1.0-FRACV)*FRACL+
     *           HREALL(2)*(1.0-FRACV)*(1.0-FRACL))*SIMOLE(1)
C
      IF (LDBUG .GE. 1) THEN
         WRITE (NPRT,15)
         WRITE (NPRT,*)  FRACV,FRACL,T,P,HOFZ,(FEED(J),J=1,NOCOMP)
   15    FORMAT (/' SUB ADBF AT FTN#15: FRACV/ FRACL / T / P /
     * HOFZ / FEED /'/)
      END IF
C
C     NOUT=1: OUTPUT STREAM COULD BE VAPOR+LIQUID+LIQUID
C
      IF (NOUT .EQ. 1) THEN
         SOTEMP(1)=T
         SOPRES(1)=P
         SOVPFR(1)=FRACV
         SOFRAL(1)=FRACL
         SOMOLE(1)=SIMOLE(1)
         SOENTH(1)=SIENTH(1)
         DO 20 I=1,NOCOMP
   20    SOCOMP(I,1)=SICOMP(I,1)
```

```
         GO TO 200
      END IF
C
C     NOUT=2 & MODE<>13:  OUTPUT STREAM (1) VAPOR & (2) 1/2 LIQUID
C     NOUT=2 & MODE=13 :  OUTPUT STREAMS ARE ONLY LIQUID
C                         (1) LIGHT PHASE
C                         (2) HEAVY PHASE
C
      IF (NOUT .EQ. 2) THEN
         GO TO (33,33,36,36,33,33,36,36,33,33,34,34,36), MODE
   33    SITEMP(1)=T
         SITEMP(2)=T
         SOTEMP(1)=T
         SOTEMP(2)=T
         GO TO 36
   34    SOPRES(1)=P
         SOPRES(2)=P
   36    CONTINUE
C
         IF (MODE .EQ. 13) THEN
            SOVPFR(1)=0.0
            SOVPFR(2)=0.0
            SOFRAL(1)=1.0
            SOFRAL(2)=1.0
            SOMOLE(1)=SIMOLE(1)*FRACL
            SOMOLE(2)=SIMOLE(1)*(1.0-FRACL)
            SOENTH(1)=HREALL(1)*SOMOLE(1)
            SOENTH(2)=HREALL(2)*SOMOLE(2)
            DO 38 I=1,NOCOMP
            SOCOMP(I,1)=X1(I)*SOMOLE(1)
   38       SOCOMP(I,2)=X2(I)*SOMOLE(2)
            GO TO 200
         ELSE
            SOVPFR(1)=1.0
            SOVPFR(2)=0.0
            SOFRAL(1)=0.0
            SOFRAL(2)=FRACL
            SOMOLE(1)=SIMOLE(1)*FRACV
            SOMOLE(2)=SIMOLE(1)*(1.0-FRACV)
            SOENTH(1)=HVAP*SOMOLE(1)
            SOENTH(2)=(HREALL(1)*FRACL+HREALL(2)*(1.0-FRACL))*SOMOLE(2)
            SOZ(1)=ZVAP
            DO 40 I=1,NOCOMP
            SOCOMP(I,1)=Y(I)*SOMOLE(1)
   40       SOCOMP(I,2)=(X1(I)*FRACL+X2(I)*(1.0-FRACL))*SOMOLE(2)
            GO TO 200
         END IF
      END IF
C
C     NOUT=3: 3 OUTPUT STREAM FROM THE EQUIPMENT
C     STRM*1 .. VAPOR / V
C     STRM*2 .. LIGHT LIQUID / EXTRACT / L1
C     STRM*3 .. HEAVY LIQUID / RAFFINATE / L2
C
      IF (NOUT .EQ. 3) THEN
         DO 56 I=1,NOUT
         GO TO (53,53,56,56,53,53,56,56,53,53,54,54,56), MODE
   53    SOTEMP(I)=T
         GO TO 56
   54    SOPRES(I)=P
```

```
   56   CONTINUE
        SOVPFR(1)=1.0
        SOFRAL(1)=0.0
        DO 60 I=2,3
        SOFRAL(I)=1.0
   60   SOVPFR(I)=0.0
C
        SOMOLE(1)=SIMOLE(1)*FRACV
        SOMOLE(2)=SIMOLE(1)*(1.0-FRACV)*FRACL
        SOMOLE(3)=SIMOLE(1)*(1.0-FRACV)*(1.0-FRACL)
        SOENTH(1)=HVAP*SOMOLE(1)
        SOENTH(2)=HREALL(1)*SOMOLE(2)
        SOENTH(3)=HREALL(2)*SOMOLE(3)
        SOZ(1)=ZVAP
        DO 70 I=1,NOCOMP
        SOCOMP(I,1)=Y(I)*SOMOLE(1)
        SOCOMP(I,2)=X1(I)*SOMOLE(2)
   70   SOCOMP(I,3)=X2(I)*SOMOLE(3)
        GO TO 200
      END IF
C
  200 CONTINUE
      NOUT=SVNOUT
      IF (KTRACE .LT. 2) GO TO 250
      WRITE (NPRT,210)
  210 FORMAT ('0 SUB ADBF AT STM*210 : NTYPE / NOUT / FRACV / FRACL /')
      WRITE (NPRT,*) MODE, NOUT, FRACV, FRACL
C
  250 RETURN
      END
      SUBROUTINE BCTL
C
C     BCTL BLOCK TAPS THE VALUES FROM THE REFERENCE STREAMS
C     [ + VE FOR INCOMING & - VE FOR OUTGOING STREAMS] AND
C     MAKE NEW ESTIMATE OF DISTILLATE OF THE TARGET DIST
C     BLOCK. AT PRESENT BLOCK IS DESIGNED FOR THE BENZENE
C     STRIPPING COLUMN.
C
      COMMON  /BLANK/  NCR, NPRT, KEEPIT(22)
      COMMON  /CMPRO/  NK, NCM1, NCP1, IDLL, IDLV, IDH, LDBUG, ISW,
     *                 NDIM, ZNAME(2,10), L(10), NTCOMP(10), NLIO, IPSET
      COMMON  /CONTL/  NIN,NOUT,NOCOMP,NE,NEN,KUNITS
      COMMON  /SYSC/   LA,LB,LC,LOOP,LOOPS
      COMMON  /SYSD/   KEFLAG(50),KSFLAG(100),KTRACE,DERROR,NPFREQ,
     *                 IPUNCH
      COMMON  /EQPA/   EQPAR(25,50),NEMAX,MAXEQP
      COMMON  /STMA/   SEXTSV(13,100),SINTSV(11,100),NSMAX,MAXSEX,MAXSIN
      COMMON  /STRMIN/ SINUM(4),SIFLAG(4),SIVPFR(4),SITEMP(4),SIPRES(4),
     *                 SIENTH(4),SIVISC(4),SITHK(4),SIZ(4),SIS(4),
     *                 SIFRAL(4),SIMOLE(4),SICOMP(10,4),SIKV(10,4)
      COMMON  /STMOUT/ SONUM(4),SOFLAG(4),SOVPFR(4),SOTEMP(4),SOPRES(4),
     *                 SOENTH(4),SOVISC(4),SOTHK(4),SOZ(4),SOS(4),
     *                 SOFRAL(4),SOMOLE(4),SOCOMP(10,4),SOKV(10,4)
      REAL             SIDUM(4,12),SODUM(4,12),COMIN(10),DR(10),XF(10)
      INTEGER          ISAVE(10), ISTRM(4), ICOMP(3)
      EQUIVALENCE      (SIDUM(1,1),SINUM(1)),(SODUM(1,1),SONUM(1))
      DATA             K, MAXDSP /0, 10/
      REAL             XB(3)/0.995, 1.E-5, 0.005/
      REAL             XD(3)/0.31642, 0.14041, 0.54317/
C
```

```
C     EQPAR(1,NE) = BLOCK/NODE #
C     EQPAR(2,NE) = DISTILLATION COLUMN BLOCK/NODE #
C     EQPAR(3,NE) = CODE FOR DIST STREAM TYPE
C            (-1:SUBCOOLED LIQUID, 0:VAPOR/LIQUID, +1:LIQ AT BUB T)
C     EQPAR(4,NE) = DISTILLATE VAPOR/(V+L) FRACTION
C     EQPAR(5,NE) = REFERENCE STREAM # 1
C     EQPAR(6,NE) = REFERENCE STREAM # 2
C     EQPAR(7,NE) = REFERENCE STREAM # 3
C     EQPAR(8,NE) = REFERENCE STREAM # 4
C
C     EQPAR(9,NE) = REFERENCE COMPONENT # 1
C     EQPAR(10,NE) = REFERENCE COMPONENT # 2
C     EQPAR(11,NE) = REFERENCE COMPONENT # 3
C     EQPAR(12,NE) = REFERENCE COMPONENT # 4
C
C     EQPAR(13,NE) TO  EQPAR(25,NE) = 0.0
C
C     LOAD THE OUTPUT STREAM WITH THE INPUT STREAM
C
C     DO LOOP ON SODUM=SIDUM
C
      DO 30 I=1,NOCOMP
      XF(I)=0.0
      DR(I)=0.0
   30 COMIN(I)=0.0
      ITAG1=0
      IF (EQPAR(9,NE) .LT. 0.0) ITAG1=1
      DO 50 I=1,NOCOMP
      DO 50 J=1,NIN
      COMIN(I)=COMIN(I)+SICOMP(I,J)
   50 SOCOMP(I,J)=SICOMP(I,J)
C
      DO 60 J=3,12
      DO 60 I=1,NIN
   60 SODUM(I,J)=SIDUM(I,J)
C
      DO 70 I=1,4
      IF (EQPAR(I+4,NE) .NE. 0.0) THEN
         ISTRM(I)=SIGN(ABS(EQPAR(I+4,NE))+0.1,EQPAR(I+4,NE))
         END IF
   70 CONTINUE
      DO 80 I=1,3
   80 ICOMP(I)=EQPAR(I+8,NE)+0.1
C
C     COMPUTE BTMS RATE OF 1 AND 2 BY ESTABLISHING MASS
C     BALANCE BASED UPON THE REFERENCE STREAMS
C
      B1=0
      B2=0
      DO 85 I=1,4
      J1=ICOMP(1)
      J2=ICOMP(2)
      IF (ISTRM(I) .GT. 0) THEN
         IF (SEXTSV(J1+3,ISTRM(I)) .GT. 0.0 .AND.
     %      (SEXTSV(J2+3,ISTRM(I)) .GT. 0.0) ) THEN
            B1=B1+SEXTSV(J1+3,ISTRM(I))
            B2=B2+SEXTSV(J2+3,ISTRM(I))
          END IF
      ELSE IF (ISTRM(I) .LT. 0) THEN
            ITEMP=IABS(ISTRM(I))
```

```
            IF (SEXTSV(J1+3,ITEMP) .GT. 0.0 .AND.
     %         (SEXTSV(J2+3,ITEMP) .GT. 0.0) ) THEN
               B1=B1-SEXTSV(J1+3,ITEMP)
               B2=B2-SEXTSV(J2+3,ITEMP)
            END IF
      END IF
C
   85 CONTINUE
C
C     COMPUTATION OF COMPONENTIAL DISTILLATE RATE
C
      IF (B1 .LT. 0.0) B1=0.0
      IF (B2 .LT. 0.0) B2=0.0
      D1=COMIN(1)-B1
      D2=COMIN(2)-B2
      D3=COMIN(3)
      DRATE=D1+D2+D3
      WRITE (NPRT,90) B1, B2
   90 FORMAT (' SUB BCTL: ESTIMATED B1 AND B2 FOR BZ
     % STRIPPING COLUMN ARE '/2E25.8)
C
C     THIS IS FOR THE 1 ST ENTRY IN BCTL BECAUSE
C     SEXTSV ARRAY IS CLEAN IF THE REFERENCE STREAMS ARE
C     NOT YET PROCESSED FOR A SINGLE TIME.
C
      IF (DRATE .EQ. 0.0) DRATE=2*COMIN(3)
C
      IF (ITAG1 .EQ. 1) GO TO 350
      FRATE=0.0
      DO 100 J=1,NIN
      SOMOLE(J)=SIMOLE(J)
  100 FRATE=FRATE+SIMOLE(J)
C
C
      IF (LDBUG .GE. 1) THEN
         WRITE (NPRT,240)
  240    FORMAT (' SUB BCTL:FEED, DIST AND BTMS COMPOSITIONS '/)
         WRITE (NPRT,*) (XF(J),J=1,NOCOMP),(XF(J),J=1,NOCOMP),
     *   (XF(J),J=1,NOCOMP)
         WRITE (NPRT,*)
         WRITE (NPRT,250) DRATE, FRATE, B1, B2
  250    FORMAT (' CHECK IN BCTL: DRATE / FRATE / B1 / B2'/4E16.5)
      END IF
C
      IF (FRATE-DRATE) 300,300,350
  300 WRITE (NPRT,310)
  310 FORMAT ('0PROGRAM STOPPED ... DISTILLATE RATE TOO HIGH. READ
     * PROPER VALUES OF XD & XB ARRAYS IN DCTL BLOCK ')
      CALL EXIT
      RETURN
C
C     DIST RATE ASSIGNED TO EQPAR OF THE PROPER DISTILLATION BLOCK
C     UNITS OF EQPAR AND DRATE ARE DIFFERENT
C
C     ISAVE ARRAY STORES THE DIST COLUMN BLOCK # WHICH HAS BEEN
C     PROCESSED ONCE. SECOND TIME, FOR THE SAME BLOCK #, UNITS
C     OF EQPAR(18,NE) & EQPAR(19,NE) REMAIN UNCHANGED.
C
  350 II=EQPAR(2,NE)+0.1
      IF (ITAG1 .EQ. 1) GO TO 500
```

```
      IF (EQPAR(3,NE)) 400,420,400
  400 EQPAR(18,II)=0.0
      EQPAR(19,II)=DRATE
      GO TO 500
  420 EQPAR(18,II)=DRATE*EQPAR(4,NE)
      EQPAR(19,II)=DRATE*(1.0-EQPAR(4,NE))
  500 IF (LDBUG .GE. 1) THEN
         WRITE (NPRT,550) EQPAR(18,II),EQPAR(19,II)
         WRITE (NPRT,*)
      END IF
  550 FORMAT (/' SUB DSPT: DESTV = ',E13.5,' & DESTL = ',E13.5)
C
C     DSPMAX IS THE MAX # OF DSPT MODULES IN A FLOWSCHEME
C
  560 K=K+1
      IF (K .GE. MAXDSP) GO TO 700
      DO 570 I=K,MAXDSP
  570 ISAVE(I)=0
      ITAG=0
C
      DO 580 I=1,K
  580 IF (II .EQ. ISAVE(I)) ITAG=1
      IF (ITAG  .EQ. 1) GO TO 700
      ISAVE(K)=II
      IF (ITAG1 .EQ. 1) GO TO 700
      EQPAR (18,II)=EQPAR(18,II)/453.59
      EQPAR (19,II)=EQPAR(19,II)/453.59
C
  700 RETURN
      END
      SUBROUTINE BZTL
C
C     BZTL BLOCK TAPS THE VALUES FROM THE REFERENCE STREAMS
C     [ + VE FOR INCOMING & - VE FOR OUTGOING STREAMS] AND
C     MAKE INITIAL ESTIMATE OF THE DISTILLATE RATE OF THE
C     SPECIFIED DISTILLATION BLOCK. FURTHER ESTIMATES OF
C     THE DISTILLATE RATE ARE BASED ON THE REQUIRED MATERIAL
C     BALANCE. AT PRESENT THIS BLOCK IS DESIGNED FOR THE BENZENE
C     STRIPPING COLUMN AND CAN BE EASILY EXTENDED TO ANY TYPE OF
C     DISTILLATION COLUMN.
C
      COMMON  /BLANK/  NCR, NPRT, KEEPIT(22)
      COMMON  /CMPRO/  NK, NCM1, NCP1, IDLL, IDLV, IDH, LDBUG, ISW,
     *                 NDIM, ZNAME(2,10), L(10), NTCOMP(10), NLIQ, IPSET
      COMMON  /CONTL/  NIN,NOUT,NOCOMP,NE,NEN,KUNITS
      COMMON  /SYSC/   LA,LB,LC,LOOP,LOOPS
      COMMON  /SYSD/   KEFLAG(50),KSFLAG(100),KTRACE,DERROR,NPFREC,
     *                 IPUNCH
      COMMON  /EQPA/   EQPAR(25,50),NEMAX,MAXEQP
      COMMON  /STMA/   SEXTSV(13,100),SINTSV(11,100),NSMAX,MAXSEX,MAXSIN
      COMMON  /STRMIN/ SINUM(4),SIFLAG(4),SIVPFR(4),SITEMP(4),SIPRES(4),
     *                 SIENTH(4),SIVISC(4),SITHK(4),SIZ(4),SIS(4),
     *                 SIFRAL(4),SIMOLE(4),SICOMP(10,4),SIKV(10,4)
      COMMON  /STMOUT/ SONUM(4),SOFLAG(4),SOVPFR(4),SOTEMP(4),SOPRES(4),
     *                 SOENTH(4),SOVISC(4),SOTHK(4),SOZ(4),SOS(4),
     *                 SOFRAL(4),SOMOLE(4),SOCOMP(10,4),SOKV(10,4)
      REAL             SIDUM(4,12),SODUM(4,12),COMIN(10),DR(10),XF(10)
      INTEGER          ISAVE(10), ISTRM(4)
      EQUIVALENCE      (SIDUM(1,1),SINUM(1)),(SODUM(1,1),SONUM(1))
      DATA             K, ISV, ERROR /0, 0, 0.01/
```

```
      DATA                BTM1, BTM2 / 10.995, 17.2726/
      INTEGER             ICOMP(3)/ 1, 2, 0/
C
C
C         EQPAR(1,NE) = EQUIPMENT NUMBER
C         EQPAR(2,NE) = NUMBER OF STAGES IN STRIPPING SECTION
C         EQPAR(3,NE) = NUMBER OF STAGES IN RECTIFYING SECTION
C         EQPAR(4,NE) = TYPE OF UNIT
C         EQPAR(5,NE) = STAGE EFFICIENCY STRIPPING SECTION ... FRACTION
C         EQPAR(6,NE) = STAGE EFFICIENCY RECTIFYING SECTION ... FRACTION
C         EQPAR(7,NE) = TOP STAGE TEMPERATURE (DEG K)
C         EQPAR(8,NE) = BOTTOM STAGE TEMPERATURE (DEG K)
C         EQPAR(9,NE) = TOP STAGE PRESSURE (ATM)
C         EQPAR(10,NE) = BOTTOM STAGE PRESSURE (ATM)
C         EQPAR(11,NE) = TEMPERATURE TOLLERANCE (DEFAULT = 0.01)
C         EQPAR(12,NE) = FLOW TOLLERANCE (DEFAULT = 0.0005)
C         EQPAR(13,NE) = NUMBER OF FEEDS
C         EQPAR(14,NE) = STAGE NUMBER FOR THE 1ST FEED
C         EQPAR(15,NE) = REFERENCE STREAM # 1
C         EQPAR(16,NE) = REFERENCE STREAM # 2
C         EQPAR(17,NE) = REFERENCE STREAM # 3
C         EQPAR(18,NE) = SPECIFIED DISTILLATE VAPOR RATE, DESTV
C         EQPAR(19,NE) = SPECIFIED DISTILLATE LIQUID RATE, DESTL
C         EQPAR(20,NE) = REFLUX RATIO OR BOILUP RATIO
C         EQPAR(21,NE) = DISTILLATE CODE (IDCODE)
C                        -1 : SUBCOOLED LIQUID
C                         0 : VAPOR/LIQUID DISTILLATE
C                        +1 : LIQUID AT BUBBLE POINT
C         EQPAR(22,NE) = ITRMAX (MAXIMUM VALUE FOR ITERATIONS)
C         EQPAR(23,NE) = DISTILLATE VAPOR/(V+L) FRACTION
C
C         INPUT VALUES    NCASE        DESCRIPTION
C              3            3     DISTILLATION COLUMN (RR SPECIFIED)
C              4            4     DISTILLATION COLUMN (BOILUP SPECIFIED)
C              5            5     SELF REFLUXING COLUMN (BOILUP SPECIFIED)
C              6            6     SELF REBOILING COLUMN (RR SPECIFIED)
C
C     IOK=0 SUCCESSFUL CALCULATIONS
C     IOK=1 EXCESS BENZENE IN THE BTMS (ACTION INC DIST RATE)
C     IOK=1 EXCESS WATER IN THE BTMS (ACTION DEC DIST RATE)
C
C
      IF (LDBUG .GE. 1) WRITE (6,9999)
 9999 FORMAT(' ',30X,'SUBROUTINE BZTL')
      ISV=0
C
C     IF (LDBUG .GE. 1) THEN
C        WRITE (NPRT,4)
C   4    FORMAT (/' PARAMETERS IN SUB. ACTL ARE:'/)
C        WRITE (NPRT,*) (C(J),J=1,12)
C        WRITE (NPRT,*) (ALPHA(J),J=1,6)
C     END IF
      DO 30 I=1,NOCOMP
   30 COMIN(I)=0.0
      DO 50 I=1,NOCOMP
      DO 50 J=1,NIN
   50 COMIN(I)=COMIN(I)+SICOMP(I,J)
C  50 SOCOMP(I,J)=SICOMP(I,J)
C
C     DO 60 J=3,12
```

```
C     DO 60 I=1,NIN
C  60 SDDUM(I,J)=SIDUM(I,J)
C
      DO 70 I=1,3
      IF (EQPAR(I+14,NE) .NE. 0.0) THEN
         ISTRM(I)=SIGN(ABS(EQPAR(I+14,NE))+0.1,EQPAR(I+14,NE))
         END IF
   70 CONTINUE
C
C     IN CASE THE BLOCK IS USED STAND ALONE
      KOUNT=0
      DO 75 I=1,3
   75 IF (ISTRM(I) .EQ. 0) KOUNT=KOUNT+1
C     ALL STREAM NUMBERS ARE 0
      IF (KOUNT .EQ. 3) THEN
         B1=BTM1*453.59
         B2=BTM2*453.59
         GO TO 85
      END IF

C     DO 80 I=1,3
C  80 ICOMP(I)=EQPAR(I+8,NE)+0.1
C
C     COMPUTE BTMS RATE OF 1 AND 2 BY ESTABLISHING MASS
C     BALANCE BASED UPON THE REFERENCE STREAMS
C
      B1=0
      B2=0
      DO 85 I=1,4
      J1=ICOMP(1)
      J2=ICOMP(2)
      IF (ISTRM(I) .GT. 0) THEN
         IF (SEXTSV(J1+3,ISTRM(I)) .GT. 0.0 .AND.
     %      (SEXTSV(J2+3,ISTRM(I)) .GT. 0.0) ) THEN
            B1=B1+SEXTSV(J1+3,ISTRM(I))
            B2=B2+SEXTSV(J2+3,ISTRM(I))
          END IF
      ELSE IF (ISTRM(I) .LT. 0) THEN
            ITEMP=IABS(ISTRM(I))
            IF (SEXTSV(J1+3,ITEMP) .GT. 0.0 .AND.
     %         (SEXTSV(J2+3,ITEMP) .GT. 0.0) ) THEN
               B1=B1-SEXTSV(J1+3,ITEMP)
               B2=B2-SEXTSV(J2+3,ITEMP)
            END IF
      END IF
C
   85 CONTINUE
C
C     COMPUTATION OF COMPONENTIAL DISTILLATE RATE
C
C     IF (B1 .LT. 0.0) B1=0.0
C     IF (B2 .LT. 0.0) B2=0.0
      D1=COMIN(1)-B1
      D2=COMIN(2)-B2
      D3=COMIN(3)
      DRATE=D1+D2+D3
      DRMIN=COMIN(3)
      WRITE (NPRT,90) B1, B2
   90 FORMAT (' SUB BZTL: ESTIMATED B1 AND B2 FOR BZ
     % STRIPPING COLUMN ARE '/2E25.8)
```

```
C
C     THIS IS FOR THE 1 ST ENTRY IN BCTL BECAUSE
C     SEXTSV ARRAY IS CLEAN IF THE REFERENCE STREAMS ARE
C     NOT YET PROCESSED FOR A SINGLE TIME.
C
      IF (DRATE .EQ. 0.0) DRATE=2*COMIN(3)
C
      FRATE=0.0
      DO 100 J=1,NIN
C     SOMOLE(J)=SIMOLE(J)
  100 FRATE=FRATE+SIMOLE(J)
C
C
      IF (LDBUG .GE. 1) THEN
C        WRITE (NPRT,240)
C 240    FORMAT (' SUB BZTL:FEED, DIST AND BTMS COMPOSITIONS '/)
C        WRITE (NPRT,*) (XF(J),J=1,NOCOMP),(XD(J),J=1,NOCOMP),
C    *   (XB(J),J=1,NOCOMP)
         WRITE (NPRT,*)
         WRITE (NPRT,250) DRATE, FRATE, B1, B2, (COMIN(I),I=1,NOCOMP)
  250    FORMAT (' CHECK IN BZTL: DRATE / FRATE / B1 / B2 / COMIN'/
     *   4E16.5/5E16.5)
      END IF
C
C     SETTING MAX AND MIN DIST RATES W.R.T. BENZENE SPECS IN THE
C     DISTILLATE/BOTTOMS
C     MAX RATE: 0.98*FRATE (ARBITRARY) OR COMPUTE BASED UPON
C               BZ SPECS
C     MIN RATE: DIST RATE (WITH BZ IN DIST=0.995 TO 0.997
C                          OF ENTERING BZ)
C     IF MIN RATE DOES NOT SATISFY THE ETHANOL SPECS IN BOTTOMS,
C     SEARCH FOR DIST RATE BETWEEN MIN AND MAX RATES FIXED.
C     IF ETOH SPECS ARE NOT MET, SELECT MIN DIST RATE FOR
C     SEPERATION.
C     LOOP STARTS HERE
      KNT=0
      DRSV=0.9*DRATE
  275 IF (FRATE-DRATE) 300,300,350
  300 DRATE=0.9*FRATE
      GO TO 275
C     WRITE (NPRT,310)
C 310 FORMAT ('0PROGRAM STOPPED ... DISTILLATE RATE TOO HIGH. READ
C    * PROPER VALUES OF XD & XB ARRAYS IN DCTL BLOCK ')
C     CALL EXIT
C     RETURN
C
C
  350 IF (EQPAR(21,NE)) 400,420,400
  400 EQPAR(18,NE)=0.0
      EQPAR(19,NE)=DRATE
      GO TO 500
  420 EQPAR(18,NE)=DRATE*EQPAR(23,NE)
      EQPAR(19,NE)=DRATE*(1.0-EQPAR(23,NE))
  500 IF (LDBUG .GE. 1) THEN
         WRITE (NPRT,550) EQPAR(18,NE),EQPAR(19,NE)
         WRITE (NPRT,*)
      END IF
C
      KUNITS=EQPAR(25,NE)+0.1
      IF (KUNITS .EQ. 0) GO TO 575
```

```
      EQPAR (18,NE)=EQPAR(18,NE)/453.59
      EQPAR (19,NE)=EQPAR(19,NE)/453.59
  575 CONTINUE
C
      CALL DIST
      IF (KNT .EQ. 0) FXSV=0.9*(SOCOMP(ICOMP(1),2)-B1)
C     IF (KNT .GT. 0) CALL ZDIST
      WRITE (NPRT,578)
  578 FORMAT (' SUB BZTL STMT#578: RETURNED FROM DIST')
C
C     CHECK WHETHER THE BTMS COMPOSITION IS CORRECT
C     SOCOMP(I,2)
      IF (LDBUG .GE. 1) THEN
         WRITE (NPRT,550) EQPAR(18,NE), EQPAR(19,NE)
         WRITE (NPRT,*)
      END IF
  550 FORMAT (/' SUB DSPT: DESTV = ',E13.5,' & DESTL = ',E13.5)
      IOK=0
      XD3=ABS(COMIN(3)-SOCOMP(3,1))/COMIN(3)
C
C     IF (XD3 .GE. 0.995 .AND. XD3 .LE. 0.997) DRMIN=DRATE
C     IF (SOCOMP(3,2) .GT. ERROR) IOK=3
C     IF (IOK .NE. 0) GO TO 600
C     IF (KNT .LE. 10) THEN
C        FX=SOCOMP(1,2)-B1
C     ELSE
C        FX=SOCOMP(3,2)
C     END IF
C
      FX=SOCOMP(1,2)-B1
      IF (FX-ERROR) 580,600,585
  580 IOK=2
      GO TO 600
  585 IOK=1
C
  600 IF (IOK .EQ. 0) GO TO 700
      IF (KNT .GT. 10 .AND. (IOK .EQ. 2 .AND. ISV .EQ. 3)) GO TO 700
      ISV=IOK
C     SECANT METHOD FOR NEW GUESS OF DRATE
C     OBJ FUNC IS CHANGED AFTER KNT>10
      IF (IOK .EQ. 1 .OR. IOK .EQ. 2) THEN
          DELTA=-(DRATE-DRSV)*FX/(FX-FXSV)
      END IF
      IF (IOK .EQ. 3) DELTA=0.08*DRATE
      FXSV=FX
      DRSV=DRATE
      DRATE=DRATE+DELTA
      IF (DRATE .LT. DRMIN) DRATE=DRMIN
      KNT=KNT+1
      WRITE (NPRT,625) LOOP, KNT, IOK, DRMIN, DRSV, DRATE, DMULT
  625 FORMAT (' IN BZTL: LOOP =',I3,' KNT =',I3,' IOK=',I3/
     *' DRMIN = ',G10.5,2X,' DRSV = ',G10.5,2X,
     *' DRATE = ',G10.5,2X,' DMULT = ',G10.5)
      IF (ABS((DRSV-DRATE)/DRSV) .LT. 1.0E-4) GO TO 700
      IF (KNT .LE. 20) GO TO 275
      WRITE (NPRT,690)
  690 FORMAT (' BZTL STOPPED: ITERATION LIMIT EXCEEDED')
      CALL EXIT
C
  700 WRITE (NPRT,710)
```

```
  710 FORMAT (' BZTL SUCCESSFULLY COMPLETED')
C
      RETURN
      END
      SUBROUTINE CNTL
C
C     OPTIONS IN CNTL
C     1. MANIPULATION OF THE COMPONENTIAL FLOW OF THE TARGET STREAM
C        BASED UPON DIFFERENCE IN TWO RATES
C     2. MANIPULATION OF THE COMPONENTIAL FLOW OF THE TARGET STREAM
C        BASED UPON RATIOS OF TWO STREAM RATES
C
C     THIS BLOCK USES SECOND STREAM AS THE TARGET STREAM, THE
C     COMP FLOW IS CHANGED WITH REFERENCE TO THE FIRST INCOMING
C     STREAM.
C
      COMMON  /BLANK/  NCR, NPRT, KEEPIT(22)
      COMMON  /CMPRO/  NK, NCM1, NCP1, IDLL, IDLV, IDH, LDBUG, ISW,
     *                 NDIM, ZNAME(2,10), L(10), NTCOMP(10), NLIQ, IPSET
      COMMON  /CONTL/  NIN,NOUT,NOCOMP,NE,NEN,KUNITS
      COMMON  /SYSC/   LA,LB,LC,LOOP,LOOPS
      COMMON  /SYSD/   KEFLAG(50),KSFLAG(100),KTRACE,DERROR,NPFREQ,
     *                 IPUNCH
      COMMON  /EQPA/   EQPAR(25,50),NEMAX,MAXEQP
      COMMON  /STRMIN/ SINUM(4),SIFLAG(4),SIVPFR(4),SITEMP(4),SIPRES(4),
     *                 SIENTH(4),SIVISC(4),SITHK(4),SIZ(4),SIS(4),
     *                 SIFRAL(4),SIMOLE(4),SICOMP(10,4),SIKV(10,4)
      COMMON  /STMOUT/ SONUM(4),SOFLAG(4),SOVPFR(4),SOTEMP(4),SOPRES(4),
     *                 SOENTH(4),SOVISC(4),SOTHK(4),SOZ(4),SOS(4),
     *                 SOFRAL(4),SOMOLE(4),SOCOMP(10,4),SOKV(10,4)
      REAL             SIDUM(4,12), SODUM(4,12), SIC(12), SID(12)
      INTEGER          ISAVE(10)
      EQUIVALENCE      (SIDUM(1,1),SINUM(1)),(SODUM(1,1),SONUM(1))
      DATA             K, MAXDSP /0, 10/
      DATA             RMIN, RMAX /1.05, 2.12/
C
C     EQPAR(1,NE) = BLOCK/NODE #
C     EQPAR(2,NE) = OPTION #
C     EQPAR(3,NE)= COMPONENT # TO BE CONTROLLED
C     EQPAR(4,NE) = MIN RATIO FOR OPTION 2
C     EQPAR(5,NE) = MAX RATIO FOR OPTION 2
C     EQPAR(6,NE) = MAX FLOW OF COMPONENT # IN EQPAR(3,NE)
C     EQPAR(7,NE) THRU EQPAR(25,NE) = 0.0
C
C     LOAD THE OUTPUT STREAM WITH THE INPUT STREAM
C
C     DO LOOP ON SODUM=SIDUM
      KUNITS=EQPAR(25,NE)+0.1
      IF (KUNITS .EQ. 0) GO TO 10
      EQPAR(6,NE)=EQPAR(6,NE)*453.59
      EQPAR(25,NE)=0.0
   10 CONTINUE
C
      IF (EQPAR(2,NE) .EQ. 2.0) GO TO 250
C
C     OPTION 1
C
      ICOMP=EQPAR(3,NE)+0.1
      IF (SICOMP(ICOMP,1) .EQ. 0.0) GO TO 350
      DIFF=SICOMP(ICOMP,1)-SICOMP(ICOMP,2)
```

```
      SOCOMP(ICOMP,2)=SICOMP(ICOMP,2)+DIFF
      IF (SOCOMP(ICOMP,2) .GT. EQPAR(6,NE)) SOCOMP(ICOMP,2)=EQPAR(6,NE)
      SUM=0.0
      DO 150 J=1,NOCOMP
      SICOMP(J,2)=SOCOMP(J,2)
  150 SUM=SUM+SOCOMP(J,2)
      SOMOLE(2)=SUM
      SIMOLE(2)=SUM
      GO TO 350
C
C     OPTION 2
C
  250 IF (EQPAR(4,NE) .NE. 0.0) RMIN=EQPAR(4,NE)
      IF (EQPAR(5,NE) .NE. 0.0) RMAX=EQPAR(5,NE)
  275 RATIO=SOMOLE(1)/SOMOLE(2)
      IF (RATIO .LT. RMIN) THEN
         SUM=0.0
         DO 280 I=1,NOCOMP
         SOCOMP(I,2)=0.99*SOCOMP(I,2)
  280    SUM=SUM+SOCOMP(I,2)
         SOMOLE(2)=SUM
         GO TO 275
      ELSE
         IF (RATIO .GE. RMAX) THEN
            SUM=0.0
            DO 300 I=1,NOCOMP
            SOCOMP(I,2)=1.01*SOCOMP(I,2)
  300       SUM=SUM+SOCOMP(I,2)
            SOMOLE(2)=SUM
            GO TO 275
         END IF
      END IF
C
  350 CONTINUE
C     ESTABLISHING STREAM # 2 VIA ISOTHERMAL FLASH
C
      ESAVE=EQPAR(2,NE)
      NSAVE=NOUT
      DO 360 I=3,12
      SID(I)=SIDUM(1,I)
  360 SIDUM(1,I)=SIDUM(2,I)
      DO 370 I=1,NOCOMP
      SIC(I)=SICOMP(I,1)
  370 SICOMP(I,1)=SICOMP(I,2)
C
      EQPAR(2,NE)=8.0
      NOUT=1
      CALL ADBF
C     RESTORE THE STREAM VARIABLES
      EQPAR(2,NE)=ESAVE
      NOUT=NSAVE
      DO 372 I=3,12
      SIDUM(2,I)=SODUM(1,I)
  372 SIDUM(1,I)=SID(I)
      DO 374 I=1,NOCOMP
      SICOMP(I,2)=SOCOMP(I,1)
  374 SICOMP(I,1)=SIC(I)
C
      DO 380 J=3,12
      DO 380 I=1,NIN
```

```
  380 SODUM(I,J)=SIDUM(I,J)
      DO 390 I=1,NIN
      DO 390 J=1,NOCOMP
  390 SOCOMP(J,I)=SICOMP(J,I)
      IF (LDBUG .GE. 1) WRITE (6,400) ICOMP, SICOMP(ICOMP,2),
     * SOCOMP(ICOMP,2)
  400 FORMAT (/' IN SUB CNTL: ICOMP, SICOMP & SOCOMP OF (ICOMP,2)
     * ARE '/I5,2E15.5)
  900 RETURN
      END
      SUBROUTINE DCTL
C
C     DCTL DYNAMICALLY SIMULATES THE FEED-FORWARD CONTROL
C     OF THE SPLIT IN AN AZEOTROPIC DISTILLATION COLUMN
C     BASED UPON THE COMPOSITE FEED COMPOSITION AND RATE
C     AND THE ASSUMED DISTILLATE AND BOTTOMS COMPOSITION.
C     THIS BLOCK CAN BE EASILY EXTENDED TO ANY DISTILLATION
C     COLUMN.
C
      COMMON  /BLANK/   NCR, NPRT, KEEPIT(22)
      COMMON  /CMPRO/   NK, NCM1, NCP1, IDLL, IDLV, IDH, LDBUG, ISW,
     *                  NDIM, ZNAME(2,10), L(10), NTCOMP(10), NLIQ, IPSET
      COMMON  /CONTL/   NIN,NOUT,NOCOMP,NE,NEN,KUNITS
      COMMON  /SYSC/    LA,LB,LC,LOOP,LOOPS
      COMMON  /SYSD/    KEFLAG(50),KSFLAG(100),KTRACE,DERROR,NPFREQ,
     *                  IPUNCH
      COMMON  /EQPA/    EQPAR(25,50),NEMAX,MAXEQP
      COMMON  /STRMIN/  SINUM(4),SIFLAG(4),SIVPFR(4),SITEMP(4),SIPRES(4),
     *                  SIENTH(4),SIVISC(4),SITHK(4),SIZ(4),SIS(4),
     *                  SIFRAL(4),SIMOLE(4),SICOMP(10,4),SIKV(10,4)
      COMMON  /STMOUT/  SONUM(4),SOFLAG(4),SOVPFR(4),SOTEMP(4),SOPRES(4),
     *                  SOENTH(4),SOVISC(4),SOTHK(4),SOZ(4),SOS(4),
     *                  SOFRAL(4),SOMOLE(4),SOCOMP(10,4),SOKV(10,4)
      REAL              SIDUM(4,12),SODUM(4,12),COMIN(10),DR(10),XF(10)
      REAL              XD(3), XB(3)
      INTEGER           ISAVE(10)
      EQUIVALENCE       (SIDUM(1,1),SINUM(1)),(SODUM(1,1),SONUM(1))
      DATA              K, MAXDSP /0, 10/
C     REAL              XB(3)/0.995, 1.E-5, 0.005/
C     REAL              XD(3)/0.31642, 0.14041, 0.54317/
C
C     EQPAR(1,NE) = BLOCK/NODE #
C     EQPAR(2,NE) = DISTILLATION COLUMN BLOCK/NODE #
C     EQPAR(3,NE) = CODE FOR DIST STREAM TYPE
C            (-1:SUBCOOLED LIQUID, 0:VAPOR/LIQUID, +1:LIQ AT BUB T)
C     EQPAR(4,NE) = DISTILLATE VAPOR/(V+L) FRACTION
C
C     EQPAR(5,NE) THRU EQPAR(NOCOMP+4,NE)           = XD (I), I=1,NOCOMP
C     EQPAR(NOCOMP+5,NE) THRU EQPAR(2*NOCOMP+4,NE) = XB (I), I=1,NOCOMP
C                 XD AND XB ARE GUESSED VALUES OF DISTILLATE
C                 AND BOTTOMS COMPONENT MOLE FRACTIONS
C     IF EQPAR(5,NE) >= 2.0 THEN DEFAULT VALUES ARE USED
C
C     IF EQPAR(5,NE) < 0 NO CHANGE IS MADE IN DIST RATE,
C     ITAG1 IS USED WITH REFERENCE TO IT.
C
C     LOAD THE OUTPUT STREAM WITH THE INPUT STREAM
C
C     DO LOOP ON SODUM=SIDUM
      IF (EQPAR(5,NE) .GE. 2.0) GO TO 20
```

```
      DO 20 I=1,NCCOMP
      XD(I)=EQPAR(I+4,NE)
      IJ=NOCOMP+4+I
      XB(I)=EQPAR(IJ,NE)
   20 CONTINUE
C
      DO 30 I=1,NCCOMP
      XF(I)=0.0
      DR(I)=0.0
   30 COMIN(I)=0.0
      ITAG1=0
      IF (EQPAR(5,NE) .LT. 0.0) ITAG1=1
C
      DO 50 I=1,NOCOMP
      DO 50 J=1,NIN
      COMIN(I)=CCMIN(I)+SICOMP(I,J)
   50 SOCOMP(I,J)=SICOMP(I,J)
C
      DO 60 J=3,12
      DO 60 I=1,NIN
   60 SODUM(I,J)=SIDUM(I,J)
C
      IF (ITAG1 .EQ. 1) GO TO 350
      DRATE=0.0
      FRATE=0.0
      DO 100 J=1,NIN
      SOMCLE(J)=SIMOLE(J)
  100 FRATE=FRATE+SIMOLE(J)
C
C
      DO 150 I=1,NOCOMP
  150 XF(I)=COMIN(I)/FRATE
      SUM1=0.0
      SUM2=0.0
      SUM3=0.0
      DO 160 I=1,NOCOMP
      SUM1=SUM1+XF(I)
      SUM2=SUM2+XD(I)
      SUM3=SUM3+XB(I)
  160 CONTINUE
      DO 170 I=1,NOCOMP
      XF(I)=XF(I)/SUM1
      XD(I)=XD(I)/SUM2
      XB(I)=XB(I)/SUM3
  170 CONTINUE
C
C     DO 180 I=1,NOCOMP
C 180 DR(I)=(XF(I)-XB(I))/(XD(I)-XB(I))*CCMIN(I)
C     DO 190 I=1,NOCOMP
C 190 DRATE=DRATE+DR(I)
C
C     DO 180 I=1,NOCOMP
C 180 DR(I)=(XF(I)-XB(I))/(XD(I)-XB(I))*FRATE
C     DO 190 I=1,NOCOMP
C 190 DRATE=DRATE+DR(I)
C     DRATE=DRATE/NOCOMP
C
C     CALCULATION OF CRATE USING ASSUMED VALUES OF DIST AND BTMS
C     COMPOSITIONS THRU EQPAR MATRIX
C
```

```
      DRATE=(XB(2)*COMIN(1)-XB(1)*COMIN(2))/
     %      (XB(2)*XD(1)-XB(1)*XD(2))
C
      IF (LDBUG .GE. 1) THEN
         WRITE (NPRT,240)
 240     FORMAT (' SUB DCTL:FEED, DIST AND BTMS COMPOSITIONS '/)
         WRITE (NPRT,*) (XF(J),J=1,NOCOMP),(XD(J),J=1,NOCOMP),
     *   (XB(J),J=1,NOCOMP)
         WRITE (NPRT,*)
         WRITE (NPRT,245)
 245     FORMAT (/' SICOMP 1&2 , SIMOLE , COMIN ')
         WRITE (NPRT,*) ((SICOMP(I,J),I=1,NOCOMP),J=1,NIN),
     *   (SIMOLE (I),I=1,NIN), (COMIN(I),I=1,NOCOMP)
         WRITE (NPRT,250) DRATE, FRATE
 250     FORMAT (' CHECK IN DCTL: DRATE & FRATE ',2E20.8)
      END IF
C
      IF (FRATE-DRATE) 300,300,350
 300  WRITE (NPRT,310)
 310  FORMAT ('0PROGRAM STOPPED ... DISTILLATE RATE TOO HIGH. READ
     * PROPER VALUES OF XD & XB ARRAYS IN DCTL BLOCK ')
      CALL EXIT
      RETURN
C
C     DIST RATE ASSIGNED TO EQPAR OF THE PROPER DISTILLATION BLOCK
C     UNITS OF EQPAR AND DRATE ARE DIFFERENT
C
C     ISAVE ARRAY STORES THE DIST COLUMN BLOCK # WHICH HAS BEEN
C     PROCESSED ONCE. SECOND TIME, FOR THE SAME BLOCK #, UNITS
C     OF EQPAR(18,NE) & EQPAR(19,NE) REMAIN UNCHANGED.
C
 350  II=EQPAR(2,NE)+0.1
      IF (ITAG1 .EQ. 1) GO TO 500
      IF (EQPAR(3,NE)) 400,420,400
 400  EQPAR(18,II)=0.0
      EQPAR(19,II)=DRATE
      GO TO 500
 420  EQPAR(18,II)=DRATE*EQPAR(4,NE)
      EQPAR(19,II)=DRATE*(1.0-EQPAR(4,NE))
 500  IF (LDBUG .GE. 1) THEN
         WRITE (NPRT,550) EQPAR(18,II),EQPAR(19,II)
         WRITE (NPRT,*)
      END IF
 550  FORMAT (/' SUB DSPT: DESTV = ',E13.5,' & DESTL = ',E13.5)
C
C     DSPMAX IS THE MAX # OF DSPT MODULES IN A FLOWSCHEME
C
 560  K=K+1
      IF (K .GE. MAXDSP) GO TO 700
      DO 570 I=K,MAXDSP
 570  ISAVE(I)=0
      ITAG=0
C
      DO 580 I=1,K
 580  IF (II .EQ. ISAVE(I)) ITAG=1
      IF (ITAG  .EQ. 1) GO TO 700
      ISAVE(K)=II
      IF (ITAG1 .EQ. 1) GO TO 700
      EQPAR (18,II)=EQPAR(18,II)/453.59
      EQPAR (19,II)=EQPAR(19,II)/453.59
```

```
C
  700 RETURN
      END
      SUBROUTINE DSPT
C
C     DSPT SIMULATES THE FEED-FORWARD CONTROL OF THE SPLIT IN A
C     DISTILLATION COLUMN. THE SPLIT (ASSUMING NO SIDE STREAMS)
C     IS COMPUTED BASED ON THE MULTIPLIERS CORRESPONDING TO EACH
C     OF THE COMPONENTS AND COMPONENTIAL FEED RATES.
C
      COMMON  /BLANK/  NCR, NPRT, KEEPIT(22)
      COMMON  /CMPRO/  NK, NCM1, NCP1, IDLL, IDLV, IDH, LDBUG, ISW,
     *                 NDIM, ZNAME(2,10), L(10), NTCOMP(10), NLIQ, IPSET
      COMMON  /CONTL/  NIN,NOUT,NOCOMP,NE,NEN,KUNITS
      COMMON  /SYSC/   LA,LB,LC,LOOP,LOOPS
      COMMON  /SYSD/   KEFLAG(50),KSFLAG(100),KTRACE,DERROR,NPFREQ,
     *                 IPUNCH
      COMMON  /EQPA/   EQPAR(25,50),NEMAX,MAXEQP
      COMMON  /STRMIN/ SINUM(4),SIFLAG(4),SIVPFR(4),SITEMP(4),SIPRES(4),
     *                 SIENTH(4),SIVISC(4),SITHK(4),SIZ(4),SIS(4),
     *                 SIFRAL(4),SIMOLE(4),SICOMP(10,4),SIKV(10,4)
      COMMON  /STMOUT/ SONUM(4),SOFLAG(4),SOVPFR(4),SOTEMP(4),SOPRES(4),
     *                 SOENTH(4),SOVISC(4),SOTHK(4),SOZ(4),SOS(4),
     *                 SOFRAL(4),SOMOLE(4),SOCOMP(10,4),SOKV(10,4)
      REAL             SIDUM(4,12),SODUM(4,12)
      INTEGER          ISAVE(10)
      EQUIVALENCE      (SIDUM(1,1),SINUM(1)),(SODUM(1,1),SONUM(1))
      DATA             K, MAXDSP /0, 10/
C
C     EQPAR(1,NE) = BLOCK/NODE #
C     EQPAR(2,NE) = DISTILLATION COLUMN BLOCK/NODE #
C     EQPAR(3,NE) = CODE FOR DIST STREAM TYPE
C           (-1:SUBCOOLED LIQUID, 0:VAPOR/LIQUID, +1:LIQ AT BUB T)
C     EQPAR(4,NE) = DISTILLATE VAPOR/(V+L) FRACTION
C
C     EQPAR(5,NE) = FEED MULTIPLIER COMPONENT 1
C     EQPAR(6,NE) = FEED MULTIPLIER COMPONENT 2
C     EQPAR(7,NE) = FEED MULTIPLIER COMPONENT 3
C     EQPAR(8,NE) = FEED MULTIPLIER COMPONENT 4
C     ....
C     EQPAR(14,NE)= FEED MULTIPLIER COMPONENT 10
C     EQPAR(15,NE) THRU EQPAR(25,NE) = 0.0
C
C     IF EQPAR(5,NE) < 0 NO CHANGE IS MADE IN DIST RATE,
C     ITAG1 IS USED WITH REFERENCE TO IT.
C
C     LOAD THE OUTPUT STREAM WITH THE INPUT STREAM
C
C     DO LOOP ON SODUM=SIDUM
      ITAG1=0
      IF (EQPAR(5,NE) .LT. 0.0) ITAG1=1
      SUM=0.0
      DO 50 J=1,NIN
      DO 50 I=1,NOCOMP
      SUM=SUM+SICOMP(I,J)
   50 SOCOMP(I,J)=SICOMP(I,J)
C
      DO 60 J=3,12
      DO 60 I=1,NIN
   60 SODUM(I,J)=SIDUM(I,J)
```

```
C
      IF (ITAG1 .EQ. 1) GO TO 175
      DRATE=0.0
      FRATE=0.0
      DO 100 J=1,NIN
      SOMOLE(J)=SIMOLE(J)
      FRATE=FRATE+SIMOLE(J)
      DO 100 I=1,NOCOMP
      DRATE=DRATE+EQPAR(I+4,NE)*SICOMP(I,J)
  100 CONTINUE
C
      IF (LDBUG .GE. 1) THEN
         WRITE (NPRT,*)
         WRITE (NPRT,120) SUM, FRATE, DRATE, FRATE
  120    FORMAT (' CHECK IN DSPT: TOTAL OF SICOMP = ',
     *     E18.8/'                TOTAL OF SIMOLE = ',E18.8/
     *           '                         DRATE  = ',E18.8/
     *           '                         FRATE  = ',E18.8)
      END IF
C
      IF (FRATE-DRATE) 150,150,175
  150 WRITE (NPRT,160)
  160 FORMAT ('0PROGRAM STOPPED ... DISTILLATE RATE TOO HIGH. READ
     * PROPER VALUES OF MULTIPLIERS FOR DSPT PROCESS')
      CALL EXIT
      RETURN
C
C     DIST RATE ASSIGNED TO EQPAR OF THE PROPER DISTILLATION BLOCK
C     UNITS OF EQPAR AND DRATE ARE DIFFERENT
C
C     ISAVE ARRAY STORES THE DIST COLUMN BLOCK # WHICH HAS BEEN
C     PROCESSED ONCE. SECOND TIME, FOR THE SAME BLOCK #, UNITS
C     OF EQPAR(18,NE) & EQPAR(19,NE) REMAIN UNCHANGED.
C
  175 II=EQPAR(2,NE)+0.1
      IF (ITAG1 .EQ. 1) GO TO 500
      IF (EQPAR(3,NE)) 200,220,200
  200 EQPAR(18,II)=0.0
      EQPAR(19,II)=DRATE
      GO TO 500
  220 EQPAR(18,II)=DRATE*EQPAR(4,NE)
      EQPAR(19,II)=DRATE*(1.0-EQPAR(4,NE))
  500 IF (LDBUG .GE. 1) THEN
         WRITE (NPRT,550) EQPAR(18,II),EQPAR(19,II)
         WRITE (NPRT,*)
      END IF
  550 FORMAT (/' SUB DSPT: DESTV = ',E13.5,' & DESTL = ',E13.5)
C
C     DSPMAX IS THE MAX # OF DSPT MODULES IN A FLOWSCHEME
C
  560 K=K+1
      IF (K .GE. MAXDSP) GO TO 700
      DO 570 I=K,MAXDSP
  570 ISAVE(I)=0
      ITAG=0
C
      DO 580 I=1,K
  580 IF (II .EQ. ISAVE(I)) ITAG=1
      IF (ITAG  .EQ. 1) GO TO 700
      ISAVE(K)=II
```

```
      IF (ITAG1 .EQ. 1) GO TO 700
      EQPAR (18,II)=EQPAR(18,II)/453.59
      EQPAR (19,II)=EQPAR(19,II)/453.59
C
  700 RETURN
      END
      SUBROUTINE ECTL
C
C     THIS BLOCK IS DEDICATED (AT PRESENT) FOR AZEOTROPIC
C     DISTILLATION COLUMN (ETOH-WATER-BENZENE).
C
C     ECTL DYNAMICALLY SIMULATES THE FEED-FORWARD CONTROL
C     OF THE SPLIT IN A AZEOTROPIC DISTILLATION COLUMN
C     BASED UPON THE COMPOSITE FEED COMPOSITION AND RATE
C     AND THE ASSUMED ENTRAINER RATE.
C
C     1. DETERMINATION OF ENTRAINER RATE (TOP FEED, WITH FIXED
C        COMPOSITION) WITH  FIXED, ETHANOL+WATER FEED
C        COMPOSITION, BOTTOMS SPECS AND THEIR RATES.
C     2. IF SATISFACTORY SOLUTION IS NOT OBTAINED FROM DIST,
C        DIST CALCULATIONS ARE REPEATED WITH NEW ESTIMATE OF THE
C        ENTRAINER RATE.
C     3. CALL EXIT IF CONVERGENCE IS IN UNSATISFACTORY.
C
      COMMON  /BLANK/  NCR, NPRT, KEEPIT(22)
      COMMON  /CMPRO/  NK, NCM1, NCP1, IDLL, IDLV, IDH, LDBUG, ISW,
     *                 NDIM, ZNAME(2,10), L(10), NTCOMP(10), NLIQ, IPSET
      COMMON  /CONTL/  NIN,NOUT,NOCOMP,NE,NEN,KUNITS
      COMMON  /SYSC/   LA,LB,LC,LOOP,LOOPS
      COMMON  /SYSD/   KEFLAG(50),KSFLAG(100),KTRACE,DERROR,NPFREQ,
     *                 IPUNCH
      COMMON  /EQPA/   EQPAR(25,50),NEMAX,MAXEQP
      COMMON  /STRMIN/ SINUM(4),SIFLAG(4),SIVPFR(4),SITEMP(4),SIPRES(4),
     *                 SIENTH(4),SIVISC(4),SITHK(4),SIZ(4),SIS(4),
     *                 SIFRAL(4),SIMOLE(4),SICOMP(10,4),SIKV(10,4)
      COMMON  /STMOUT/ SONUM(4),SOFLAG(4),SOVPFR(4),SOTEMP(4),SOPRES(4),
     *                 SOENTH(4),SOVISC(4),SOTHK(4),SOZ(4),SOS(4),
     *                 SOFRAL(4),SOMOLE(4),SOCOMP(10,4),SOKV(10,4)
      REAL             SIDUM(4,12),SODUM(4,12),COMIN(10),ZF(10),XF(10)
      REAL             SCC(12), SOC(12)
      REAL             XBT(3), XE(3), XBTSV(3)
      INTEGER          ISAVE(10)
      EQUIVALENCE      (SIDUM(1,1),SINUM(1)),(SODUM(1,1),SONUM(1))
      REAL             XBSET(3)/0.99, 1.0E-4, 0.01/
      REAL             XB(3)/0.99, 1.E-4, 0.01/
      REAL             XD(3)/0.28, 0.18, 0.54/
      INTEGER          KMAX / 10 /
C
C          EQPAR(1,NE) = EQUIPMENT NUMBER
C          EQPAR(2,NE) = NUMBER OF STAGES IN STRIPPING SECTION
C          EQPAR(3,NE) = NUMBER OF STAGES IN RECTIFYING SECTION
C          EQPAR(4,NE) = TYPE OF UNIT
C          EQPAR(5,NE) = STAGE EFFICIENCY STRIPPING SECTION ... FRACTION
C          EQPAR(6,NE) = STAGE EFFICIENCY RECTIFYING SECTION ... FRACTION
C          EQPAR(7,NE) = TOP STAGE TEMPERATURE (DEG K)
C          EQPAR(8,NE) = BOTTOM STAGE TEMPERATURE (DEG K)
C          EQPAR(9,NE) = TOP STAGE PRESSURE (ATM)
C          EQPAR(10,NE) = BOTTOM STAGE PRESSURE (ATM)
C          EQPAR(11,NE) = TEMPERATURE TOLLERANCE (DEFAULT = 0.01)
C          EQPAR(12,NE) = FLOW TOLLERANCE (DEFAULT = 0.0005)
```

```
C          EQPAR(13,NE) = NUMBER OF FEEDS
C          EQPAR(14,NE) = STAGE NUMBER FOR THE 1ST FEED
C          EQPAR(15,NE) = STAGE NUMBER FOR THE 2ND FEED
C          EQPAR(16,NE) = STAGE NUMBER FOR THE 3RD FEED
C          EQPAR(17,NE) = STAGE NUMBER FOR THE 4TH FEED
C          EQPAR(18,NE) = SPECIFIED DISTILLATE VAPOR RATE, DESTV
C          EQPAR(19,NE) = SPECIFIED DISTILLATE LIQUID RATE, DESTL
C          EQPAR(20,NE) = REFLUX RATIO OR BOILUP RATIO
C          EQPAR(21,NE) = DISTILLATE CODE (IDCODE)
C                         -1 : SUBCOOLED LIQUID
C                          0 : VAPOR/LIQUID DISTILLATE
C                         +1 : LIQUID AT BUBBLE POINT
C          EQPAR(22,NE) = ITRMAX (MAXIMUM VALUE FOR ITERATIONS)
C          EQPAR(23,NE) = DISTILLATE VAPOR/(V+L) FRACTION
C          EQPAR(24,NE) = SPECIFIED BOTTOMS RATE
C                         (DEFAULT: SUM OF ALL THE INCOMING STREAMS
C                          EXCEPT THE FIRST ONE)
C
C          INPUT VALUES    NCASE         DESCRIPTION
C               3             3     DISTILLATION COLUMN (RR SPECIFIED)
C               4             4     DISTILLATION COLUMN (BOILUP SPECIFIED)
C               5             5     SELF REFLUXING COLUMN (BOILUP SPECIFIED)
C               6             6     SELF REBOILING COLUMN (RR SPECIFIED)
C
C      IOK=0 SUCCESSFUL CALCULATIONS      .
C      IOK=1 EXCESS BENZENE IN THE BTMS (ACTION INC DIST RATE)
C      IOK=1 EXCESS WATER IN THE BTMS (ACTION DEC DIST RATE)
C
C      DO LOOP ON SODUM=SIDUM
C
       IF (LDBUG .GE. 1) WRITE (6,9999)
 9999  FORMAT(' ',30X,'SUBROUTINE ECTL')
C
C      IF (LDBUG .GE. 1) THEN
C         WRITE (NPRT,4)
C   4     FORMAT (/' PARAMETERS IN SUB. ECTL ARE:'/)
C         WRITE (NPRT,*) (C(J),J=1,12)
C         WRITE (NPRT,*) (ALPHA(J),J=1,6)
C      END IF
       IOK=0
       KNT=0
       ERATE=0
       BRATE=0
       ISW=0
       SUM1=0.0
       SUM2=0.0
       ERATE=SIMOLE(1)
       IF (EQPAR(24,NE) .EQ. 0.0) THEN
          DO 15 I=2,NIN
   15     BRATE=BRATE+SIMOLE(I)
       ELSE
          KUNITS=EQPAR(25,NE)+0.1
          IF (KUNITS .EQ. 0) GO TO 17
          EQPAR(24,NE)=EQPAR(24,NE)*453.59
   17     BRATE=EQPAR(24,NE)
       END IF
C
       DO 20 I=1,NCCOMP
   20  XE(I)=0.0
       DO 23 I=1,NCCOMP
```

```
   23 XE(I)=SICOMP(I,1)/ERATE
      ERSV=0.9*ERATE
      FXNSV=XB(2)
C
C     LOOP STARTS HERE
C
   25 SIMOLE(1)=ERATE
      DO 30 I=1,NOCOMP
      XF(I)=0.0
   30 COMIN(I)=0.0
      DO 50 I=1,NOCOMP
      SICOMP(I,1)=XE(I)*SIMOLE(1)
      DO 50 J=1,NIN
   50 COMIN(I)=COMIN(I)+SICOMP(I,J)
C     UPDATING ENTHALPY OF INCOMING ENTRAINER STREAM VIA ADBF
      NSAVE=NOUT
      ESAVE=EQPAR(2,NE)
      NOUT=1
C     SAVE OUTPUT STREAM # 1
      DO 100 I=3,12
  100 SOD(I)=SODUM(1,I)
      DO 110 I=1,NOCOMP
  110 SOC(I)=SOCOMP(I,1)
C     ENTHALPY CALCULATION VIA ISOTHERMAL FLASH
      EQPAR(2,NE)=8.0
      CALL ADBF
C     RESTORING VALUES
      NOUT=NSAVE
      EQPAR(2,NE)=ESAVE
      DO 120 I=3,12
      SIDUM(1,I)=SODUM(1,I)
  120 SODUM(1,I)=SOD(I)
      DO 130 I=1,NOCOMP
  130 SOCOMP(I,1)=SOC(I)
      FRATE=0.0
      DO 140 J=1,NIN
  140 FRATE=FRATE+SIMOLE(J)
C
      DO 150 I=1,NOCOMP
  150 XF(I)=COMIN(I)/FRATE
      DRATE=FRATE-BRATE
C
  155 CONTINUE
      SUM1=0.0
      SUM2=0.0
      SUM3=0.0
      DO 160 I=1,NOCOMP
      SUM1=SUM1+XF(I)
      SUM2=SUM2+XD(I)
      SUM3=SUM3+XB(I)
  160 CONTINUE
      DO 170 I=1,NOCOMP
      XF(I)=XF(I)/SUM1
      XD(I)=XD(I)/SUM2
      XB(I)=XB(I)/SUM3
  170 CONTINUE
C
      IF (LDBUG .GE. 1) THEN
         WRITE (NPRT,240)
  240    FORMAT (' SUB ECTL:FEED, DIST AND BTMS COMPOSITIONS '/)
```

```
         WRITE (NPRT,*) (XF(J),J=1,NOCOMP),(XD(J),J=1,NOCOMP),
     *   (XB(J),J=1,NOCOMP)
         WRITE (NPRT,*)
         WRITE (NPRT,250) FRATE, ERATE, DRATE, BRATE
  250    FORMAT (' CHECK IN ECTL: FRATE / ERATE / DRATE / BARTE '/
     *   4E16.5)
      END IF
C
  290 IF (FRATE-DRATE) 300,300,350
  300 WRITE (NPRT,310)
  310 FORMAT ('0PROGRAM STOPPED IN ECTL: DISTILLATE RATE TOO HIGH. ')
      CALL EXIT
      RETURN
C
  350 IF (EQPAR(21,NE)) 400,420,400
  400 EQPAR(18,NE)=0.0
      EQPAR(19,NE)=DRATE
      GO TO 500
  420 EQPAR(18,NE)=DRATE*EQPAR(23,NE)
      EQPAR(19,NE)=DRATE*(1.0-EQPAR(23,NE))
  500 IF (LDBUG .GE. 1) THEN
         WRITE (NPRT,550) EQPAR(18,NE),EQPAR(19,NE)
         WRITE (NPRT,*)
      END IF
  550 FORMAT (/' SUB DSPT: DESTV = ',E13.5,' & DESTL = ',E13.5)
C
      KUNITS=EQPAR(25,NE)+0.1
      IF (KUNITS .EQ. 0) GO TO 575
      EQPAR (18,NE)=EQPAR(18,NE)/453.59
      EQPAR (19,NE)=EQPAR(19,NE)/453.59
  575 CONTINUE
C
      CALL DIST
C     IF (KNT .GT. 0) CALL ZDIST
      WRITE (NPRT,578)
  578 FORMAT (' SUB ECTL STMT#578: RETURNED FROM DIST')
C
C     CHECK WHETHER THE BTMS COMPOSITION IS CORRECT
C     SOCOMP(I,2)
      DO 600 I=1,NOCOMP
  600 XBT(I)=SOCOMP(I,2)/SOMOLE(2)
      IF (XBT(1) .GE. XBSET(1) .AND.
     %    XBT(2) .LE. XBSET(2) .AND.
     %    XBT(3) .LE. XBSET(3)) GO TO 700
C
      IF (XBT(1) .LT. XBSET(1)) THEN
         IF (XBT(3) .GT. XBSET(3)) ICK=1
         IF (XBT(3) .GT. 0.02) ICK=10
         IF (XBT(3) .GT. 0.04) ICK=11
         IF (XBT(3) .GT. 0.10) ICK=12
      END IF
C
      IF (ICK .NE. 0) GO TO 605
      IF (XBT(1) .LT. XBSET(1) .AND.
     %    XBT(2) .GT. XBSET(2)) ICK=2
C
      IF (ICK .NE. 0) GO TO 605
      IF (XBT(1) .LT. XBSET(1) .AND.
     %    XBT(2) .GT. XBSET(2) .AND.
     %    XBT(3) .LT. XBSET(3)) ICK=3
```

```
      IF (IOK .EQ. 0) GO TO 700
C
C     SECANT METHOD FOR NEW VALUE OF ORATE
  605 CONTINUE
      SUMA=0.0
      DO 610 I=1,NOCOMP
  610 SUMA=SUMA+XBT(I)
      DO 612 I=1,NOCOMP
  612 XBT(I)=XBT(I)/SUMA
      FXN=XBT(2)-XBSET(2)
      IF (IOK .EQ. 2 .OR. IOK .EQ. 3) THEN
         DELTA=-FXN*(ERATE-ERSV)/(FXN-FXNSV)
      END IF
      IF (IOK .EQ. 1)  DELTA=0.010*ERATE
      IF (IOK .EQ. 10) DELTA=0.02*ERATE
      IF (IOK .EQ. 11) DELTA=0.075*ERATE
      IF (IOK .EQ. 12) DELTA=0.20*ERATE
      FXNSV=FXN
      ERSV=ERATE
      ELIMIT=0.25*ERATE
      DELTA=SIGN( AMIN1(ABS(DELTA),ELIMIT), DELTA)
      ERATE=ERATE-DELTA
      KNT=KNT+1
      WRITE (NPRT,625) LOOP, KNT, IOK, ERATE, DELTA
  625 FORMAT (' IN ECTL: LOOP =',I3,' KNT =',I3,' IOK=',I3/
     *' ERATE = ',G15.5,2X,' DELTA = ',G15.5)
      IF (KNT .LE. KMAX) GO TO 25
      CALL EXIT
C
  700 WRITE (NPRT,710)
  710 FORMAT (' ECTL SUCCESSFULLY COMPLETED')
      RETURN
      END
      SUBROUTINE RCTL
C
C     RCTL BLOCK TAPS THE VALUES FROM THE REFERENCE STREAMS
C     [ + VE FOR INCOMING & - VE FOR OUTGOING STREAMS] AND
C     MAKE NEW ESTIMATE OF COMPONENTIAL RATES OF THE OUTPUT
C     STREAM.
C     ONLY 1 INPUT AND 1 OUTPUT STREAM ALLOWED
C
      COMMON  /BLANK/  NCR, NPRT, KEEPIT(22)
      COMMON  /CMPRO/  NK, NCM1, NCP1, IOLL, IOLV, IOH, LOBUG, ISW,
     *                 NDIM, ZNAME(2,10), L(10), NTCOMP(10), NLIQ, IPSET
      COMMON  /CONTL/  NIN,NOUT,NOCOMP,NE,NEN,KUNITS
      COMMON  /SYSC/   LA,LB,LC,LOOP,LOOPS
      COMMON  /SYSD/   KEFLAG(50),KSFLAG(100),KTRACE,DERROR,NPFREQ,
     *                 IPUNCH
      COMMON  /EQPA/   EQPAR(25,50),NEMAX,MAXEQP
      COMMON  /STMA/   SEXTSV(13,100),SINTSV(11,100),NSMAX,MAXSEX,MAXSIN
      COMMON  /STRMIN/ SINUM(4),SIFLAG(4),SIVPFR(4),SITEMP(4),SIPRES(4),
     *                 SIENTH(4),SIVISC(4),SITHK(4),SIZ(4),SIS(4),
     *                 SIFRAL(4),SIMOLE(4),SICOMP(10,4),SIKV(10,4)
      COMMON  /STMOUT/ SONUM(4),SOFLAG(4),SOVPFR(4),SOTEMP(4),SOPRES(4),
     *                 SOENTH(4),SOVISC(4),SOTHK(4),SOZ(4),SOS(4),
     *                 SOFRAL(4),SOMOLE(4),SOCOMP(10,4),SOKV(10,4)
      REAL             SIDUM(4,12),SODUM(4,12),COMIN(10),CR(10),XF(10)
      INTEGER          ISAVE(10), ISTRM(4), ICOMP(4)
      EQUIVALENCE      (SIDUM(1,1),SINUM(1)),(SODUM(1,1),SONUM(1))
C
```

```
C     EQPAR(1,NE) = BLOCK/NODE #
C     EQPAR(2,NE) = }
C     EQPAR(3,NE) = } EMPTY
C     EQPAR(4,NE) = }
C     EQPAR(5,NE) = REFERENCE STREAM # 1
C     EQPAR(6,NE) = REFERENCE STREAM # 2
C     EQPAR(7,NE) = REFERENCE STREAM # 3
C     EQPAR(8,NE) = REFERENCE STREAM # 4
C
C     EQPAR(9,NE) = REFERENCE COMPONENT # 1
C     EQPAR(10,NE) = REFERENCE COMPONENT # 2
C     EQPAR(11,NE) = REFERENCE COMPONENT # 3
C     EQPAR(12,NE) = REFERENCE COMPONENT # 4
C
C     EQPAR(13,NE) TO  EQPAR(25,NE) = 0.0
C
C     LOAD THE OUTPUT STREAM WITH THE INPUT STREAM
C
C     DO LOOP ON SODUM=SIDUM
C
      DO 30 I=1,NOCOMP
      XF(I)=0.0
      DR(I)=0.0
   30 COMIN(I)=0.0
      ITAG1=0
      IF (EQPAR(9,NE) .LT. 0.0) ITAG1=1
      DO 50 I=1,NOCOMP
      DO 50 J=1,NIN
      COMIN(I)=COMIN(I)+SICOMP(I,J)
   50 SOCOMP(I,J)=SICOMP(I,J)
C
      DO 60 J=3,12
      DO 60 I=1,NIN
   60 SODUM(I,J)=SIDUM(I,J)
C
      DO 70 I=1,4
      IF (EQPAR(I+4,NE) .NE. 0.0) THEN
         ISTRM(I)=SIGN(ABS(EQPAR(I+4,NE))+0.1,EQPAR(I+4,NE))
         END IF
   70 CONTINUE
      DO 80 I=1,4
   80 ICOMP(I)=EQPAR(I+8,NE)+0.1
C
C     COMPUTE BTMS RATE OF 1 AND 2 BY ESTABLISHING MASS
C     BALANCE BASED UPON THE REFERENCE STREAMS
C     B1=SUM OF INPUT STREAM RATES
C     B2=SUM OF OUTPUT STREAM RATES
C
      B1=0
      B2=0
      DO 85 I=1,4
      J1=ICOMP(1)
      J2=ICOMP(2)
      IF (ISTRM(I) .GT. 0) THEN
         IF (SEXTSV(J1+3,ISTRM(I)) .GT. 0.0 .AND.
     %      (SEXTSV(J2+3,ISTRM(I)) .GT. 0.0) ) THEN
            B1=B1+SEXTSV(J1+3,ISTRM(I))
            B2=B2+SEXTSV(J2+3,ISTRM(I))
          END IF
      ELSE IF (ISTRM(I) .LT. 0) THEN
```

```
            ITEMP=IABS(ISTRM(I))
            IF (SEXTSV(J1+3,ITEMP) .GT. 0.0 .AND.
     %         (SEXTSV(J2+3,ITEMP) .GT. 0.0) ) THEN
               B1=B1-SEXTSV(J1+3,ITEMP)
               B2=B2-SEXTSV(J2+3,ITEMP)
            END IF
      END IF
C
   85 CONTINUE
C
      WRITE (NPRT,90) B1, B2
   90 FORMAT (' SUB RCTL: B1 AND B2 = '2E20.8)
      ADD1=B1
      ADD2=B2
C     IF (B1 .LE. 0.0) ADD1=0.0
C     IF (B2 .LE. 0.0) ADD2=0.0
C     ITAR=EQPAR(2,NE)+0.1
      IF (J1 .NE. 0) SOCOMP(J1,1)=ADD1+COMIN(1)
      IF (J2 .NE. 0) SOCOMP(J2,1)=ADD2+COMIN(2)
      IF (SOCOMP(1,1) .LT. 0.0) SOCOMP(1,1)=0.0
      IF (SOCOMP(2,1) .LT. 0.0) SOCOMP(2,1)=0.0
C
C     THIS IS FOR THE 1 ST ENTRY IN RCTL BECAUSE
C     SEXTSV ARRAY IS CLEAN IF THE REFERENCE STREAMS ARE
C     NOT YET PROCESSED FOR A SINGLE TIME.
C
      IF (ITAG1 .EQ. 1) GO TO 200
      SUM=0.0
      DO 100 I=1,NOCOMP
      SUM=SUM+SOCOMP(I,1)
  100 SICOMP(I,1)=SOCOMP(I,1)
      SOMOLE(1)=SUM
  120 SIMOLE(1)=SOMOLE(1)
C
  200 IF (LDBUG .GE. 1) THEN
         WRITE (NPRT,*)
         WRITE (NPRT,250) B1, B2
  250    FORMAT (' SUB RCTL STMT#250: B1 AND B2 = ',2E16.5)
      END IF
C
  700 RETURN
      END
      SUBROUTINE SBOX
C
C     SBOX BLOCK CAN BE USED AS A DUMMY DISTILLATION COLUMN.
C     THE SPLIT IS COMPUTED AND THE STREAM CONDITIONS ARE
C     ESTABLISHED VIA ADBF BLOCK. SBOX BLOCK TAPS THE VALUES
C     FROM THE REFERENCE STREAMS [ + VE FOR INCOMING & - VE
C     FOR OUTGOING STREAMS] AND MAKE NEW ESTIMATE OF COMPONENTIAL
C     RATE OF THE OUTPUT STREAM. TARGET STREAM IS READ THRU EQPAR
C     VECTOR.
C
C     NIN (INPUT) AND NOUT (OUTPUT) STREAMS ALLOWED
C
      COMMON  /BLANK/  NCR, NPRT, KEEPIT(22)
      COMMON  /CMPRO/  NK, NCM1, NCP1, IDLL, IDLV, IDH, LDBUG, ISW,
     *                 NDIM, ZNAME(2,10), L(10), NTCOMP(10), NLIQ, IPSET
      COMMON  /CONTL/  NIN,NOUT,NOCOMP,NE,NEN,KUNITS
      COMMON  /SYSC/   LA,LB,LC,LCOP,LOOPS
      COMMON  /SYSD/   KEFLAG(50),KSFLAG(100),KTRACE,DERROR,NPFREQ,
```

```
     *                 IPUNCH
      COMMON  /EQPA/   EQPAR(25,50),NEMAX,MAXEQP
      COMMON  /STMA/   SEXTSV(13,100),SINTSV(11,100),NSMAX,MAXSEX,MAXSIN
      COMMON  /STRMIN/ SINUM(4),SIFLAG(4),SIVPFR(4),SITEMP(4),SIPRES(4),
     *                 SIENTH(4),SIVISC(4),SITHK(4),SIZ(4),SIS(4),
     *                 SIFRAL(4),SIMOLE(4),SICOMP(10,4),SIKV(10,4)
      COMMON  /STMOUT/ SONUM(4),SOFLAG(4),SOVPFR(4),SOTEMP(4),SOPRES(4),
     *                 SOENTH(4),SOVISC(4),SOTHK(4),SOZ(4),SOS(4),
     *                 SOFRAL(4),SOMOLE(4),SOCOMP(10,4),SOKV(10,4)
      REAL             SIDUM(4,12),SODUM(4,12),COMIN(10),DR(10),XF(10)
      REAL             SIC(12), SID(12), SOD1(12), SOC1(12)
      INTEGER          ISAVE(10), ISTRM(4), ICOMP(4)
      EQUIVALENCE      (SIDUM(1,1),SINUM(1)),(SODUM(1,1),SONUM(1))
C
C     EQPAR(1,NE) = BLOCK/NODE #
C     EQPAR(2,NE) = }
C     EQPAR(3,NE) = HEAT (OUT-IN) STORED
C     EQPAR(4,NE) = # WHICH GOES IN SOMOLE(*)
C                   (DEFAULT TARGET STREAM SOCOMP(I,2))
C     EQPAR(5,NE) = REFERENCE STREAM # 1
C     EQPAR(6,NE) = REFERENCE STREAM # 2
C     EQPAR(7,NE) = REFERENCE STREAM # 3
C     EQPAR(8,NE) = REFERENCE STREAM # 4
C
C     EQPAR(9,NE) = REFERENCE COMPONENT # 1
C     EQPAR(10,NE) = REFERENCE COMPONENT # 2
C     EQPAR(11,NE) = REFERENCE COMPONENT # 3
C     EQPAR(12,NE) = REFERENCE COMPONENT # 4
C
C     EQPAR(13,NE) = DISTILLATE TEMPERATURE
C     EQPAR(14,NE) = DISTILLATE PRESSURE
C     EQPAR(15,NE) = DISTILLATE VAPOR FRACTION
C     EQPAR(16,NE) = BOTTOMS TEMPERATURE
C     EQPAR(17,NE) = BOTTOMS PRESSURE
C
C     EQPAR(18,NE) TO  EQPAR(25,NE) = 0.0
C
C     LOAD THE OUTPUT STREAM WITH THE INPUT STREAM
C
C     DO LOOP ON SODUM=SIDUM
C
      KUNITS=EQPAR(25,NE)+0.1
      IF (KUNITS .EQ. 0) GO TO 10
      EQPAR(13,NE)=(EQPAR(13,NE)-32.0)/1.8+273.16
      EQPAR(14,NE)=EQPAR(14,NE)/14.696
      EQPAR(16,NE)=(EQPAR(16,NE)-32.0)/1.8+273.16
      EQPAR(17,NE)=EQPAR(17,NE)/14.696
      EQPAR(25,NE)=0.0
   10 CONTINUE
      DO 30 I=1,NCCOMP
   30 COMIN(I)=0.0
C     ITAG1=0
C     IF (EQPAR(9,NE) .LT. 0.0) ITAG1=1
      DO 50 I=1,NCCOMP
      DO 50 J=1,NIN
   50 COMIN(I)=COMIN(I)+SICOMP(I,J)
C
      DO 70 I=1,4
      IF (EQPAR(I+4,NE) .NE. 0.0) THEN
         ISTRM(I)=SIGN(ABS(EQPAR(I+4,NE))+0.1,EQPAR(I+4,NE))
```

```
         END IF
   70 CONTINUE
      DO 80 I=1,4
   80 ICOMP(I)=EQPAR(I+8,NE)+0.1
C
C     COMPUTE BTMS RATE OF 1 AND 2 BY ESTABLISHING MASS
C     BALANCE BASED UPON THE REFERENCE STREAMS
C     B1=SUM OF INPUT STREAM RATES
C     B2=SUM OF OUTPUT STREAM RATES
C
      B1=0
      B2=0
      DO 85 I=1,4
      J1=ICOMP(1)
      J2=ICOMP(2)
      IF (ISTRM(I) .GT. 0) THEN
         IF (SEXTSV(J1+3,ISTRM(I)) .GT. 0.0 .AND.
     %      (SEXTSV(J2+3,ISTRM(I)) .GT. 0.0) ) THEN
            B1=B1+SEXTSV(J1+3,ISTRM(I))
            B2=B2+SEXTSV(J2+3,ISTRM(I))
          END IF
      ELSE IF (ISTRM(I) .LT. 0) THEN
            ITEMP=IABS(ISTRM(I))
            IF (SEXTSV(J1+3,ITEMP) .GT. 0.0 .AND.
     %         (SEXTSV(J2+3,ITEMP) .GT. 0.0) ) THEN
               B1=B1-SEXTSV(J1+3,ITEMP)
               B2=B2-SEXTSV(J2+3,ITEMP)
            END IF
      END IF
   85 CONTINUE
C
      WRITE (NPRT,90) B1, B2
   90 FORMAT (' SUB SBOX: B1 AND B2 = '2E20.8)
      ADD1=B1
      ADD2=B2
C     IF (B1 .LE. 0.0) ADD1=0.0
C     IF (B2 .LE. 0.0) ADD2=0.0
C     DEFAULT TARGET STREAM
C     IF (ITAG1 .EQ. 1) GO TO 200
      ITAR=EQPAR(4,NE)+0.1
      IF (ITAR .EQ. 0) ITAR=2
      DO 95 J=1,NIN
      SOMOLE(J)=0.0
      DO 95 I=1,NOCOMP
   95 SOCOMP(I,J)=0.0
      IF (J1 .NE. 0) SOCOMP(J1,ITAR)=ADD1
      IF (J2 .NE. 0) SOCOMP(J2,ITAR)=ADD2
      DO 98 I=1,NOCOMP
      IF (I .EQ. J1 .OR. I .EQ. J2) GO TO 98
      SOCOMP(I,1)=COMIN(I)
   98 CONTINUE
C
      SUM=0.0
      SUM1=0.0
      DO 100 I=1,NOCOMP
      SUM1=SUM1+SOCOMP(I,ITAR)
      SOCOMP(I,1)=COMIN(I)-SOCOMP(I,ITAR)
      IF (SOCOMP(I,1) .LT. 0.0)SOCOMP(I,1)=0.0
  100 SUM=SUM+SOCOMP(I,1)
      SOMOLE(ITAR)=SUM1
```

```
      SOMOLE(1)=SUM
C     IF (LDBUG .GE. 0) THEN
         WRITE (NPRT,105) (SOMOLE(J),(SOCOMP(I,J),I=1,NOCOMP),
     *   J=1,NIN)
 105     FORMAT (' SUB SBOX STMT#105: SOMOLE / SOCOMP ARE '/
     *   10((4G18.5)/))
C     END IF
      DO 130 I=1,NIN
      IF (SOMOLE (I) .LT. 0.0) THEN
         WRITE (NPRT,110) I, SOMOLE(I)
 110     FORMAT (' SUB SBOX: NEGATIVE FLOWS, I / SOMOLE ARE ',
     *   I3,2X,G13.5)
         CALL EXIT
      END IF
 130  CONTINUE
C
C     THE OUT GOING STREAMS ARE ESTABLISHED BY
C     COMPUTING BUBBLE/DEW POINT TEMPERATURE
C     ENTHALPIES
C     1 - DISTILLATE (VAPOR)
C     2 - BOTTOMS
C
      NSAVE=NOUT
      NSAVE1=NIN
      ESAVE=EQPAR(2,NE)
      NIN=1
      NOUT=1
C     SAVE INPUT STREAM # 1 AND MOVE OUTPUT STREAM # 1
C     INTO INPUT STREAM # 1
      DO 150 I=3,12
      SID(I)=SIDUM(1,I)
 150  SIDUM(1,I)=SODUM(1,I)
      DO 155 I=1,NOCOMP
      SIC(I)=SICOMP(I,1)
 155  SICOMP(I,1)=SOCOMP(I,1)
      SITEMP(1)=EQPAR(13,NE)
      SIPRES(1)=EQPAR(14,NE)
      SIVPFR(1)=EQPAR(15,NE)
C     DEW POINT AND ENTHALPY CALCULATION
      EQPAR(2,NE)=1.0
      CALL ADBF
C
C     SAVE OUTPUT STREAM # 1 AND MOVE OUTPUT STREAM # 2
C     INTO INPUT STREAM # 1
      DO 160 I=3,12
 160  SOD1(I)=SODUM(1,I)
      DO 165 I=1,NOCOMP
 165  SOC1(I)=SOCOMP(I,1)
C     SECOND STREAM
      DO 170 I=3,12
 170  SIDUM(1,I)=SODUM(2,I)
      DO 175 I=1,NOCOMP
 175  SICOMP(I,1)=SOCOMP(I,2)
      SITEMP(1)=EQPAR(16,NE)
      SIPRES(1)=EQPAR(17,NE)
      SIVPFR(1)=0.0
C     BUBBLE POINT AND ENTHALPY
      EQPAR(2,NE)=2.0
      CALL ADBF
C     RESTORE THE SAVED VALUES
```

```
      EQPAR(2,NE)=ESAVE
      NOUT=NSAVE
      NIN=NSAVE1
C     RESTORE INPUT STREAM # 1
      DO 180 I=3,12
  180 SIDUM(1,I)=SID(I)
      DO 185 I=1,NOCOMP
  185 SICOMP(I,1)=SIC(I)
C
      DO 190 I=3,12
      SODUM(2,I)=SODUM(1,I)
  190 SODUM(1,I)=SOD1(I)
      SUM=0.0
      DO 195 I=1,NOCOMP
      SOCOMP(I,2)=SOCOMP(I,1)
      SUM=SUM+SOCOMP(I,2)
  195 SOCOMP(I,1)=SOC1(I)
      SOMOLE(2)=SUM
      SUM=0.0
      DO 197 I=1,NIN
  197 SUM=SUM+SOENTH(I)+SIENTH(I)
C     STORING HEAT BALANCE
      EQPAR(3,NE)=SUM
C     THIS IS FOR THE 1 ST ENTRY IN SBOX BECAUSE
C     SEXTSV ARRAY IS CLEAN IF THE REFERENCE STREAMS ARE
C     NOT YET PROCESSED FOR A SINGLE TIME.
C
  200 CONTINUE
C     IF (LDBUG .GE. 0) THEN
         DO 230 I=1,NIN
  230    WRITE (NPRT,240) I, SOMOLE(I)
  240    FORMAT (' SUB SBOX STMT#240: SOMOLE(',I2,') =',G15.5)
         WRITE (NPRT,*)
         WRITE (NPRT,245) EQPAR(3,NE)*3.96887E-6, SUM
  245    FORMAT (' HEAT BALANCE IN (K BTU) =',G15.5/
     *           ' HEAT BALANCE IN (CAL)   =',G15.5)
         WRITE (NPRT,250) B1, B2
  250    FORMAT (' SUB SBOX STMT#250: B1 AND B2 = ',2E16.5)
C     END IF
C
  700 RETURN
      END
      SUBROUTINE SMIX
C
C     SPECIAL MIXER: THIS BLOCK MIXES INPUT STREAMS AND
C     PERFORM TWO LIQUID PHASE CALCULATIONS TO ESTABLISH
C     TWO OUTPUT STREAMS WHICH ARE IN EQUILIBRIUM. THE
C     HEAT ADDED/REMOVED IS SAVED IN EQPAR(4,NE).
C
      COMMON  /BLANK/  NCR, NPRT, KEEPIT(22)
      COMMON  /CONTL/  NIN,NOUT,NOCOMP,NE,NEN,KUNITS
      COMMON  /CMPRO/  NK, NCM1, NCP1, IDLL, IDLV, IDH, LDBUG, ISW,
     *                 NDIM, ZNAME(2,10), L(10), NTCOMP(10), NLIQ, IPSET
      COMMON  /SYSB/   KRET(66),KCNT,KDUM(4),IRDMAN(56)
      COMMON  /SYSC/   LA,LB,LC,LOOP,LOOPS
      COMMON  /SYSD/   KEFLAG(50),KSFLAG(100),KTRACE,DERROR,NPFREQ,
     *                 IPUNCH
      COMMON  /EQPA/   EQPAR(25,50),NEMAX,MAXEQP
      COMMON  /STRMIN/ SINUM(4),SIFLAG(4),SIVPFR(4),SITEMP(4),SIPRES(4),
     *                 SIENTH(4),SIVISC(4),SITHK(4),SIZ(4),SIS(4),
```

```
     *                   SIFRAL(4),SIMOLE(4),SICOMP(10,4),SIKV(10,4)
      COMMON  /STMOUT/  SONUM(4),SOFLAG(4),SOVPFR(4),SOTEMP(4),SOPRES(4),
     *                   SOENTH(4),SOVISC(4),SOTHK(4),SOZ(4),SOS(4),
     *                   SOFRAL(4),SOMOLE(4),SOCOMP(10,4),SOKV(10,4)
      COMMON  /STRM/    T, P, Z(10), Y(10), X(10), FRACV, ZVAP,
     *                   EK(10), VP(10), FUG(10), GAM(10), SVAP,
     *                   HOFZ, HVAP, HLIQ, DHV, XSH, NOBUB, NODEW
      COMMON  /TWOLQ/   X1(10), X2(10), DUMB1(40), DHL(2), HIDLL(2),
     +                   HREALL(2), FRACL, DUMB2(4)
      COMMON  /ZFEEDZ/  PF, TF, FEED(10), AAAA(3)
C
      REAL               SIDUM(4,12), SODUM(4,12), SIC(12), SID(12)
C
      EQUIVALENCE        (SINUM,SIDUM), (SONUM,SODUM)
C
C          EQPAR(1,NE) = EQUIPMENT NUMBER
C          EQPAR(2,NE) = TEMPERATURE (F) OF ALL OUTPUT STRMS
C          EQPAR(3,NE) = PRESSURE (PSIA) OF ALL OUTPUT STRMS
C          EQPAR(4,NE) = HEAT REMOVED/ADDED IN THE OPERATION
C                        (VALUE IS STORED)
C          EQPAR(5,NE) = MODE OF FLASH CALCULATION
C                        (DEFAULT MODE=13)
C          EQPAR(6,NE) TO EQPAR(25,NE) = 0.0
C
C     MODE=NTYPE
C
C       NTYPE    DESCRIPTION
C
C          1     DEW POINT TEMPERATURE
C          2     BUBBLE POINT TEMPERATURE (1/2 LIQ)
C          3     ALL VAPOR ENTHALPY WITH PRIOR DEW POINT
C          4     ALL LIQUID ENTHALPY WITH PRIOR BUBBLE POINT (1/2 LIQ)
C          5     ALL VAPOR ENTHALPY
C          6     ALL LIQUID ENTHALPY (1/2 LIQ)
C          7     ISOTHERMAL FLASH (1/2 LIQ)
C          8     ISOTHERMAL FLASH ... NO DEW/BUBBLE POINT (1/2 LIQ)
C          9     ADIABATIC FLASH (1/2 LIQ)
C         10     ADIABATIC FLASH ... NO DEW/BUBBLE POINT (1/2 LIQ)
C         11     DEW POINT PRESSURE
C         12     BUBBLE POINT PRESSURE (1/2 LIQUID)
C         13     LIQ - LIQ SEPERATION BELOW BUBBLE POINT (2 LIQ)
C
D     WRITE (6,9999)
 9999 FORMAT(' ',30X,'SUBROUTINE SMIX')
C
      KUNITS=EQPAR(25,NE)+0.1
      IF (KUNITS .EQ. 0) GO TO 11
      EQPAR(2,NE)=(EQPAR(2,NE)-32.0)/1.8+273.16
      EQPAR(3,NE)=EQPAR(3,NE)/14.696
      EQPAR(25,NE)=0.0
   11 CONTINUE
C
      T=EQPAR(2,NE)
      P=EQPAR(3,NE)
      MODE=EQPAR(5,NE)+0.1
      IF (MODE .EQ. 0) MODE=13
C
      DO 1 I=1,NIN
      IF (SIMOLE(I) .GT. 0.) GO TO 2
1     CONTINUE
```

```
      RETURN
2     SMALL=SIPRES(I)
      J=I+1
      IF (J.GT.NIN) GO TO 4
      DO 3 I=J,NIN
3     IF (SIPRES(I).LT.SMALL.AND.SIMOLE(I).GT.0.) SMALL=SIPRES(I)
4     SOPRES(1)=SMALL
      SOENTH(1)=0.
      SOMOLE(1)=0.
      DO 5 J=1,NOCOMP
5     SOCOMP(J,1)=0.
      DO 6 I=1,NIN
      SOENTH(1)=SOENTH(1)+SIENTH(I)
      SOMOLE(1)=SOMOLE(1)+SIMOLE(I)
      DO 6 J=1,NOCOMP
6     SOCOMP(J,1)=SOCOMP(J,1)+SICOMP(J,I)
      IF (SOTEMP(1).EQ.0.) SOTEMP(1)=273.16
      DO 12 I=3,12
      SID(I)=SIDUM(1,I)
12    SIDUM(1,I)=SODUM(1,I)
      DO 13 I=1,NOCOMP
      SIC(I)=SICOMP(I,1)
  13  SICOMP(I,1)=SOCOMP(I,1)
C
      SVNOUT=NOUT
      DO 17 I=1,NOUT
      SOPRES(I)=P
   17 SOTEMP(I)=T
C
      HOFZ=SIENTH(1)/SIMOLE(1)
      FRACV=SIVPFR(1)
      FRACL=SIFRAL(1)
      DO 19 I=1,NOCOMP
   19 FEED(I)=SICOMP(I,1)
C
      IF (LDBUG .GE. 0) THEN
         WRITE (NPRT,21)
         WRITE (NPRT,*)  FRACV,FRACL,T,P,HOFZ,(FEED(J),J=1,NOCOMP)
   21    FORMAT (/' SUB SMIX AT FTN*21: FRACV/ FRACL / T / P /
     * HOFZ / FEED /'/)
      END IF
C
      CALL ANYONE (MODE)
C
      IF (LDBUG .GE. 0) THEN
         WRITE (NPRT,25)
         WRITE (NPRT,*)  FRACV,FRACL,T,P,HOFZ,(FEED(J),J=1,NOCOMP)
   25    FORMAT (/' SUB SMIX AT FTN*25: FRACV/ FRACL / T / P /
     *   HOFZ / FEED /'/)
      END IF

C
C     NOUT=2 & MODE<>13: OUTPUT STREAM (1) VAPOR & (2) 1/2 LIQUID
C     NOUT=2 & MODE=13 : OUTPUT STREAMS ARE ONLY LIQUID
C                        (1) LIGHT PHASE
C                        (2) HEAVY PHASE
C
      IF (NOUT .EQ. 2) THEN
         IF (MODE .EQ. 13) THEN
            SOVPFR(1)=0.0
```

```
                SOVPFR(2)=0.0
                SOFRAL(1)=1.0
                SOFRAL(2)=1.0
                SOMOLE(1)=SIMOLE(1)*FRACL
                SOMOLE(2)=SIMOLE(1)*(1.0-FRACL)
                SOENTH(1)=HREALL(1)*SOMOLE(1)
                SOENTH(2)=HREALL(2)*SOMOLE(2)
                DO 38 I=1,NOCOMP
                SOCOMP(I,1)=X1(I)*SOMOLE(1)
   38           SOCOMP(I,2)=X2(I)*SOMOLE(2)
                GO TO 200
             ELSE
                SOVPFR(1)=1.0
                SOVPFR(2)=0.0
                SOFRAL(1)=0.0
                SOFRAL(2)=FRACL
                SOMOLE(1)=SIMOLE(1)*FRACV
                SOMOLE(2)=SIMOLE(1)*(1.0-FRACV)
                SOENTH(1)=HVAP*SOMOLE(1)
                SOENTH(2)=(HREALL(1)*FRACL+HREALL(2)*(1.0-FRACL))*SOMOLE(2)
                SOZ(1)=ZVAP
                DO 40 I=1,NOCOMP
                SOCOMP(I,1)=Y(I)*SOMOLE(1)
   40           SOCOMP(I,2)=(X1(I)*FRACL+X2(I)*(1.0-FRACL))*SOMOLE(2)
                GO TO 200
             END IF
          END IF
C
  200     CONTINUE
          DO 202 I=3,12
  202     SIDUM(1,I)=SID(I)
          DO 203 I=1,NOCOMP
  203     SICOMP(I,1)=SIC(I)
C
          SUM1=0.0
          SUM2=0.0
          DO 207 I=1,NIN
  207     SUM1=SUM1+SIENTH(I)
          DO 208 I=1,NOUT
  208     SUM2=SUM2+SOENTH(I)
          EQPAR(4,NE)=SUM1-SUM2
C
          NOUT=SVNOUT
          IF (LDBUG .GE. 0) THEN
             WRITE (NPRT,209)
             WRITE (NPRT,*) (SOMOLE(I),(SOCOMP(J,I),J=1,NOCOMP),I=1,NOUT)
  209        FORMAT (/' SUB SMIX AT FTN#209: SOMOLE / SOCOMP / '/
     *       4E15.5/4E15.5)
          END IF
          IF (KTRACE .LT. 2) GO TO 250
          WRITE (NPRT,210)
  210     FORMAT ('0 SUB SMIX AT STM#210 : NTYPE / NOUT / FRACV / FRACL /')
          WRITE (NPRT,*) MODE, NOUT, FRACV, FRACL
C
  250     RETURN
          END
```

```
      PROGRAM  FLASH2
C
C     GENERALIZED VAPOR-LIQUID-LIQUID FLASH PROGRAM FOR
C     THE NON-IDEAL NON-ELECTROLYTIC SYSTEMS
C
C     VERSION #  2 ..  AUGUST 1984.
C     VERSION #  3 ..  FEBRUARY 1985. INCLUSION OF SUBROUTINE SWITCH
C                      FOR THE OPTION OF TWO DIFFERENT SETS OF PARAMETERS
C                      FOR GAMMA MODEL
C
      COMMON  /BLANK/  NCR, NPRT, NSTART, KUNITS, TITLE(20)
      COMMON  /CMPRO/  NC, NCM1, NCP1, IDLL, IDLV, IDH, LDBUG, ISW,
     *                 NDIM, ZNAME(2,10), L(10), NTCOMP(10), NLIQ, IPSET
      COMMON  /ZDATA/  CPL(10,4), CPV(10,4), ENP(10,10), ANT(6,10),
     *                 W(10), AX, BX, OMEGA(10), AVAL(10), BVAL(10),
     *                 AK(10,10), R(10), Q(10), QP(10), XL(10),
     *                 VOL(10), C(180), ALPHA(45), VC(10), TC(10),
     *                 PC(10), ZC(10), TNBP(10), OA(10), OB(10),
     *                 A(10,10), G(10,10), ZRA(10), RD(10), DMU(10),
     *                 ETA(10)
      COMMON  /STRM/   T, P, Z(10), Y(10), X(10), FRACV, ZVAP,
     *                 EK(10), VP(10), FUG(10), GAM(10), SVAP,
     *                 HOFZ, HVAP, HLIQ, DHV, XSH, NOBUB, NODEW
      COMMON  /CONTRL/ ITF, IPF,  N, NTYPE, JCODE
      COMMON  /TWOLQ/  X1(10), X2(10), GAM1(10), GAM2(10), EK1(10),
     +                 EK2(10), DHL(2), HIDLL(2), HREALL(2), FRACL,
     +                 IE, IR, XMAX, XMIN
      COMMON  /ZFEEDZ/ PF, TF, FEED(10), FMOL, TREF, HI
      COMMON  /DUMMY/  XX(10,2), SX(10,2), XC(10,2), YY(10), SY(10),
     +                 YC(10), RMAX, RMIN
      DIMENSION        DEWC(10), BUBC(10), IJK(7), HLIQD(2)
      REAL             FD(11), BUBVAP(10), DEWLIQ(10)
      EQUIVALENCE      (FEED(1),FD(1))
C
      DATA             IJK /'T','P','F','Q','M','N',' '/
      DATA             DOLLAR /'$$$$'/
C
      CALL ERRSET (73,.TRUE.,.TRUE.,.FALSE.,.FALSE.,999)
      CALL ERRSET (74,.TRUE.,.TRUE.,.FALSE.,.FALSE.,999)
   10 DO 5 II=1,10
      Y(II)=0.0
      YY(II)=0.0
      X1(II)=0.0
      X2(II)=0.0
      XX(II,1)=0.0
      XX(II,2)=0.0
      EK1(II)=1.0
      EK2(II)=1.0
      FUG(II)=1.0
      GAM1(II)=1.0
      GAM2(II)=1.0
    5 CONTINUE
      KUNITS=1
      NCR=5
      NPRT=6
C
C     READ IN THE MAIN TITLE
C
      READ (NCR,16,END=1500,ERR=7) TITLE
      WRITE (NPRT,17) TITLE
```

```
C
  7   CALL START (IDATA,MFEEDS,MCASES,&1500)
C
C     THE FOLLOWING CODES AND VALUES ARE READ IN ADDITION TO THOSE
C     READ IN START.
C
C     PARAMETERS READ CARDS
C
C         JCODE     CASE CALCULATION CODE
C                        0    USE THE USER INTERACTIVE MODE
C                        1    BYPASS THE USER INTERACTIVE MODE
C
C         IE        COMPONENT # : E-PHASE RICH IN THAT COMPONENT
C
C         IR        COMPONENT # : R-PHASE RICH IN THAT COMPONENT
C
C         XMAX      X TO INITIALIZE XE(IE) & XR(IR) IN INTLIZ
C
C         XMIN      X TO INITIALIZE XE(IR) & XR(IE) IN INTLIZ
C
C
      READ (NCR,*) JCODE, IE, IR, XMAX, XMIN
      WRITE (NPRT,8) JCODE, IE, IR, XMAX, XMIN
    8 FORMAT ('0DEFINED CODES AND VALUES:'//
     *        5X, 'JCODE =',                    I23//
     *        5X, 'E-PHASE RICH IN =',          I13//
     *        5X, 'R-PHASE RICH IN =',          I13//
     *        5X, 'E-PHASE: MAIN COMP X =',     F6.3//
     *        5X, 'R-PHASE: MAIN COMP X =',     F6.3//)
C
      IF (NLIQ .EQ. 0) NLIQ=1
      NLIQSV=NLIQ
      IF (IDATA.NE.0) GO TO 11
      CALL CDATA
      WRITE (NPRT, 9)
    9 FORMAT ('0GENERALIZED NONIDEAL FLASH (1/2 LIQ) PROGRAM')
      GO TO 665
C
C     ACCESS DATA RETREVIAL PROGRAMS
C
  11  WRITE (NPRT,8)
      CALL ZPVT
      CALL ZNRTL
      WRITE (NPRT,13)
   13 FORMAT ('0COMPONENTS USED ARE:'/
     *    2X, '#',2X,'NAME',6X,'ID#')
      WRITE (NPRT,14) (J,(ZNAME(K,J),K=1,2),NTCOMP(J),J=1,NC)
   14 FORMAT (I3,2X,2A4,4X,I3)
C
C     *** *** *** RETURN POINT FOR MULTIPLE CASES *** *** ***
C
   15 READ (NCR,16,END=1500,ERR=7) TITLE
   16 FORMAT (20A4)
      IF (TITLE(1) .EQ. DOLLAR) GO TO 10
      WRITE (NPRT,17) TITLE
   17 FORMAT ('1',20A4)
      READ (NCR,*,END=1500,ERR=1500)  PF,TF,FRACV,HRUN,NTYPE
      PRES=PF
C
      HVAP=0.0
```

```
      HLIQ=0.0
      DHV=0.0
      XSH=0.0
C
      WRITE (NPRT,20) PF,TF,FRACV,HRUN,NTYPE
   20 FORMAT ('0 PARAMETERS FOR EQUILIBRIUM CALCULATION:'/
     *    5X, 'P, PSIA =',  F14.3/
     *    5X, 'T, DEG F =', F13.2/
     *    5X, 'FRACV =',    F16.5/
     *    5X, 'H, K-BTU =', 1PE13.5/
     *    5X, 'NTYPE =',    I16)
C
C     CONVERT PSIA, F, BTU TO ATM, K, CAL (INTERNAL UNITS)
C
      PF=PF/14.696
      P=PF
      TF=(TF-32.0)/1.8+273.16
      TSAVE=TF
      HRUN=HRUN*252.16*1.0E3
      HOFZ=HRUN
C
C     INITIAL SETTING OF GAMMA, FUGACITY AND DISTRIBUTION COEFF. BASED
C     UPON THE TYPE OF COMPONENT
C
      DO 30 I=1,NC
      GAM1(I)=1.0
      GAM2(I)=1.0
      VP(I)=0.0
      EK1(I) = 0.0
      EK2(I) = 0.0
      FUG(I)=0.0
      IF (L(I) .GT. 0) FUG(I)=1.0
   30 CONTINUE
C
C     READ IN LB-MOLES OF COMPONENT FLOWRATES IN THE FEED
C
      READ (NCR,*) (FD(J),J=1,NC)
      FMOL=0.0
      DO 35 J=1,NC
   35 FMOL=FMOL+FD(J)
      DO 40 I=1,NC
   40 Z(I)=FD(I)/FMOL
C
      WRITE (NPRT,80)
   80 FORMAT ('0FEED SUMMARY:'/
     *          '  *  NAME',15X,'MOLS',9X,'MOL FRAC')
      DO 90 J=1,NC
   90 WRITE (NPRT,100) J,(ZNAME(K,J),K=1,2),FD(J),Z(J)
  100 FORMAT (I3,2X,2A4,F17.4,F15.6)
      WRITE (NPRT,110) FMOL
  110 FORMAT (' TOTAL',F24.4)
C
C     CONVERT MOLAR UNITS FROM LB-MOLE TO GM-MOLE
C
      FMOL=FMOL*453.59
      FD(NC+1)=FMOL
      HRUN=HRUN/FMOL
      TERM=FMOL/252.16/1.0E3
C
C     FRACV USED AS SWITCH
```

```
C        -1   SUBCOOLED LIQUID
C        +2   SUPERHEATED VAPOR
C
      IF (NTYPE .GT. 0) GO TO 115
      IF (FRACV .EQ. 2.0) GO TO 1000
      IF (FRACV .EQ. -1.0) GO TO 1000
      IF (ABS(FRACV-0.5) .LT. 0.001) GO TO 500
      GO TO 500
C
C        NTYPE    DESCRIPTION
C
C           1     DEW POINT TEMPERATURE
C           2     BUBBLE POINT TEMPERATURE (1/2 LIQ)
C           3     ALL VAPOR ENTHALPY WITH PRIOR DEW POINT
C           4     ALL LIQUID ENTHALPY WITH PRIOR BUBBLE POINT (1/2 LIQ)
C           5     ALL VAPOR ENTHALPY
C           6     ALL LIQUID ENTHALPY (1/2 LIQ)
C           7     ISOTHERMAL FLASH (1/2 LIQ)
C           8     ISOTHERMAL FLASH ... NO DEW/BUBBLE POINT (1/2 LIQ)
C           9     ADIABATIC FLASH (1/2 LIQ)
C          10     ADIABATIC FLASH ... NO DEW/BUBBLE POINT (1/2 LIQ)
C          11     DEW POINT PRESSURE
C          12     BUBBLE POINT PRESSURE (1/2 LIQUID)
C          13     LIQ - LIQ SEPERATION BELOW BUBBLE POINT (2 LIQ)
C
  115 IF (NTYPE .GT. 13) GO TO 1000
C
C     SETTING MIN & MAX VAPOR FRACTION
C
      RMIN=0.0
      RMAX=1.0
      DO119I=1,NC
      IF (L(I)) 116,117,118
  116 RMAX=RMAX-Z(I)
      GO TO 118
  117 RMIN=RMIN+Z(I)
  118 CONTINUE
C
C     SETTING DEW POINT AND BUBBLE POINT CALCULATION SWITCHES
C
      NODEW=0
      NOBUB=0
C
      DO 140 I=1,NC
      IF (FD(I)) 140,140,119
  119 IF (L(I)) 120,130,140
  120 NODEW=1
      GO TO 140
  130 NOBUB=1
  140 CONTINUE
C
C     INTIALIZATION OF THE RESPECTIVE COMPOSITIONS OF TWO LIQUID PHASES
C
      IF (NTYPE .EQ. 13) NLIQ=2
      IF (NLIQ .NE. 2) GO TO 146
      T=TF
      CALL INTLIZ
C
C     WRITE (NPRT,145) T, TF, TSAVE
C 145 FORMAT ('  T , TF & TSAVE  IN FLASH2 ARE  ',3F12.4)
```

```
C
  146 GO TO (150,220,150,220,350,410,150,440,150,440,1000,
     *                                              1000,612),NTYPE
C
C     *** DEW POINT TEMPERATURE DETERMINATION ***
C               NTYPE=1, 3, 7 & 9
C
  150 WRITE (NPRT,151)
  151 FORMAT ('1RESULTS OF DEW POINT CALCULATION')
      IF (NODEW.EQ.0) GO TO 170
      WRITE (NPRT,160)
  160 FORMAT ('ONO DEW POINT SINCE NONVOLATILE COMPONENTS ARE PRESENT')
      TDEW=1.0E6
      DO 165 I=1,NC
  165 DEWC(I)=0.0
      IF (NTYPE.EQ.3) GO TO 350
      IF (NTYPE.EQ.7) GO TO 220
      IF (NTYPE.EQ.9) GO TO 220
      GO TO 665
C
  170 DO 180 I=1,NC
  180 Y(I)=Z(I)
      T=TF
C     WRITE (NPRT,185) T, TF, TSAVE
C 185 FORMAT ('  T , TF & TSAVE  IN FLASH2 AT STM# 185 ARE  ',3F12.4)
      NHOLD=NLIQ
      NLIQ=1
      CALL DEWT1
      TDEW=T
      TDEG=(TDEW-273.16)*1.8+32.0
      DO 190 I=1,NC
  190 DEWC(I)=X1(I)
      WRITE (NPRT,200) PRES, TDEG
  200 FORMAT ('ODEW POINT OF FEED AT',F7.2,' PSIA IS',F7.2,' DEG F')
      WRITE (NPRT,205) ((ZNAME(J,I),J=1,2),I=1,NC)
  205 FORMAT (25X,10(2A4,2X))
      WRITE (NPRT,210) (DEWC(I),I=1,NC)
  210 FORMAT (' DEW PT LIQ MOLE FRAC', 2X, 10F10.5)
      CALL PRINT2
      NLIQ=NHCLD
      IF (NTYPE.EQ.3) GO TO 320
      IF (NTYPE.EQ.7) GO TO 220
      IF (NTYPE.EQ.9) GO TO 220
      GO TO 665
C
C     *** BUBBLE POINT TEMPERATURE DETERMINATION ***
C
C             NTYPE=2, 4, 6, 7 & 9
C
  220 WRITE (NPRT,221)
  221 FORMAT (////'ORESULTS OF BUBBLE POINT CALCULATION')
      IF (NOBUB.EQ.0) GO TO 240
      WRITE (NPRT,230)
  230 FORMAT('ONO BUBBLE POINT SINCE NONCONDENSIBLE COMPONENTS ARE PRESE
     *NT')
  231 TBUB=-459.0
      DO 235 I=1,NC
  235 BUBC(I)=0.0
      IF (NTYPE.EQ.4) GO TO 410
      IF (NTYPE.EQ.7) GO TO 440
```

```
      IF (NTYPE.EQ.9) GO TO 440
      GO TO 665
C
  240 IF (NLIQ.EQ.2) GO TO 280
      DO 241 I=1,NC
  241 X1(I)=Z(I)
      T=TF
      FRACL=1.0
      CALL BUBT1
C
  245 IF (NOBUB.EQ.0) GO TO 255
      WRITE (NPRT,250)
  250 FORMAT('0FEED REPRESENTS A HYPOTHETICAL LIQUID OR IS IN THE RETROG
     +RADE REGION. BUBBLE POINT CALCULATIONS TERMINATED.')
      GO TO 231
C
  255 TBUB=T
      TDEG=(TBUB-273.16)*1.8+32.0
      WRITE (NPRT,260) PRES, TDEG
  260 FORMAT ('0BUBBLE POINT OF FEED AT',F7.2,' PSIA IS',F7.2,' DEG F')
      DO 265 I=1,NC
  265 BUBC(I)=Y(I)
      WRITE (NPRT,205) ((ZNAME(J,I),J=1,2),I=1,NC)
      WRITE (NPRT,270) (BUBC(I),I=1,NC)
  270 FORMAT (' BUB PT VAP MOLE FRAC', 2X, 10F10.5)
      CALL PRINT2
      IF (NTYPE.EQ.4) GO TO 380
      IF (NTYPE.EQ.7) GO TO 440
      IF (NTYPE.EQ.9) GO TO 440
      GO TO 665
  280 CONTINUE
      T=TF
C
C     ISO FLASH TEMP TF MAY NOT BE SUITABLE AS INTIAL GUESS FOR BUBT2
C
      IF (NTYPE .EQ. 7) T=0.98*TF
      FRACL=0.50
      CALL INTLIZ
      CALL BUBT2
      IF (NLIQ.EQ.1) GO TO 245
      WRITE (NPRT,285) FRACL
  285 FORMAT ('0TWO LIQ PHASE REGION, LIQUID PHASE MOLE RATIO', F12.6)
      GO TO 245
C
C     *** ALL VAPOR ENTHALPY WITH PRIOR DEW POINT ***
C
C         NTYPE=3 & 5
C
  320 IF (TF .LT. TDEW) GO TO 665
  330 WRITE (NPRT,340)
  340 FORMAT ('0FEED AT OR ABOVE DEW POINT')
  350 T=TF
      DO 360 I=1,NC
  360 Y(I)=Z(I)
      TDEG=(T-273.16)*1.8+32.0
      H = HVAP*TERM
      DHV=DHV*TERM
      HIDLV=H-DHV
      WRITE (NPRT,370) PRES,TDEG,H,HIDLV,DHV
  370 FORMAT ('0VAPOR PHASE ENTHALPY SUMMARY:'/
```

```
     *    5X,'P, PSIA =',F21.3/
     *    5X,'T, DEG F =',F20.2/
     *    5X,'HVAP (REAL), K-BTU =',F13.5/
     *    5X,'HVAP (IDEAL),K-BTU =',F13.5/
     *    5X,'DELTA HVAP , K-BTU =',F13.5)
      GO TO 665
C
C     *** ALL LIQUID ENTHALPY WITH PRIOR BUBBLE POINT ***
C
C         NTYPE= 4 & 6
C
  380 IF (TF .GT. TBUB) GO TO 665
  390 WRITE (NPRT,400)
  400 FORMAT ('0FEED AT OR BELOW BUBBLE POINT')
  410 T=TF
      NLIQ=NLIQSV
      GO TO (415,420), NLIQ
C
  415 DO 416 I=1,NC
  416 X1(I)=Z(I)
      DO 418 I=1,NC
  418 X(I)=X1(I)
      CALL LIQH
      HREALL(1)=HLIQ
      H=HREALL(1)
      HIDLL(1)=HLIQ-XSH
      DHL(1)=XSH
      GO TO 429
C
  420 CONTINUE
      CALL INTLIZ
      CALL TWOLIQ
      WRITE (NPRT,285) FPACL
  421 DO 423 I=1,NC
  423 X(I)=X1(I)
      CALL LIQH
      HREALL(1)=HLIQ
      HIDLL(1)= HLIQ-XSH
      DHL(1)  = XSH
      DO 424 I=1,NC
  424 X(I)=X2(I)
      CALL LIQH
      HREALL(2)=HLIQ
      HIDLL(2)= HLIQ-XSH
      DHL(2)  = XSH
      H=HREALL(1)*FRACL+HREALL(2)*(1.0-FRACL)
C
C     UNITS CONVERSION FROM CAL/G-MOLE TO TOTAL K-BTU
C
  429 TDEG=(T-273.16)*1.8+32.0
      H=H*TERM
      DO 430 N =1,NLIQ
      HREALL(N)=HREALL(N)*TERM
      HIDLL(N)=HIDLL(N)*TERM
      DHL(N)=DHL(N)*TERM
  430 CONTINUE
C
      CALL PRINT2
      WRITE (NPRT,435) PRES,TDEG,H
  435 FORMAT ('0LIQUID PHASE ENTHALPY SUMMARY:'/
```

```
     *    5X,'P, PSIA =',F21.3/
     *    5X,'T, DEG F =',F20.2/
     *    5X,'HLIQ (REAL), K-BTU =',F13.5)
C
      DO 439 N=1,NLIQ
      WRITE (NPRT,437) N
  437 FORMAT ('0ENTHALPY SUMMARY OF LIQUID PHASE # ',I1)
      WRITE (NPRT,438) HREALL(N),HIDLL(N),DHL(N)
  438 FORMAT ('      HLIQ (REAL), K-BTU =',F13.5/
     *          5X,'HLIQ (IDEAL),K-BTU =',F13.5/
     *          5X,'DELTA HLIQ , K-BTU =',F13.5)
  439 CONTINUE
      GO TO 665
C
C     INITIALIZE VAPOR & LIQUID PHASES FOR ISO & ADIABATIC FLASH
C
  440 CONTINUE
      IF (NOBUB.EQ.0) GO TO 480
      IF (NODEW.EQ.0) GO TO 550
C
  460 DO 470 I=1,NC
  470 Y(I)=BUBC(I)
      GO TO 570
C
  480 NLIQ=NLIQSV
      GO TO (490,520), NLIQ
  490 DO 500 I=1,NC
      IF (L(I)) 492,494,496
  492 Y(I)=0.0
      X1(I)=Z(I)
      GO TO 500
  494 Y(I)=Z(I)
      X1(I)=0.0
      GO TO 500
  496 Y(I)=Z(I)*0.5
      X1(I)=Y(I)
  500 CONTINUE
      UY=0.0
      UX=0.0
      DO 505 I=1,NC
      UY=UY+Y(I)
  505 UX=UX+X1(I)
      DO 510 I=1,NC
      Y(I)=Y(I)/UY
  510 X1(I)=X1(I)/UX
      GO TO 570
C
  520 DO 540 I=1,NC
      IF (L(I)) 522,528,530
  522 Y(I)=0.0
      IF (I .EQ. IE) GO TO 524
      IF (I .EQ. IR) GO TO 526
      X1(I)=Z(I)*0.5
      X2(I)=X1(I)
      GO TO 540
  524 X1(I)=Z(I)
      X2(I)=0.02
      GO TO 540
  526 X1(I)=0.02
      X2(I)=Z(I)
```

```
      GO TO 540
  528 Y(I)=Z(I)
      X1(I)=0.0
      X2(I)=0.0
      GO TO 540
  530 Y(I)=Z(I)*0.5
      IF (I .EQ. IE) GO TO 532
      IF (I .EQ. IR) GO TO 534
      X1(I)=Z(I)*0.25
      X2(I)=X1(I)
      GO TO 540
  532 X1(I)=Z(I)*0.5
      X2(I)=0.02
      GO TO 540
  534 X1(I)=0.02
      X2(I)=Z(I)*0.5
  540 CONTINUE
      SUM=0.0
      UY=0.0
      UX=0.0
      DO 542 I=1,NC
      SUM=SUM+Y(I)
      UY=UY+X1(I)
  542 UX=UX+X2(I)
      DO 544 I=1,NC
      Y(I)=Y(I)/SUM
      X1(I)=X1(I)/UY
  544 X2(I)=X2(I)/UX
      GO TO 570
C
  550 DO 552 I=1,NC
  552 Y(I)=Z(I)
      GO TO (554,558), NLIQ
  554 DO 556 I=1,NC
  556 X1(I)=DEWC(I)
      GO TO 570
  558 X1(IE)=DEWC(IE)
      X2(IE)=0.02
      X1(IR)=0.02
      X2(IR)=DEWC(IR)
      DO 560 I=1,NC
      IF (I .EQ. IE) GO TO 560
      IF (I .EQ. IR) GO TO 560
      X1(I)=DEWC(I)*0.5
      X2(I)=X1(I)
  560 CONTINUE
      SUM1=0.0
      SUM2=0.0
      DO 562 I=1,NC
      SUM1=SUM1+X1(I)
      SUM2=SUM2+X2(I)
  562 CONTINUE
      DO 564 I =1,NC
      X1(I)=X1(I)/SUM1
      X2(I)=X2(I)/SUM2
  564 CONTINUE
  570 CONTINUE
      IF (NTYPE .EQ.7) GO TO 585
      IF (NTYPE .EQ. 6) GO TO 590
C
```

```
C     *** ADIABATIC FLASH ***
C
C         NTYPE=9 & 10
C
      IF (HRUN .EQ. 0.0) GO TO 1000
      WRITE (NPRT,581)
  581 FORMAT ('1RESULTS OF ADIABATIC FLASH CALCULATION')
      T=TF
      HI=HRUN
      CALL AFLSH2
      GO TO 600
C
C     *** ISOTHERMAL FLASH ***
C
C         NTYPE=7 & 8
C
  585 CONTINUE
      IF (TF .GT. TDEW) GO TO 330
      IF (TF .LT. TBUB) GO TO 390
  590 T=TF
      WRITE (NPRT,591)
  591 FORMAT ('1RESULTS OF ISOTHERMAL FLASH CALCULATION')
      IF (LDBUG .GE. 2) WRITE (NPRT,594) (X1(I),I=1,NC),(X2(I),I=1,NC)
  594 FORMAT ('0IN FLASH2 AT STMT#594 X1 & X2 ARE ='/10(F7.5,2X)/
     *10(F7.5,2X))
      NLIQ=NLIQSV
      GO TO (592,593), NLIQ
  592 CALL FLSH1
      GO TO 600
  593 CALL FLSH2
C
  600 TDEG=(T-273.16)*1.8+32.0
      WRITE (NPRT,610) TDEG,PRES,FRACV
  610 FORMAT('0SYSTEM IS IN THE V/L PHASE REGION AT',F7.2,' DEG F AND',
     * F7.2,' PSIA'/'                    VAPOR/FEED MOLE RATIO',2X,F9.6)
      IF (NLIQ.EQ.2) WRITE(NPRT,285) FRACL
C
      CALL PRINT2
      GO TO 620
C
C     *** LIQ - LIQ SEPERATION AT T BELOW BUBBLE POINT ***
C
C         NTYPE=13
C
  612 T=TF
      FRACL=0.5
      CALL TWOLIQ
      WRITE (NPRT,614)
  614 FORMAT ('0LIQUID - LIQUID SEPERATION BELOW BUBBLE POINT')
      TDEG=(T-273.16)*1.8+32.0
      WRITE (NPRT,616) NLIQ,TDEG
  616 FORMAT ('0SYSTEM IS IN THE ',I1,' LIQUID PHASE REGION AT',
     * F7.2,' DEG F')
      IF (NLIQ.EQ.2) WRITE(NPRT,285) FRACL
      GO TO 421
C
C     CALCULATION OF VAP/LIQ ENTHALPIES AFTER ISO/ADIAB FLASH
C
  620 DO 622 I=1,NC
  622 X(I)=X1(I)
```

```
      CALL LIQH
      HREALL(1)=HLIQ
      HIDLL(1)= HLIQ-XSH
      DHL(1)  = XSH
      IF (NLIQ .NE. 2)GO TO 625
      DO 624 I=1,NC
  624 X(I)=X2(I)
      CALL LIQH
      HREALL(2)=HLIQ
      HIDLL(2)= HLIQ-XSH
      DHL(2)  = XSH
  625 CALL VAPH
C
      TDEG=(T-273.16)*1.8+32.0
      HVAPOR=HVAP*TERM
      DHV=DHV*TERM
      HIDLV=HVAPOR-DHV
      WRITE (NPRT,370) PRES,TDEG,HVAPOR,HIDLV,DHV
      GO TO (631,632),NLIQ
  631 HLIQD(1)=HREALL(1)
      HLIQD(2)=0.0
      GO TO 633
  632 HLIQD(1)=HREALL(1)
      HLIQD(2)=HREALL(2)
C
  633 DO 635 N=1,NLIQ
      HIDLL(N)=HIDLL(N)*TERM
      HLIQD(N)=HLIQD(N)*TERM
      DHL(N)=(HLIQD(N)-HIDLL(N))
      WRITE (NPRT,437) N
      WRITE (NPRT,438)HLIQD(N),HIDLL(N),DHL(N)
  635 CONTINUE
      H=HVAPOR*FRACV+HLIQD(1)*(1.0-FRACV)*FRACL
      IF (NLIQ .EQ. 2) H=H+HLIQD(2)*(1.0-FRACV)*(1.0-FRACL)
C
      WRITE (NPRT,640) PRES,TDEG,H
  640 FORMAT ('OTOTAL ENTHALPY SUMMARY:'/
     *    5X,'P, PSIA =',F21.3/
     *    5X,'T, DEG F =',F20.2/
     *    5X,'H  (REAL), K-BTU =',F13.5)
C
C     HI IS THE ENTHALPY ASSOCIATED WITH THE ADIABATIC
C     FLASH FEED STREAM.
C     ISOTHERMAL FLASH CAN BE PERFORMED BEFORE THE ADIABATIC
C     FLASH TO ESTABLISH FEED, IN THE MULTIPLE CASE PROBLEM.
C
      IF (NTYPE .EQ. 7 .OR. NTYPE .EQ. 8) THEN
         HI=HVAP*FRACV+HREALL(1)*(1.0-FRACV)*FRACL+
     %      HREALL(2)*(1.0-FRACV)*(1.0-FRACL)
      END IF
C
  665 IF (JCODE.NE.0) GO TO 15
C
C     CODE FOR INTERACTIVE MODE HAS TO BE MODIFIED.
C
      INDX=3
  670 WRITE (6,680)
  680 FORMAT (' ENTER CHANGES'/' ')
      WRITE (6,690)
  690 FORMAT (////)
```

```
  700 READ (5,710) I,S
  710 FORMAT (A1,F10.9)
      DO 720 J=1,7
      IF (I-IJK(J)) 720,740,720
  720 CONTINUE
      WRITE (6,730)
  730 FORMAT (' INVALID DATA'/' ')
      GO TO 700
  740 GO TO (760,750,770,840,860,10,830), J
  750 IF (INDX .GT. 2) INDX=2
      P=S
C     CALL M19P (IPF,P)
      GO TO 700
  760 IF (INDX .GT. 3) INDX=3
      TF=S
C     CALL M19T (ITF,TF)
      GO TO 700
  770 IF (INDX .GT. 1) INDX=1
      write (6,780)
  780 FORMAT (' ENTER FEED COMPOSITION (8F10.0)'/' ')
      read (5,790) (FD(I),I=1,NC)
  790 FORMAT (10F10.5)
      S=0.0
      DO 800 I=1,NC
  800 S=S+FD(I)
      IF (S.NE.0.0) GO TO 700
      read (5,790,END=810) (FD(I),I=1,NC)
      GO TO 700
  810 write (6,820)
  820 FORMAT(' ERROR:  NO FEED COMPOSITION THRU EITHER KEY BOARD OR INPU
     *T DATA CARDS')
C
  830 GO TO (15,150,320), INDX
C
  840 NTYPE=1
      HI=HI+S
      write (6,850) S
  850 FORMAT('ONONISOTHERMAL MODE ENTERED.   Q =',F10.2,' BTU/LBMOL'/
     * ' ')
      GO TO 700
  860 NTYPE=S
      GO TO 700
C
 1000 WRITE (NPRT,1100)
 1100 FORMAT(' EXITING FLASH2 WITH INCOMPLETE CALCULATIONS')
 1500 CALL EXIT
      STOP
      END
```

```
      SUBROUTINE TWOLIQ
C
C     TWO PHASE MATERIAL BALANCE USED FOR
C         *  BUBBLE POINT
C         *  SUBCOOLED LIQUID
C     OPTION OF DIFFERENT PARAMETER SETS FOR VLE AND LLE INCLUDED
C     THROUGH IPSET.
C
      COMMON  /BLANK/  NCR, NPRT, NSTART, KUNITS, TITLE(20)
      COMMON  /CMPRO/  NC, NCM1, NCP1, IDLL, IDLV, IDH, LDBUG, ISW,
     *                 NDIM, ZNAME(2,10), L(10), NTCOMP(10), NLIQ, IPSET
      COMMON  /ZDATA/  CPL(10,4), CPV(10,4), ENP(10,10), ANT(6,10),
     *                 W(10), AX, BX, OMEGA(10), AVAL(10), BVAL(10),
     *                 AK(10,10), R(10), Q(10), QP(10), XL(10),
     *                 VOL(10), C(180), ALPHA(45), VC(10), TC(10),
     *                 PC(10), ZC(10), TNBP(10), OA(10), OB(10),
     *                 A(10,10), G(10,10), ZRA(10), RD(10), DMU(10),
     *                 ETA(10)
      COMMON  /STRM/   T, P, Z(10), Y(10), X(10), FRACV, ZVAP,
     *                 EK(10), VP(10), FUG(10), GAM(10), SVAP,
     *                 HOFZ, HVAP, HLIQ, DHV, XSH, NOBUB, NODEW
      COMMON  /CONTRL/ ITF, IPF,  N, NTYPE, JCODE
      COMMON  /TWOLQ/  X1(10), X2(10), GAM1(10), GAM2(10), EK1(10),
     +                 EK2(10), DHL(2), HIDLL(2), HREALL(2), FRACL,
     +                 IE, IR, XMAX, XMIN
      COMMON  /ZFEEDZ/ PF, TF, FEED, FMOL, TREF, HI
      COMMON   /DUMMY/ XX(10,2),SX(10,2),XC(10,2),YY(10),SY(10),YC(10),
     +                 RMAX, RMIN
      DIMENSION        RG(10), XTEMP(10,2)
C
      DATA             CONV/1.0E-5/, CONV1/1.E-5/, CONV2/1.E-3/,
     *                 NOBJ /3/, GUESS /0.50/, KMAX/100/
C
C     ENTRY TO SUBROUTINE SWITCH IS MADE TO LOAD LLE PARAMETERS IF
C     SEPERATE SETS OF PARAMETERS ARE USED
C
      IF (IPSET .EQ. 0) GO TO 3
      IPSET=2
      CALL SWITCH
    3 INDEX=0
      KNT=0
      IDX=1
      ISAVE=ISW
      ISW=0
      DO 5 I =1,NC
      GAM1(I)=1.0
      GAM2(I)=1.0
    5 CONTINUE
      FRACL=0.5
      IF (LDBUG .GT. 2) THEN
        WRITE (NPRT,6)
    6   FORMAT (/' CHECK ON PARAMETER VALUES IN TWOLIQ SMT * 6'/)
        CALL PRCHK
        END IF
      IF (X1(IE).LE.1.E-12 .OR. X2(IR).LE.1.E-12) CALL INTLIZ
      IF (LDBUG .GE. 2) WRITE (NPRT,7) IDLL
    7 FORMAT(' IDLL AT THE BEGINING OF TWOLIQ IS ',I4)
      CALL ACTVY(T,P,X1,GAM1)
C
      KNTX=0
```

```
      IZEROS=0
      DO 8 I=1,NC
      IF (X2(I) .GT. 0.0) GO TO 8
      KNTX=KNTX+1
    8 CONTINUE
      IF (KNTX .GE. NC) THEN
         DO 9 I=1,NC
    9    GAM2(I)=1.0
         IZEROS=1
         GO TO 11
      ELSE
         CALL ACTVY(T,P,X2,GAM2)
      END IF
C
   11 ISW=1
      IF (LDBUG.GE.2)WRITE (NPRT,15)(GAM1(I),I=1,NC),(GAM2(I),I=1,NC)
   15 FORMAT('  GAM1 & GAM2 FOR ALL COMPONENTS ARE ',/6F12.4)
      GO TO 30
C
   20 CALL ACTVY(T,P,X1,GAM1)
      IF (IZEROS .EQ. 0) CALL ACTVY(T,P,X2,GAM2)
   30 DO 40 I=1,NC
   40 RG(I)=GAM1(I)/GAM2(I)
      K=0
C
      IF (LDBUG.GE.1) THEN
         WRITE(NPRT,45) (X1(I),I=1,NC)
         WRITE(NPRT,46) (X2(I),I=1,NC)
         WRITE(NPRT,47) (GAM1(I),I=1,NC)
         WRITE(NPRT,48) (GAM2(I),I=1,NC)
   45    FORMAT ('0X1-ASS ',10E13.5)
   46    FORMAT ('0X2-ASS ',10E13.5)
   47    FORMAT ('0GAM1   ',10E13.5)
   48    FORMAT ('0GAM2   ',10E13.5)
      END IF
C
C     INNER LOOP: SOLVING FOR FRACL FOR A SET OF COMPOSITIONS
C
C
C     FRACL=GUESS
   50 F2=0.0
      DF2=0.0
      DDF2=0.0
      DO 60 I=1,NC
      IF (L(I).EQ.0 .OR. Z(I).LT.1.0E-12) GO TO 60
      B=Z(I)*(1.0-RG(I))
      WW=FRACL+(1.0-FRACL)*RG(I)
      DWW=1.0-RG(I)
      F2=F2+B/WW
      DF2=DF2-B/WW**2*DWW
C     DDF2=DDF2+2.0*B/WW**3*DWW**2
   60 CONTINUE
C     CC=F2*DF2
C     FF=DF2**2-F2*DDF2
C     DEL=-CC/FF
      DEL=-F2/DF2
      K=K+1
C
      IF (LDBUG.GE.1) WRITE(NPRT,62) KNT,T,F2,FRACL,DEL
   62 FORMAT (' KNT-T-F2-FRACL-DEL', I3,F12.4,3E14.5)
```

```
C
      IF (K .LT. 20) GO TO 70
   63 WRITE(NPRT,64)
   64 FORMAT ('0TWOLIQ CALCULATION TERMINATED'/
     +         ' CALCULATION CONTINUING' /)
      DO 66 I=1,NC
      WW=FRACL+(1.0-FRACL)*RG(I)
      X1(I)=Z(I)/WW
   66 X2(I)=X1(I)*RG(I)
      SUM1=0.0
      SUM2=0.0
      DO 67 I =1,NC
      SUM1=SUM1+X1(I)
      SUM2=SUM2+X2(I)
  67  CONTINUE
      DO 68 I =1,NC
      X1(I)=X1(I)/SUM1
      X2(I)=X2(I)/SUM2
  68  CONTINUE
      ISW=ISAVE
C
C     ENTRY TO SUBROUTINE SWITCH IS MADE TO LOAD BACK VLE PARAMETERS
C     IF SEPERATE SETS OF PARAMETERS ARE USED
C
      IF (IPSET .EQ. 0) GO TO 69
      IPSET=1
      CALL SWITCH
   69 RETURN
C
   70 NCVRG=0
   75 IF (FRACL+DEL.LT.1.0 .AND. FRACL+DEL.GT.0.0) GO TO 80
      NCVRG=1
      DEL=DEL*0.5
      GO TO 75
C
C  80 IF (FRACL.LT.0.99999) GO TO 85
   80 IF (FRACL .GT. 1.0E-5) GO TO 85
      FRACL=1.0-FRACL
      DO 81 I=1,NC
      HOLD=X1(I)
      X1(I)=X2(I)
      X2(I)=HOLD
      HOLD=XX(I,1)
      XX(I,1)=XX(I,2)
      XX(I,2)=HOLD
      HOLD=SX(I,1)
      SX(I,1)=SX(I,2)
      SX(I,2)=HOLD
      HOLD=XC(I,1)
      XC(I,1)=XC(I,2)
      XC(I,2)=HOLD
      HOLD=GAM1(I)
      GAM1(I)=GAM2(I)
   81 GAM2(I)=HOLD
C  85 IF (FRACL.LT.1.0E-5) GO TO 166
   85 IF (FRACL .GT. 0.99999) GO TO 166
C
   90 IF (ABS(F2).LT.CONV .AND. ABS(DEL).LT.CONV .AND. NCVRG.EQ.0)
     +    GO TO 95
      FRACL=FRACL+DEL
```

```
      GO TO 50
C
   95 DO 100 I=1,NC
      WW=FRACL+(1.0-FRACL)*RG(I)
      XX(I,1)=Z(I)/WW
  100 XX(I,2)=XX(I,1)*RG(I)
C
      IF (LDBUG.GE.1) THEN
         WRITE(NPRT,102) (XX(I,1),I=1,NC)
         WRITE(NPRT,103) (XX(I,2),I=1,NC)
  102    FORMAT ('0X1-CALC ',10E13.5)
  103    FORMAT ('0X2-CALC ',10E13.5)
      END IF
C
C     INNER LOOP: SOLVING FOR FRACL FOR A SET OF COMPOSITIONS
C
      KNT=KNT+1
      IF (KNT .EQ. KMAX) GO TO 63
      GO TO (110,150), IDX
C
C     THE VALUE OF KNT=1
  110 IDX=2
      DO 115 N = 1,2
      DO 115 I =1,NC
  115 XC(I,N)=XX(I,N)
      SUM1=0.0
      SUM2=0.0
      DO 120 I =1,NC
      SX (I,1)=X1(I)
      SX(I,2)=X2(I)
      X1(I)=(X1(I)+XX(I,1))/2.0
      X2(I)=(X2(I)+XX(I,2))/2.0
      SUM1=SUM1+X1(I)
 120  SUM2=SUM2+X2(I)
      DO 130 I=1,NC
      X1(I)=X1(I)/SUM1
  130 X2(I)=X2(I)/SUM2
      GO TO 20
C
  150 CONTINUE
C     PERFORM TEST FOR CONVERGENCE ONLY ON RESULTS OF
C     NON-ACCELERATED DATA USED FOR GAMMA
C     KAC=0 CHECK X VALUES .. IF NOT CONV. GO TO WEG
C     KAC>0 DO NOT CHECK X VALUES, USE DIRECT SUBSTITUTION
C           TO GET NEXT VALUES OF X'S
      KAC=0
      IF (MOD(KNT,2) .EQ. 0) KAC=2
      IF (KAC .NE. 0) GO TO 240
C
C     ONE OF THE THREE OBJECTIVE FUNCTIONS CAN BE CHOSEN TO
C     SATISFY THE LIQ-LIQ EQUILIBRIUM CRITERIA.
C
C     NOBJ=1 : TEST ON ACTIVITIES
C     NOBJ=2 : TEST ON COMPOSITIONS
C     NOBJ=3 : TEST ON SUMMATION OF ACTIVITIES
C     NOBJ=4 : TEST ON ACTIVITIES AND COMPOSITIONS
C
      SUM=0.0
      DO 164 I=1,NC
      IF (L(I).EQ.0 .OR. Z(I).LT.1.0E-12) GO TO 164
```

```
      GO TO (155,157,159,161), NOBJ
C     NOBJ=1 : TEST ON ACTIVITIES
  155 IF (ABS(X1(I)*GAM1(I)-X2(I)*GAM2(I))/(X2(I)*GAM2(I)) .GT.
     +    CONV1) GO TO 190
      GO TO 164
C     NOBJ=2 : TEST ON COMPOSITIONS
C
  157 IF (ABS((X1(I)-XX(I,1))/X1(I)) .GT. CONV1 .OR.
     *ABS((X2(I)-XX(I,2))/X2(I)) .GT. CONV1)GO TO 190
      GO TO 164
C
C     NOBJ=3 : TEST ON SUMMATION OF ACTIVITIES
  159 SUM=SUM+ABS(X1(I)*GAM1(I)-X2(I)*GAM2(I))
      GO TO 164
C
C     NOBJ=4 : TEST ON ACTIVITIES AND COMPOSITIONS
  161 IF (ABS(X1(I)*GAM1(I)-X2(I)*GAM2(I))/(X2(I)*GAM2(I)) .GT.
     +    CONV1) GO TO 190
      IF (ABS((X1(I)-XX(I,1))/X1(I)) .GT. CONV1 .OR.
     *ABS((X2(I)-XX(I,2))/X2(I)) .GT. CONV1)GO TO 190
  164 CONTINUE
C
      IF (NOBJ .EQ. 3 .AND. SUM .GT. CONV2)GO TO 190
      INDEX=1
      GO TO 170
C
  166 DO 167 I=1,NC
      X1(I)=Z(I)
  167 X2(I)=0.0
      NLIQ=1
      WRITE(NPRT,168)
  168 FORMAT (// 5X, 'LIQUID HAS GONE TO A ONE PHASE SYSTEM' //)
C
C     ENTRY TO SUBROUTINE SWITCH IS MADE TO LOAD BACK VLE PARAMETERS
C     IF SEPERATE SETS OF PARAMETERS ARE USED
C
      IF (IPSET .EQ. 0) GO TO 169
      IPSET=1
      CALL SWITCH
  169 RETURN
C
  170 SUM1=0.0
      SUM2=0.0
      DO 172 I=1,NC
      SUM1=SUM1+X1(I)
      SUM2=SUM2+X2(I)
  172 CONTINUE
      DO 174 I =1,NC
      X1(I)=X1(I)/SUM1
      X2(I)=X2(I)/SUM2
  174 CONTINUE
      ISW=ISAVE
      IF (INDEX .EQ. 1) WRITE(NPRT,180)
  180 FORMAT('0TWO LIQUID CALCULATIONS SUCCESSFULLY COMPLETED')
C
C     ENTRY TO SUBROUTINE SWITC1 IS MADE TO LOAD BACK VLE PARAMETERS
C     IF SEPERATE SETS OF PARAMETERS ARE USED
C
      IF (IPSET .EQ. 0) GO TO 185
      IPSET=1
```

```
      CALL SWITCH
  185 RETURN
C
  190 CONTINUE
C     WEG BYPASSED
C     IF (KNT .GE. 0) GO TO 240
      IF (LDBUG .GE. 1) WRITE (NPRT,192)KNT
  192 FORMAT(1X,I4,4X,' BEFORE CALL WEG IN TWOLIQ:')
      DO 220 N=1,2
      SUM1=0.0
      SUM2=0.0
      DO 200 I=1,NC
      IF (L(I).EQ.0 .OR. Z(I).LT.1.0E-12) GO TO 200
      IF (N .EQ.1) XTEMP(I,N)=X1(I)
      IF (N .EQ. 2) XTEMP(I,N)=X2(I)
C
      IF (LDBUG .GE. 1) WRITE (NPRT,195)XTEMP(I,N),XX(I,N),SX(I,N),
     * XC(I,N)
  195 FORMAT(' XTEMP=',E13.5,'  XX=',E13.5,'  SX=',E13.5,'  XC=',E13.5)
C
      XXSAVE=XTEMP(I,N)
      CALL WEG (XTEMP(I,N),XX(I,N),SX(I,N),XC(I,N))
      IF (XTEMP(I,N) .LT. 0.0) XTEMP(I,N)=XXSAVE
      IF (XTEMP(I,N) .GT. 1.0) XTEMP(I,N)=XXSAVE
C*    XDIFF=ABS(XTEMP(I,N)-XXSAVE)
C*    IF (XDIFF .GT. 0.25*XXSAVE) XTEMP(I,N)=XXSAVE+XDIFF
      IF (LDBUG .GE. 1) WRITE (NPRT,195)XTEMP(I,N),XX(I,N),SX(I,N),
     * XC(I,N)
      IF (N .EQ. 1) SUM1=SUM1+XTEMP(I,N)
      IF (N .EQ. 2) SUM2=SUM2+XTEMP(I,N)
  200 CONTINUE
      DO 210 I=1,NC
      IF (N .EQ.1) X1(I)=XTEMP(I,N)/SUM1
  210 IF (N .EQ.2) X2(I)=XTEMP(I,N)/SUM2
  220 CONTINUE
      IF (LDBUG.GE.1) THEN
         WRITE(NPRT,225) (X1(I),I=1,NC)
         WRITE(NPRT,227) (X2(I),I=1,NC)
  225    FORMAT ('0X1-WEG ',10E13.5)
  227    FORMAT ('0X2-WEG ',10E13.5)
      END IF
C
C     INNER LOOP: SOLVING FOR FRACL FOR A SET OF COMPOSITIONS
C
C     KAC>0 .. USE DIRECT SUBSTITUTION & NORMALIZE
C
  240 CONTINUE
      SUM1=0.0
      SUM2=0.0
      DO 270 I=1,NC
C     X1(I)=XX(I,1)
C     X2(I)=XX(I,2)
      X1(I)=(XX(I,1)+X1(I))/2.0
      X2(I)=(XX(I,2)+X2(I))/2.0
      SUM1=SUM1+X1(I)
      SUM2=SUM2+X2(I)
  270 CONTINUE
      DO 280 I =1,NC
      X1(I)=X1(I)/SUM1
      X2(I)=X2(I)/SUM2
```

```
  280 CONTINUE
C
      GO TO 20
      END
      SUBROUTINE FLSH1
C
C     ISOTHERMAL FLASH *** ONE LIQUID
C
C
      COMMON  /BLANK/  NCR, NPRT, NSTART, KUNITS, TITLE(20)
      COMMON  /CMPRO/  NC, NCM1, NCP1, IDLL, IDLV, IDH, LDBUG, ISW,
     *                 NDIM, ZNAME(2,10), L(10), NTCOMP(10), NLIQ, IPSET
      COMMON  /ZDATA/  CPL(10,4), CPV(10,4), ENP(10,10), ANT(6,10),
     *                 W(10), AX, BX, OMEGA(10), AVAL(10), BVAL(10),
     *                 AK(10,10), R(10), Q(10), QP(10), XL(10),
     *                 VCL(10), C(180), ALPHA(45), VC(10), TC(10),
     *                 PC(10), ZC(10), TNBP(10), DA(10), DB(10),
     *                 A(10,10), G(10,10), ZRA(10), RD(10), DMU(10),
     *                 ETA(10)
      COMMON  /STRM/   T, P, Z(10), Y(10), X(10), FRACV, ZVAP,
     *                 EK(10), VP(10), FUG(10), GAM(10), SVAP,
     *                 HOFZ, HVAP, HLIQ, DHV, XSH, NDBUG, NODEW
      COMMON  /CONTRL/ ITF, IPF,  N, NTYPE, JCODE
      COMMON  /TWOLQ/  X1(10), X2(10), GAM1(10), GAM2(10), EK1(10),
     +                 EK2(10), DHL(2), HIDLL(2), HREALL(2), FRACL,
     +                 IE, IR, XMAX, XMIN
      COMMON  /ZFEEDZ/ PF, TF, FEED(10), FMOL, TREF, HI
      COMMON  /DUMMY/  XX(20), SX(20), XC(20), YY(10), SY(10),YC(10),
     +                 RMAX, RMIN
C
      EQUIVALENCE      (RVF,FRACV)
C
      DATA             CONV/1.0E-4/,  CONV1/1.E-5/
C
C     RVF IS VAPOR FRACTION
C     CALLING PROGRAM MUST SUPPLY INITIAL VALUE FOR RVF,X,Y
C
      KNT=0
      IDX=1
      ISW=0
      CALL KCALC2
      ISW=1
      IF (NC.GT.1) GO TO  21
C
      Y(1)=1.0
      X1(1)=1.0
      RETURN
C
   20 CALL KCALC2
C
   21 IF (LDBUG.GE.1) WRITE(NPRT,25) KNT,T,RVF
   25 FORMAT ('0KNT = ',I3,'  FLSH*1  T&RVF', F12.4,E14.5)
      IF (LDBUG.GE.2) WRITE(NPRT,26) (Y(I),I=1,NC),(X1(I),I=1,NC)
   26 FORMAT ('0Y-ASS   ',3E13.5/' X-ASS   ',3E13.5)
C
   29 K=0
   30 AMAX=RMAX
      AMIN=RMIN
      F=0.0
      DF=0.0
```

```
      DO 80 I=1,NC
      IF (L(I)) 40,50,60
   40 S=1.0/(1.0-RVF)
      GO TO 70
   50 S=-1.0/RVF
      GO TO 70
   60 S=(1.0-EK1(I ))/(1.0+RVF*(EK1(I )-1.0))
   70 F=F+Z(I)*S
   80 DF=DF+Z(I)*S*S
      K=K+1
C
      IF (LDBUG.GE.2) WRITE(NPRT,90) K,F,DF,RVF
   90 FORMAT (5X,'K = ',I2,' F-DF-RVF',3E14.5 )
C
      IF (K.LT.20) GO TO 99
   91 WRITE (NPRT,92)
   92 FORMAT ('OFLASH#1 CALCULATION TERMINATED'/
     +      ' CALCULATION CONTINUING' /)
      GO TO 320
C
   99 IF (ABS(F) .LT. CONV1) GO TO 190
C  99 IF (F) 100,190,110
C 100 AMIN=RVF
C     GO TO 120
C 110 AMAX=RVF
C 120 IF ((AMAX-AMIN).LT.CONV1)GO TO 170
C     DF=-F/DF
C 130 F=RVF+DF
C     IF (F-AMIN)140,150,150
C 140 DF=DF*.50
C     GO TO 130
C 150 IF (F-AMAX)160,160,140
C 160 RVF=F
C
      IF (ABS(RVF-AMIN).LT.CONV1 .OR. ABS(RVF-AMAX).LT.CONV1) GO TO 190
      DR=-F/DF
  130 RNEXT=RVF+DR
      IF (RNEXT .GE. AMIN) GO TO 150
  140 DR=DR*0.5
      GO TO 130
  150 IF (RNEXT .GT. AMAX) GO TO 140
      RVF=RNEXT
C
C     IF (ABS(DF)-CONV1)190,30,30
      IF (ABS(DR) .GT. CONV1) GO TO 30
C
C 170 CONTINUE
C     SUM=0.0
C     DO 180 I=1,NC
C     X1(I)=(X1(I)+SX(I))/2.0
C 180 SUM=SUM+X1(I)
C     DO 185 I=1,NC
C 165 X1(I)=X1(I)/SUM
C     GO TO 20
C
  190 IF (LDBUG .GE. 2) WRITE (NPRT,200) RVF
  200 FORMAT (5X, 'RVF', E14.5)
      DO 240 I=1,NC
      IF (L(I)) 210,220,230
  210 XX(I )=Z(I)/(1.0-RVF)
```

```
      YY(I)=0.0
      GO TO 240
  220 XX(I )=0.0
      YY(I)=Z(I)/RVF
      GO TO 240
  230 XX(I)=Z(I)/(1.0+RVF*(EK1(I)-1.0))
      YY(I)=EK1(I)*XX(I)
  240 CONTINUE
      IF (IDLL+IDLV.EQ.0) GO TO 320
C
  250 KNT=KNT+1
      IF (KNT.EQ.50) GO TO 91
      GO TO (340,260), IDX
C
  260 IF (IDLL.EQ.0) GO TO 290
      DO 280 I=1,NC
      IF ((L(I) .EQ. 0) .OR. (Z(I) .LT. 1.0E-12)) GO TO 280
      IF (ABS(X1(I)-XX(I))/X1(I) .GT. CONV) GO TO 410
  280 CONTINUE
C
  290 IF (IDLV .EQ. 0) GO TO 320
      DO 310 I=1,NC
      IF ((L(I) .LT. 0) .OR. (Z(I) .LT. 1.0E-12)) GO TO 310
      IF (ABS(Y(I)-YY(I))/Y(I)-CONV) 310,410,410
  310 CONTINUE
C
  320 UX=0.0
      UY=0.0
      DO 330 I=1,NC
      X1(I)=XX(I)
      Y(I)=YY(I)
      UX=UX+X1(I)
  330 UY=UY+Y(I)
      DO 335 I=1,NC
      X1(I)=X1(I)/UX
  335 Y(I)=Y(I)/UY
      ISW=0
      RETURN
C
  340 IF (IDLL.EQ.0) GO TO 370
      DO 360 I=1,NC
      SX(I)=X1(I)
      XC(I)=XX(I)
  360 X1(I)=(XX(I)+X1(I))/2.0
  370 IF (IDLV.EQ.0) GO TO 400
      DO 390 I=1,NC
      SY(I)=Y(I)
      YC(I)=YY(I)
  390 Y(I)=(YY(I)+Y(I))/2.0
  400 IDX=2
      FRACV=0.5*(RMAX+RMIN)
      GO TO 20
C
  410 IF (IDLL.EQ.0) GO TO 450
      SUM=0.0
      DO 430 I=1,NC
      IF ((L(I) .EQ. 0) .OR. (Z(I) .LT. 1.0E-12)) GO TO 430
      CALL WEG (X1(I),XX(I),SX(I),XC(I))
      SUM=SUM+X1(I)
  430 CONTINUE
```

```
      DO 440 I=1,NC
  440 X1(I)=X1(I)/SUM
C
  450 IF (IDLV.EQ.0) GO TO 500
      SUM=0.0
      DO 470 I=1,NC
      IF ((L(I) .LT. 0) .OR. (Z(I) .LT. 1.0E-12)) GO TO 470
      CALL WEG(Y(I),YY(I),SY(I),YC(I))
      SUM=SUM+Y(I)
  470 CONTINUE
      DO480I=1,NC
  480 Y(I)=Y(I)/SUM
  500 FRACV=(RMAX+RMIN)*0.5
      GO TO 20
C
      END
      SUBROUTINE FLSH2
C
C     ISOTHERMAL FLASH *** TWO LIQUIDS
C
C
C
      COMMON  /BLANK/  NCR, NPRT, NSTART, KUNITS, TITLE(20)
      COMMON  /CMPRO/  NC, NCM1, NCP1, IDLL, IDLV, IDH, LDBUG, ISW,
     *                 NDIM, ZNAME(2,10), L(10), NTCOMP(10), NLIQ, IPSET
      COMMON  /ZDATA/  CPL(10,4), CPV(10,4), ENP(10,10), ANT(6,10),
     *                 W(10), AX, BX, OMEGA(10), AVAL(10), BVAL(10),
     *                 AK(10,10), R(10), Q(10), QP(10), XL(10),
     *                 VOL(10), C(180), ALPHA(45), VC(10), TC(10),
     *                 PC(10), ZC(10), TNBP(10), CA(10), OB(10),
     *                 A(10,10), G(10,10), ZRA(10), RD(10), DMU(10),
     *                 ETA(10)
      COMMON  /STRM/   T, P, Z(10), Y(10), X(10), FRACV, ZVAP,
     *                 EK(10), VP(10), FUG(10), GAM(10), SVAP,
     *                 HOFZ, HVAP, HLIQ, DHV, XSH, NOBUB, NODEW
      COMMON  /CONTRL/ ITF, IPF,  N, NTYPE, JCODE
      COMMON  /TWOLQ/  X1(10), X2(10), GAM1(10), GAM2(10), EK1(10),
     +                 EK2(10), DHL(2), HIDLL(2), HREALL(2), FRACL,
     +                 IE, IR, XMAX, XMIN
      COMMON  /ZFEEDZ/ PF, TF, FEED(10), FMOL, TREF, HI
      COMMON   /DUMMY/ XX(10,2),SX(10,2),XC(10,2),YY(10),SY(10),YC(10),
     +                 RMAX, RMIN
C
      DIMENSION        RKS(10), ZJ(2,2), RHS(2), XTEMP(10,2)
      EQUIVALENCE      (U,FRACV), (V,FRACL)
C
      DATA             CONV/1.0E-4/,  CONV1/1.E-5/,  CONV2/1.E-5/
C
      KNT=0
      IDX=1
      ISW=0
      FRACV=0.5
      FRACL=0.5
      IF (LDBUG .GE. 2) WRITE (NPRT,5) (Z(I),I=1,NC)
    5 FORMAT ('0IN FLSH2 Z(I) ARE = ',10(F7.5,2X))
      CALL KCALC2
      ISW=1
      IF (NC .GT. 2) GO TO 26
C
      CALL TWOLIQ
```

```
      IF (LDBUG .GT. 2) THEN
        WRITE (NPRT,7)
    7   FORMAT (/' CHECK ON PARAMETER VALUES IN FLSH2 SMT * 7'/)
        CALL PRCHK
        END IF
      CALL KCALC2
      DO 11 I=1,NC
   11 Y(I)=EK1(I)*X1(I)
      IF (IDLV .EQ. 0) GO TO 240
      GO TO 13
   12 CALL KCALC2
   13 CALL TWCLIQ
      GO TO (14,17), IDX
   14 SUM=0.0
      DO 15 I=1,NC
      YY(I)=EK1(I)*X1(I)
      SY(I)=Y(I)
      YC(I)=YY(I)
      Y(I)=(Y(I)+YY(I))/2.0
   15 SUM=SUM+Y(I)
      DO 16 I=1,NC
   16 Y(I)=Y(I)/SUM
      IDX=2
      GO TO 12
   17 DO 18 I=1,NC
      IF (L(I).LT.0 .OR. Z(I).LT.1.0E-12) GO TO 18
      IF (ABS(Y(I)-YY(I))/Y(I).GT.CONV) GO TO 19
   18 CONTINUE
      GO TO 240
   19 SUM=0.0
      DO 21 I=1,NC
      IF (L(I).LT.0 .OR. Z(I).LT.1.0E-12) GO TO 21
      CALL WEG (Y(I),YY(I),SY(I),YC(I))
      SUM=SUM+Y(I)
   21 CONTINUE
      DO 22 I=1,NC
   22 Y(I)=Y(I)/SUM
      GO TO 12
C
   25 CALL KCALC2
   26 DO 27 I=1,NC
   27 RKS(I)=EK1(I)/EK2(I)
      K=0
C
      IF (LDBUG.GE.1) WRITE(NPRT,28) T,U,V
   28 FORMAT ('0FLASH*2   T-U-V', F12.4,2E14.5)
      IF (LDBUG.GE.2) WRITE(NPRT,29) (Y(I),I=1,NC),(X1(I),I=1,NC),
     +                             (X2(I),I=1,NC)
   29 FORMAT ('0Y-ASS  ',3E13.5/' X1-ASS ',3E13.5/' X2-ASS ',3E13.5)
C
   30 F1=0.0
      F2=0.0
      DF1U=0.0
      DF2U=0.0
      DF1V=0.0
      DF2V=0.0
C     DDF1UU=0.0
C     DDF1VV=0.0
C     DDF1UV=0.0
C     DDF2UU=0.0
```

```
C     DDF2VV=0.0
C     DDF2UV=0.0
C
      DO 50 I=1,NC
C
      AA=Z(I)*(1.0-EK1(I))
      BB=Z(I)*(1.0-RKS(I))
      WW=V*(1.0-U)+(1.0-V)*(1.0-U)*RKS(I)+U*EK1(I)
      F1=F1+AA/WW
      F2=F2+BB/WW
C
      DWU=V*(RKS(I)-1.0)-RKS(I)+EK1(I)
      DWV=(1.0-U)*(1.0-RKS(I))
      DDWUV=RKS(I)-1.0
C
      DF1U=DF1U-AA/WW**2*DWU
      DF2U=DF2U-BB/WW**2*DWU
      DF1V=DF1V-AA/WW**2*DWV
      DF2V=DF2V-BB/WW**2*DWV
C
C     DDF1UU=DDF1UU+2.0*AA/WW**3*DWU**2
C     DDF2UU=DDF2UU+2.0*BB/WW**3*DWU**2
C     DDF1VV=DDF1VV+2.0*AA/WW**3*DWV**2
C     DDF2VV=DDF2VV+2.0*BB/WW**3*DWV**2
C     DDF1UV=DDF1UV+2.0*AA/WW**3*DWU*DWV-AA/WW**2*DDWUV
C     DDF2UV=DDF2UV+2.0*BB/WW**3*DWU*DWV-BB/WW**2*DDWUV
C
   50 CONTINUE
C
      RHS(1)=-F1
      RHS(2)=-F2
      ZJ(1,1)=DF1U
      ZJ(1,2)=DF1V
      ZJ(2,1)=DF2U
      ZJ(2,2)=DF2V
C
C     RHS(1)=2.0*(F1*DF1U+F2*DF2U)
C     RHS(2)=2.0*(F1*DF1V+F2*DF2V)
C     ZJ(1,1)=2.0*(DF1U**2+F1*DDF1UU+DF2U**2+F2*DDF2UU)
C     ZJ(2,2)=2.0*(DF1V**2+F1*DDF1VV+DF2V**2+F2*DDF2VV)
C     ZJ(1,2)=2.0*(DF1U*DF1V+F1*DDF1UV+DF2U*DF2V+F2*DDF2UV)
C     ZJ(2,1)=ZJ(1,2)
C
      DETRM=ZJ(1,1)*ZJ(2,2)-ZJ(1,2)*ZJ(2,1)
      DU=(RHS(1)*ZJ(2,2)-RHS(2)*ZJ(1,2))/DETRM
      DV=(ZJ(1,1)*RHS(2)-ZJ(2,1)*RHS(1))/DETRM
      K=K+1
C
      IF (LDBUG.GE.2) WRITE(NPRT,55) F1,F2,U,DU,V,DV
   55 FORMAT ( 5X,'IN FLSH2 AT STMT#55 F1-F2-U-DU-V-DV'/ 6E14.5)
C
      IF (K.LT.20) GO TO 59
   57 WRITE(NPRT,58)
   58 FORMAT ('OFLASH2 CALCULATION TERMINATED' /
     +        ' CALCULATION CONTINUING' /)
      IF (KNT .EQ. 0 .AND. U .LE. 1.0E-10) THEN
         CALL TWOLIQ
         GO TO 275
      END IF
      GO TO 240
```

```
C
C     COMPUTE NEW VALUES OF U & V
C
   59 NCVRG=0
      GO TO (60,70), ID
   60 SDU=DU
      SDV=DV
      ID=2
      GO TO 80
   70 CONTINUE
D     SSDU=SDU
D     SSDV=SDV
D     SDU=DU
D     SDV=DV
D     TOP=SSDU*SSDV+SDU*SDV
D     BTM=(SSDU**2+SSDV**2)*(SDU**2+SDV**2)
D     COSANG=TOP/SQRT(BTM)
D     BETA=1.0+COSANG
      BETA=1.0
      DU=BETA*DU
      DV=BETA*DV
C
C     CHECK TO INSURE THAT U & V ARE .LT. 1.0 AND .GT. 0.0
C
   80 IF ((U+DU.LT.1.0 .AND. U+DU.GT.0.0) .AND.
     +    (V+DV.LE.1.0 .AND. V+DV.GE.0.0)) GO TO 90
      NCVRG=1
      DU=DU*0.5
      DV=DV*0.5
      GO TO 80
C
C  90 IF (V .LT.0.9999) GO TO 94
   90 IF (V .GT. 1.0E-8) GO TO 94
      V=1.0-V
      DO 91 I=1,NC
      HOLD=X1(I)
      X1(I)=X2(I)
      X2(I)=HOLD
      HOLD=XX(I,1)
      XX(I,1)=XX(I,2)
      XX(I,2)=HOLD
      HOLD=SX(I,1)
      SX(I,1)=SX(I,2)
      SX(I,2)=HOLD
      HOLD=XC(I,1)
      XC(I,1)=XC(I,2)
      XC(I,2)=HOLD
      HOLD=EK1(I)
      EK1(I)=EK2(I)
      EK2(I)=HOLD
      RKS(I)=EK1(I)/EK2(I)
      HOLD=GAM1(I)
      GAM1(I)=GAM2(I)
   91 GAM2(I)=HOLD
C
C  94 IF (V.LT.1.0E-10) GO TO 231
   94 IF (V .GT. 0.99999) GO TO 231
      IF (ABS(DU).LT.CONV1 .AND. ABS(DV).LT.CONV1 .AND. NCVRG.EQ.0)
     +    GO TO 110
C
```

```
   95 U=U+DU
      V=V+DV
      GO TO 30
C
  110 IF (ABS(F1).LT.CONV2.AND.ABS(F2).LT.CONV2) GO TO  120
      GO TO 95
C
C     CALCULATE COMPOSITIONS
C
  120 DO 180 I=1,NC
      IF (Z(I).LT.1.0-12) GO TO  170
      IF (L(I)) 130,140,150
C     NONVOLATILE
  130 WW=V+(1.0-V)*RKS(I)
      YY(I)=0.0
      XX(I,1)=Z(I)/WW
      XX(I,2)=XX(I,1)*RKS(I)
      GO TO  180
C     NONCONDENSIBLE
  140 YY(I)=Z(I)/U
      XX(I,1)=0.0
      XX(I,2)=0.0
      GO TO  180
C     NORMAL AND SUPERCRITCAL
  150 WW=V*(1.0-U)+(1.0-V)*(1.0-U)*RKS(I)+U*EK1(I)
      XX(I,1)=Z(I)/WW
      XX(I,2)=X1(I)*RKS(I)
      YY(I)=EK1(I)*XX(I,1)
      GO TO  180
  170 YY(I)=0.0
      XX(I,1)=0.0
      XX(I,2)=0.0
  180 CONTINUE
C
      KNT=KNT+1
      IF (KNT.EQ.50) GO TO 57
      GO TO  (280,190), IDX
C
  190 IF (IDLL.EQ.0)GO TO  220
      DO 210 I=1,NC
      IF (L(I).EQ.0 .OR. Z(I).LT.1.0E-12) GO TO 210
C     IF (ABS(X1(I)*GAM1(I)-X2(I)*GAM2(I))/(X2(I)*GAM2(I)) .GT.
C    +    CONV) GO TO 360
      IF (ABS((X1(I)-XX(I,1))/X1(I)) .GT. CONV .OR.
     *ABS((X2(I)-XX(I,2))/X2(I)) .GT. CONV)GO TO 360
  210 CONTINUE
  220 IF (IDLV.EQ.0) GO TO  240
      DO 230 I=1,NC
      IF (L(I).LT.0 .OR. Z(I).LT.1.0E-12) GO TO 230
      IF (ABS(Y(I)-YY(I))/Y(I).GT.CONV) GO TO  360
  230 CONTINUE
      GO TO 240
C
  231 DO 232 I=1,NC
      HOLD=X1(I)
      X1(I)=X2(I)
  232 X2(I)=HOLD
      WRITE(NPRT,238)
  238 FORMAT (// 5X, 'LIQUID HAS GONE TO A ONE PHASE SYSTEM' //)
      NLIQ=1
```

```
      FRACV=0.5
      CALL FLSH1
C
  240 SUM=0.0
      SUM1=0.0
      SUM2=0.0
      DO260I=1,NC
      Y(I)=YY(I)
      SUM=SUM+Y(I)
      X1(I)=XX(I,1)
      X2(I)=XX(I,2)
      SUM1=SUM1+X1(I)
      SUM2=SUM2+X2(I)
  260 CONTINUE
      DO270I=1,NC
      Y(I)=Y(I)/SUM
      X1(I)=X1(I)/SUM1
  270 X2(I)=X2(I)/SUM2
  275 ISW=0
      RETURN
C
  280 IF (IDLL.EQ.0) GO TO 320
      DO 290 N = 1,2
      DO 290 I =1,NC
  290 XC(I,N)=XX(I,N)
      SUM1=0.0
      SUM2=0.0
      DO 300 I =1,NC
      SX (I,1)=X1(I)
      SX(I,2)=X2(I)
      X1(I)=(X1(I)+XX(I,1))/2.0
      X2(I)=(X2(I)+XX(I,2))/2.0
      SUM1=SUM1+X1(I)
 300  SUM2=SUM2+X2(I)
      DO 310 I=1,NC
      X1(I)=X1(I)/SUM1
  310 X2(I)=X2(I)/SUM2
  320 IF (IDLV.EQ.0) GO TO  350
      SUM=0.0
      DO 330 I=1,NC
      SY(I)=Y(I)
      YC(I)=YY(I)
      Y(I)=(Y(I)+YY(I))/2.0
      SUM=SUM+Y(I)
  330 CONTINUE
      DO 340 I=1,NC
      Y(I)=Y(I)/SUM
  340 CONTINUE
  350 IDX=2
      GO TO 25
C
  360 IF (IDLL.EQ.0) GO TO 400
      DO 390 N=1,2
      SUM1=0.0
      SUM2=0.0
      DO 370 I=1,NC
      IF (L(I).EQ.0 .OR. Z(I).LT.1.0E-12) GO TO 370
      IF (N .EQ.1) XTEMP(I,N)=X1(I)
      IF (N .EQ. 2) XTEMP(I,N)=X2(I)
      CALL WEG (XTEMP(I,N),XX(I,N),SX(I,N),XC(I,N))
```

```
      IF (N .EQ. 1)SUM1=SUM1+XTEMP(I,N)
      IF (N .EQ. 2)SUM2=SUM2+XTEMP(I,N)
  370 CONTINUE
      DO 380 I=1,NC
      IF ( N .EQ. 1)X1(I)=XTEMP(I,N)/SUM1
      IF ( N .EQ. 2)X2(I)=XTEMP(I,N)/SUM2
  380 CONTINUE
  390 CONTINUE
  400 IF (IDLV.EQ.0) GO TO 420
      SUM=0.0
      DO 410 I=1,NC
      IF (L(I).LT.0 .OR. Z(I).LT.1.0E-12) GO TO 410
      CALL WEG (Y(I),YY(I),SY(I),YC(I))
      SUM=SUM+Y(I)
  410 CONTINUE
      GO TO 440
  420 SUM=0.0
      DO 430 I=1,NC
      Y(I)=YY(I)
      SUM=SUM+Y(I)
 430  CONTINUE
  440 DO 450 I=1,NC
      Y(I)=Y(I)/SUM
  450 CONTINUE
      GO TO 25
C
      END
      SUBROUTINE AFLSH2
C
C     ADIABATIC FLASH
C
C
      COMMON  /BLANK/  NCR, NPRT, NSTART, KUNITS, TITLE(20)
      COMMON  /CMPRO/  NC, NCM1, NCP1, IDLL, IDLV, IDH, LDBUG, ISW,
     *                 NDIM, ZNAME(2,10), L(10), NTCOMP(10), NLIQ, IPSET
      COMMON  /ZDATA/  CPL(10,4), CPV(10,4), ENP(10,10), ANT(6,10),
     *                 W(10), AX, BX, OMEGA(10), AVAL(10), BVAL(10),
     *                 AK(10,10), R(10), Q(10), QP(10), XL(10),
     *                 VOL(10), C(180), ALPHA(45), VC(10), TC(10),
     *                 PC(10), ZC(10), TNBP(10), DA(10), DB(10),
     *                 A(10,10), G(10,10), ZRA(10), RD(10), DMU(10),
     *                 ETA(10)
      COMMON  /STRM/   T, P, Z(10), Y(10), X(10), FRACV, ZVAP,
     *                 EK(10), VP(10), FUG(10), GAM(10), SVAP,
     *                 HOFZ, HVAP, HLIQ, DHV, XSH, NOBUB, NODEW
      COMMON  /CONTRL/ ITF, IPF,  N, NTYPE, JCODE
      COMMON  /TWOLQ/  X1(10), X2(10), GAM1(10), GAM2(10), EK1(10),
     +                 EK2(10), DHL(2), HIDLL(2), HREALL(2), FRACL,
     +                 IE, IR, XMAX, XMIN
      COMMON  /ZFEEDZ/ PF, TF, FEED(10), FMOL, TREF, HI
      COMMON  /DUMMY/  XX(10,2),SX(10,2),XC(10,2),YY(10),SY(10),YC(10),
     +                 RMAX, RMIN
C
      DATA             KMAX, STEP, TINC, CONV /300,20.0,10.0,1.5E-3/
      DATA             STEPMX / 20.0 /
C
      ID=1
      S=T
      KOUNT=0
      KTEN=1
```

```
      STEP=STEPMX
      TBUB=0.0
      TDEW=2000.0
      IF (NTYPE .EQ. 9) GO TO 10
      SUM1=0.0
      SUM2=0.0
      DO 2 I=1,NC
      XX(I,1)=X1(I)
      XX(I,2)=X2(I)
      SUM1=SUM1+XX(I,1)
    2 SUM2=SUM2+XX(I,2)
      DO 5 I=1,NC
      XX(I,1)=XX(I,1)/SUM1
    5 XX(I,2)=XX(I,2)/SUM2
C
   10 GO TO (11,12), NLIQ
   11 CONTINUE
      FRACV=0.5*(RMAX+RMIN)
      CALL FLSH1
      FRACL=1.0
      GO TO 15
   12 CONTINUE
      FRACV=0.5*(RMAX+RMIN)
      CALL FLSH2
   15 DO 14 I=1,NC
   14 X(I)=X1(I)
      CALL LIQH
      HREALL(1)=HLIQ
      HIDLL(1) =HLIQ-XSH
      IF (NLIQ .NE. 2) GO TO 18
      DO 16 I=1,NC
   16 X(I)=X2(I)
      CALL LIQH
      HREALL(2)=HLIQ
      HIDLL(2) =HLIQ-XSH
   18 CALL VAPH
      HTOT=HVAP*FRACV+HREALL(1)*(1.0-FRACV)*FRACL+
     %     HREALL(2)*(1.0-FRACV)*(1.0-FRACL)
      H=HTOT-HI
      IF (ABS(H/HI)-CONV) 70,20,20
   20 NLIQ=2
      GO TO (30,40), ID
   30 T=S-SIGN(TINC,H)
      HO=H
      ID=2
      GO TO 63
   40 SLOPE=(HO-H)/(S-T)
      DT=-H/SLOPE
      S=T
      IF (ABS(DT)-STEP) 60,60,50
   50 DT=SIGN(STEP,DT)
   60 T=T+DT
      HO=H
   63 T=AMIN1(T,TDEW-0.5)
      T=AMAX1(T,TBUB+0.5)
      IF (LDBUG .GE. 1) WRITE (NPRT,65) KOUNT,HTOT,HI,H
   65 FORMAT ('0IN AFLSH2 : KOUNT-HTOT-HI-DIFF ',I4,3(E12.5,2X))
      KOUNT=KOUNT+1
      IF (KOUNT .EQ. KTEN) THEN
         KTEN=KTEN+5
```

```
         STEP=0.935*STEP
         STEP=AMAX1(STEP,0.0005)
      END IF
      IF (KOUNT .GE. KMAX) THEN
          WRITE (NPRT,68) KOUNT
   68     FORMAT (/' PROGRAM TERMINATED IN AFLSH2 AFTER ',
     *    I5,' TRIALS'/)
          CALL EXIT
      END IF
C
      GO TO 10
   70 WRITE (NPRT,80)
   80 FORMAT ('0FOLLOWING IS THE RESULT OF AN ADIABATIC FLASH.')
      RETURN
C
      END
      SUBROUTINE KCALC2
C
C     ROUTINE TO CALCULATE K VALUES
C
C
      COMMON  /BLANK/  NCR, NPRT, NSTART, KUNITS, TITLE(20)
      COMMON  /CMPRO/  NC, NCM1, NCP1, IDLL, IDLV, IDH, LDBUG, ISW,
     *                 NDIM, ZNAME(2,10), L(10), NTCOMP(10), NLIQ, IPSET
      COMMON  /ZDATA/  CPL(10,4), CPV(10,4), ENP(10,10), ANT(6,10),
     *                 W(10), AX, BX, OMEGA(10), AVAL(10), BVAL(10),
     *                 AK(10,10), R(10), Q(10), QP(10), XL(10),
     *                 VOL(10), C(180), ALPHA(45), VC(10), TC(10),
     *                 PC(10), ZC(10), TNBP(10), OA(10), OB(10),
     *                 A(10,10), G(10,10), ZRA(10), RD(10), DMU(10),
     *                 ETA(10)
      COMMON  /STRM/   T, P, Z(10), Y(10), X(10), FRACV, ZVAP,
     *                 EK(10), VP(10), FUG(10), GAM(10), SVAP,
     *                 HOFZ, HVAP, HLIQ, DHV, XSH, NOBUB, NODEW
      COMMON  /CONTRL/ ITF, IPF,  N, NTYPE, JCODE
      COMMON  /TWOLQ/  X1(10), X2(10), GAM1(10), GAM2(10), EK1(10),
     +                 EK2(10), DHL(2), HIDLL(2), HREALL(2), FRACL,
     +                 IE, IR, XMAX, XMIN
      COMMON  /ZFEEDZ/ PF, TF, FEED(10), FMOL, TREF, HI
      COMMON   /DUMMY/  XX(10,2),SX(10,2),XC(10,2),YY(10),SY(10),YC(10),
     +                   RMAX, RMIN
C
      IF (T .LE. 0.0) T=273.16
      DHV=0.0
      IF (ISW.NE.0) GO TO 40
      IF (LDBUG.GE.2) THEN
         WRITE (NPRT,5) T, ISW, (L(I),I=1,NC)
    5    FORMAT (/' SUB KCALC2 : T-ISW-L = ',F7.2,5I5/)
         WRITE(NPRT,7) (ANT(1,I),ANT(2,I),ANT(3,I),I=1,NC)
    7    FORMAT('0SUB KCALC2 ANTOINES :', 10((3E12.5)/))
      END IF
C
   10 DO30I=1,NC
      IF (L(I))30,30,20
  20  VP(I)=EXP(ANT(1,I)+ANT(2,I)/(T+ANT(3,I))+ANT(4,I)*ALOG(T)+
     *          ANT(5,I)*T+ANT(6,I)*T*T)
   30 CONTINUE
C
40    DO 60 I=1,NC
      IF (L(I))60,60,50
```

```
   50 EK1(I)=VP(I)/P
   60 CONTINUE
C
      IF (IDLV.EQ.0) GO TO 100
      CALL FUGCY (T,P,Y,VP,FUG,DHV)
      DO90I=1,NC
      IF (L(I))90,90,80
   80 EK1(I)=EK1(I)/FUG(I)
   90 CONTINUE
C
100   IF (IDLL.EQ.0) RETURN
      CALL ACTVY (T,P,X1,GAM1)
      IF (NLIQ .EQ. 2) THEN
         KNTX=0
         DO 110 I=1,NC
         IF (X2(I) .GT. 0.0) GO TO 110
         KNTX=KNTX+1
  110    CONTINUE
         IF (KNTX .GE. NC) THEN
            DO 115 I=1,NC
  115       GAM2(I)=1.0
            GO TO 130
         ELSE
            CALL ACTVY(T,P,X2,GAM2)
         END IF
      END IF
C
  130 DO150I=1,NC
      IF (L(I))150,150,140
140   IF (NLIQ.EQ.2) EK2(I) = EK1(I)*GAM2(I)
      EK1(I) = EK1(I)*GAM1(I)
  150 CONTINUE
      RETURN
C
      END
      SUBROUTINE PRINT2
C
C
      COMMON  /BLANK/  NCR, NPRT, NSTART, KUNITS, TITLE(20)
      COMMON  /CMPRO/  NC, NCM1, NCP1, IDLL, IDLV, IDH, LDBUG, ISW,
     *                 NDIM, ZNAME(2,10), L(10), NTCOMP(10), NLIQ, IPSET
      COMMON  /ZDATA/  CPL(10,4), CPV(10,4), ENP(10,10), ANT(6,10),
     *                 W(10), AX, BX, OMEGA(10), AVAL(10), BVAL(10),
     *                 AK(10,10), R(10), Q(10), QP(10), XL(10),
     *                 VCL(10), C(180), ALPHA(45), VC(10), TC(10),
     *                 PC(10), ZC(10), TNBP(10), OA(10), OB(10),
     *                 A(10,10), G(10,10), ZRA(10), RD(10), DMU(10),
     *                 ETA(10)
      COMMON  /STRM/   T, P, Z(10), Y(10), X(10), FRACV, ZVAP,
     *                 EK(10), VP(10), FUG(10), GAM(10), SVAP,
     *                 HOFZ, HVAP, HLIQ, DHV, XSH, NOBUB, NODEW
      COMMON  /CONTRL/ ITF, IPF,  N, NTYPE, JCODE
      COMMON  /TWOLQ/  X1(10), X2(10), GAM1(10), GAM2(10), EK1(10),
     +                 EK2(10), DHL(2), HIDLL(2), HREALL(2), FRACL,
     +                 IE, IR, XMAX, XMIN
      COMMON  /ZFEEDZ/ PF, TF, FEED(10), FMOL, TREF, HI
      COMMON   /DUMMY/  XX(10,2),SX(10,2),XC(10,2),YY(10),SY(10),YC(10),
     +                   RMAX, RMIN
C
      DIMENSION           ACT(10),VPRES(10)
```

```
      IF (LDBUG .GE. 1)WRITE (NPRT,2)IDLV, IDLL
    2 FORMAT ( ' IN PRINT2 : IDLV = ',I3,'& IDLL=',I3)
      DO80 N=1,NLIQ
      WRITE(NPRT,5) N
    5 FORMAT (/'0"VLE" DATA FOR VAPOR AND LIQUID PHASE #', I3)
      WRITE(NPRT,1) ((ZNAME(J,I),J=1,2),I=1,NC)
    1 FORMAT (/25X,9(2A4,2X))
      WRITE(NPRT,6) (Y(I),I=1,NC)
    6 FORMAT (' VAP MCLE FRAC', 9X, 10F10.5)
      IF (N .EQ. 1) WRITE (NPRT,7) (X1(I),I=1,NC)
      IF (N .EQ. 2) WRITE (NPRT,7) (X2(I),I=1,NC)
    7 FORMAT (' LIQ MOLE FRAC', 9X, 10F10.5)
      IF (N .EQ. 1) WRITE (NPRT,10) (EK1(I),I=1,NC)
      IF (N .EQ. 2) WRITE (NPRT,10) (EK2(I),I=1,NC)
   10 FORMAT(' VALUES OF K=Y/X',7X,10F10.5)
      DO 15 I=1,NC
      VPRES(I)=VP(I)*760.0
 15   CONTINUE
      WRITE(NPRT,20)(VPRES(I),I=1,NC)
   20 FORMAT(' VAPOR PRESSURE (MM HG)',1X,10F10.3)
      IF (IDLV)30,50,30
   30 WRITE(NPRT,40)(FUG(I),I=1,NC)
   40 FORMAT(' FUGACITY FACTORS',6X,10F10.5)
   50 IF (IDLL)60,80,60
   60 IF (N .EQ. 1) WRITE (NPRT,70) (GAM1(I),I=1,NC)
      IF (N .EQ. 2) WRITE (NPRT,70) (GAM2(I),I=1,NC)
   70 FORMAT(' ACTIVITY COEFFICIENTS ',10F10.4)
      DO 71 I=1,NC
      IF (N .EQ. 1)ACT(I)=GAM1(I)*X1(I)
      IF (N .EQ. 2)ACT(I)=GAM2(I)*X2(I)
   71 CONTINUE
      WRITE(NPRT,72) (ACT(I),I=1,NC)
   72 FORMAT (' ACTIVITY (2 LIQ)', 6X, 10F10.4)
   80 CONTINUE
      RETURN
C
      END
```

```
      SUBROUTINE FOFX (IDPT,XVAR,ADJUST,YYY,ZZZ)
C
C     THIS SUBPROGRAM IS USED IN CONJUNCTION WITH NLFITS
C     (MARQUARDT'S NON-LINEAR REGRESSION) PROGRAM.
C
C     VERSION # 2 ...  MARCH 1984,  PROGRAMMED BY HARPREET CHAWLA
C     VERSION # 3 ...  AUGUST 1984, PROGRAMMED BY HARPREET CHAWLA
C
C     THE ARGUMENTS IN THE CALL LIST ARE:
C         IDPT   -  INTEGER; THE DATA POINT NUMBER
C         XVAR   -  ARRAY;   CONTAINS THE COMPOSITION VALUES
C         ADJUST -  ARRAY;   CONTAINS THE CURRENT VALUES OF THE
C                            ADJUSTABLE PARAMETERS
C         YYY    -  REAL;    CONTAINS THE DESIRED RESULT
C         ZZZ    -  REAL;    CONTAINS THE CALCULTED RESULT ON RETURN
C
C
      COMMON   /BLANK/  NCR, NPRT, NSTART, KUNITS, TITLE(20)
      COMMON   /CMPRO/  NC, NCM1, IDLL, IDLV, IDH, LDBUG, ISW, NDIM,
     *                  ZNAME(2,10), L(10), NTCOMP(10)
      COMMON   /ZDATA/  CPL(10,4), CPV(10,4), ENP(10,10), ANT(6,10),
     *                  W(10), AX, BX, OMEGA(10), AVAL(10), BVAL(10),
     *                  AK(10,10), R(10), Q(10), QF(10), XL(10),
     *                  VOL(10), C(180), ALPHA(45), VC(10), TC(10),
     *                  PC(10), ZC(10), TNBP(10), DA(10), DB(10),
     *                  A(10,10), G(10,10), ZRA(10), RD(10), DMU(10),
     *                  ETA(10)
      COMMON   /STRM/   T, P, Z(10), Y(10), X(10), FRACV, ZVAP,
     *                  EK(10), VP(10), FUG(10), GAM(10), SVAP,
     *                  HOFZ, HVAP, HLIQ, DHV, XSH, NOBUB, NODEW
      COMMON   /CONTRL/ ITF, IPF,  N, NTYPE, JCODE, NLIQ
      COMMON   /TWCLQ/  X1(10), X2(10), GAM1(10), GAM2(10), EK1(10),
     +                  EK2(10), DHL(2), HIDLL(2), HREALL(2), FRACL,
     +                  IE, IR, XMAX, XMIN
      COMMON   /ZFEEDZ/ PF, TF, FEED, FMOL, TREF, HI, NK1, NFEED
      COMMON   /DUMMY/  XX(10,2),SX(10,2),XC(10,2),YY(10),SY(10),YC(10),
     +                  RMAX, RMIN
      COMMON   /FOX/    X1EXP(10), X2EXP(10), GAM1E(10), GAM2E(10),
     *                  GAM1IE(10), GAM2IE(10),GAM1IC(10), GAM2IC(10),
     *                  ACT1C(10), ACT2C(10), ACT1E(10), ACT2E(10),
     *                  KE(10), KC(10), KIE(10), KIC(10), W1(10),
     *                  W2(10), YEXP(10), TEXP, PEXP, WT, WT1, VLEFN,
     *                  LLEFN, VLLFN, NVLPT, NLLPT, NCVLE, NCLLE,
     *                  NMODEL, INX, RECODE, NDTALE(15,10), NDSET
      COMMON   /OUTPUT/ X1ED(10,200), X2ED(10,200), X1C(10,200),
     *                  X2D(10,200), G1ED(10,200), G2ED(10,200),
     *                  G1D(10,200), G2D(10,200), G1IED(10,5),
     *                  G2IED(10,5), G1ICD(10,5), G2ICD(10,5),
     *                  KED(10,200), KCD(10,200), KIED(10,5),
     *                  KICD(10,5), YED(10,200), YCD(10,200),
     *                  TED(200), PED(200), TCD(200), PCD(200),
     *                  ACT1ED(10,200), ACT2ED(10,200), ACT1CD(10,200),
     *                  ACT2CD(10,200)
C
      DIMENSION         DEWC(10), BUBC(10), IJK(7), HLIQD(2)
      DIMENSION         XVAR(8), ADJUST(20), ALPHAS(3), PICKUP(400)
C
      REAL              FD(11), BUBVAP(10), DEWLIQ(10), KE, KC, KIE,
     *                  KIC, KED, KCD, KIED, KICD
      REAL*8            ADJUST
```

```
      INTEGER           VLEFN, LLEFN, VLLFN, RECODE, ISKIP(20)
C
      DATA              DOLLAR /'$$$$'/, ICALL/1/, KOUNT/1/
C
      NCR=5
      NPRT=6
      IF (ICALL .EQ. 0) GO TO 50
C     CALL ERRSET (48,.TRUE.,.TRUE.,.FALSE.,.FALSE.,999)
C     CALL ERRSET (38,.TRUE.,.TRUE.,.FALSE.,.FALSE.,999)
C     CALL ERRSET (60,.TRUE.,.TRUE.,.FALSE.,.FALSE.,999)
      CALL ERRSET (63,.TRUE.,.TRUE.,.FALSE.,.FALSE.,999)
      CALL ERRSET (68,.TRUE.,.TRUE.,.FALSE.,.FALSE.,999)
      CALL ERRSET (72,.TRUE.,.TRUE.,.FALSE.,.FALSE.,999)
      CALL ERRSET (73,.TRUE.,.TRUE.,.FALSE.,.FALSE.,999)
      CALL ERRSET (74,.TRUE.,.TRUE.,.FALSE.,.FALSE.,999)
      CALL ERRSET (83,.TRUE.,.TRUE.,.FALSE.,.FALSE.,999)
      CALL ERRSET (88,.TRUE.,.TRUE.,.FALSE.,.FALSE.,999)
      CALL ERRSET (89,.TRUE.,.TRUE.,.FALSE.,.FALSE.,999)
      CALL ERRSET (93,.TRUE.,.TRUE.,.FALSE.,.FALSE.,999)
   10 DO 5 I = 1,10
      Y(I)=0.0
      YY(I)=0.0
      X1(I)=0.0
      X2(I)=0.0
      XX(I,1)=0.0
      XX(I,2)=0.0
      EK1(I)=0.0
      EK2(I)=0.0
      FUG(I)=0.0
      GAM1(I)=0.0
      GAM2(I)=0.0
    5 CONTINUE
C
    7 CALL START (IDATA,MFEEDS,MCASES,&1500)
C
C     REMAINING CCNTRCL PARAMETERS
C     RECORD # 1
C         NMODEL    MODEL WHOSE PARAMETERS ARE TO BE REGRESSEC
C         NTYPE     TYPE CF REGRESSION TO BE PERFCRMED
C         ITDEP     CODE FOR TEMPERATURE DEPENDENCE OF THE PARAMETERS
C                    0  -  ALL PARAMETERS T INDEPENDENT
C                    1  -  ONE PARAMETER  T DEPENDENT
C                    0  -  TWO PARAMETERS T DEPENDENT
C                   INTERNAL ITDEP CODES ARE, ITDEP+ITDEP+1
C
C         NDSET     NO. OF EXPERIMENTAL DATA SETS (WITH N POINTS)
C         NSKIP     NO. OF DATA POINTS TO BE SKIPPED FOR REGRESSION
C         RECODE    CODE FOR READING IN EXPERIMENTAL CEPENDENT
C                   VARIABLE DATA
C                    0   NO EXPERIMENTAL DATA
C                    1   TEXP'S      2   PEXP'S
C                    3   YEXP'S      4   X2EXP'S
C                    5   TEXP'S & YEXP'S        (1 ST READ T'S)
C                    6   PEXP'S & YEXP'S        (1 ST READ P'S)
C                    7   TEXP'S & X2EXP'S       (1 ST READ T'S)
C                    8   PEXP'S & X2EXP'S       (1 ST READ P'S)
C                    9   YEXP'S & X2EXP'S       (1 ST READ Y'S)
C                   10   TEXP'S & YEXP'S & X2EXP'S (1 ST READ T'S,
C                                                   2 ND READ Y'S)
C                   11   PEXP'S & YEXP'S & X2EXP'S (1 ST READ P'S,
```

```
C                                                     2 ND READ Y'S)
C          VLEFN     CODE FOR OBJECTIVE FUNCTION IN VLE
C          LLEFN     CODE FOR OBJECTIVE FUNCTION IN LLE
C          VLLFN     CODE FOR OBJECTIVE FUNCTION IN VLLE
C          IE        COMPONENT # : COMPONENT IE RICH PHASE
C          IR        COMPONENT # : COMPONENT IR RICH PHASE
C                    (IF IE AND/OR IR = 0, PROGRAM FINDS IT)
C          XMAX      INITIALIZATION VALUE ; MOLE FRACTION OF
C                    IE OR IR IN EXTRACT OR RAFFINATE PHASE RESPECTIVELY
C                    ( IF XMAX <= 0.0, IT DEFAULTS TO 0.98)
C          XMIN      INITIALIZATION VALUE ; MOLE FRACTION OF
C                    IR OR IE IN EXTRACT OR RAFFINATE PHASE RESPECTIVELY
C                    ( IF XMIN <= 0.0, IT DEFAULTS TO 0.02)
C
C     RECORD # 2     IF NSKIP<>0
C         ISKIP      READ (IN ANY ORDER) ALL THE DATA POINT NUMBERS
C                    TO BE SKIPPED FOR THE REGRESSION
C
C     RECORD # 3,4...
C         NDTALE(I,J) MATRIX IS READ, J = DATASET NO.
C         FOR EACH VALUE OF J:
C           I=1: J,
C           I=2: DATA TYPE CODE,
C           I=3: CONDITION CODE,
C           I=4: # OF COMP.,
C           I=5: # OF DATA POINTS,
C           I=6-TO- 5+NC ... COMPID'S OF ALL COMPONENTS
C           NOTE: IN TOTAL  J  RECORDS ARE TO BE READ
C
C
      READ (NCR,*) NMODEL, NTYPE, ITDEP, NDSET, NSKIP, RECODE, VLEFN,
     *             LLEFN, VLLFN, IE, IR, XMAX, XMIN
      IF (NSKIP .NE. 0) READ (NCR,*) (ISKIP(I),I=1,NSKIP)
      DO 3 J=1,NDSET
   3  READ (NCR,*) (NDTALE(I,J),I=1,5+NC)
C
C
C     VARIOUS SETTINGS ARE MADE
C
      NCVLE=NC
      NCLLE=NC
      NVLPT=0
      NLLPT=0
      DO 4 J=1,NDSET
      IF (NDTALE(2,J) .EQ. 1) THEN
         NVLPT=NVLPT+NDTALE(5,J)
C        NCVLE=NDTALE(4,J)
      END IF
      IF (NDTALE(2,J) .EQ. 2) THEN
         NLLPT=NLLPT+NDTALE(5,J)
C        NCLLE=NDTALE(4,J)
      END IF
   4  CONTINUE
C
      WRITE(NPRT,8)NTYPE,NCVLE,VLEFN,IE,NDSET,NCLLE,LLEFN,IR,
     *             NMODEL,NVLPT,VLLFN,XMAX,ITDEP,NLLPT,RECODE,
     *             XMIN
   8  FORMAT('0','NTYPE =',I2,T15,'NCVLE =',I2,T30,'VLEFN =',I2,T45,
     *'IE  =',I2/' NDSET =',I2,T15,'NCLLE =',I2,T30,'LLEFN =',I2,T45,
     *'IR  =',I2/' NMODEL=',I2,T15,'NVLPT =',I2,T30,'VLLFN =',I2,T45,
```

```
     *'XMAX=',F5.3/' ITDEP =',I2,T15,'NLLPT =',I2,T30,'RECODE=',I2,T45,
     *'XMIN=',F5.3/' NSKIP =',I3)
      IF (NSKIP .NE. 0)WRITE (NPRT,9) (ISKIP(I),I=1,NSKIP)
    9 FORMAT ('0','THE FOLLOWING DATA POINTS HAVE BEEN IGNORED'/
     *20I4)
C
      ITDEP=ITDEP+1
      IF (IDATA.NE.0) GO TO 11
      CALL CDATA
      GO TO 15
C
C     NMODEL CODES FOR CDATA TO BE USED WITH FOFX, FOR REGRESSION .
C
C       1  -  VAN LAAR EQUATION                          (2 PARAMETER)
C       2  -  3 SUFFIX MARGULES EQUATION                 (2 PARAMETER)
C       3  -  4 SUFFIX MARGULES EQUATION                 (3 PARAMETER)
C       4  -  5 SUFFIX MARGULES EQUATION                 (4 PARAMETER)
C       5  -  MODIFIED 5 SUFFIX MARGULES EQUATION        (4 PARAMETER)
C       6  -  MODIFIED MARGULES EQUATION                 (4 PARAMETER)
C       7  -  WILSON EQUATION                            (2 PARAMETER)
C       8  -  NRTL EQUATION                              (2 PARAMETER)
C       9  -  NRTL EQUATION                              (3 PARAMETER)
C      10  -  UNIQUAC EQUATION                           (2 PARAMETER)
C      11  -  MODIFIED UNIQUAC EQUATION                  (2 PARAMETER)
C      12  -  UNIFAC EQUATION
C      13  -  KNOX EQUATION
C      14  -  HENRY'S EQUATION                           (2 PARAMETER)
C      15  -  ANTOINE EQUATION                           (6 PARAMETER)
C
C     PRESENTLY PROGRAM TAKES CARE OF NMODEL=7 TO 11 ONLY.
C
C     NDTALE(I,J) MATRIX CONSISTS OF CODES & NUMBERS FOR ALL DATA SETS
C             # OF COLUMNS (VECTORS) = # OF DATA SETS READ IN
C             1 ST ROW: NO. OF DATASETS TO BE REGRESSED
C                       1,2,3,4,..ETC.
C             2 ND ROW: DATA TYPE, VLE/LLE/HE
C                       1 = VLE, 2 = LLE, 3 = HE
C             3 RD ROW: DATA CONDITION, CONSTANT T/P
C                       1 = CONSTANT TEMPERATURE DATA
C                       2 = CONSTANT PRESSURE DATA
C             4 TH ROW: # OF COMPONENTS IN THE DATASET
C             5 TH ROW: # OF POINTS IN THE DATASET
C             6 TH ROW: ID OF FIRST COMPONENT
C             7 TH ROW: ID OF SECOND COMPONENT
C             & SO ON UPTO THE ID OF THE LAST COMPONENT
C                       0 = ABSENCE OF THE COMPONENT IN THE DATA SET
C             EXAMPLE: IN CASE OF REGRESSING BINARY & TERNARY DATASETS
C                      8 (5+3) ROWS ARE TO BE FILLED
C             RESTRICTIONS: 1. ALL VLE DATASETS SHOULD APPEAR BEFORE LLE
C                              DATASETS.
C                           2. CONSTANT T & CONSTANT P VLE DATA NOT
C                              ALLOWED TO BE REGRESSED TOGETHER.
C
C     ACCESS DATA RETREVIAL PROGRAMS
C
   11 CONTINUE
      CALL ZPVT
      CALL ZNRTL
      WRITE (NPRT,13)
   13 FORMAT ('0COMPONENTS USED ARE:'/
```

```
     *    2X, '*',2X,'NAME',6X,'ID*')
      WRITE (NPRT,14) (J,(ZNAME(K,J),K=1,2),NTCOMP(J),J=1,NC)
   14 FORMAT (I3,2X,2A4,4X,I3)
C
   15 READ (NCR,16,END=1500,ERR=7) TITLE
   16 FORMAT (20A4)
      IF (TITLE(1) .EQ. DOLLAR) GO TO 7
      WRITE (NPRT,17) TITLE
   17 FORMAT ('1',20A4)
      READ (NCR,*,END=1500,ERR=1500) PF, TF, WT, WT1
C
      PRES=PF
C
C     TF    = SYSTEM TEMP OR INTIAL T DEG C
C     PF    = SYSTEM PRESSURE OR INTIAL P IN MM HG
C     WT    = WEIGHT USED IN FX2LIQ SUBROUTINE
C     WT1   = WEIGHT USED IN FX2LIQ SUBROUTINE
C
      WRITE (NPRT,19) PF,TF,NTYPE
   19 FORMAT ('0 PARAMETERS FOR EQUILIBRIUM CALCULATION:'/
     *    5X, 'P, MMHG =',  F14.3/
     *    5X, 'T, DEG C =', F13.2/
     *    5X, 'NTYPE =',    I16)
      WRITE (NPRT,20) WT, WT1
   20 FORMAT ('0 WEIGHTS USED IN OBJECTIVE FUNCTION:'/
     *    5X, 'WEIGHT WITH TIE LINE,    WT  =',F10.2/
     *    5X, 'WEIGHT WITH PARAMETERS, WT1 =',F10.2)
C
C     CONVERT MMHG, C, TO ATM, K, CAL
C
      PF=PF/760.0
      P=PF
      TF=TF+273.16
      TSAVE=TF
C
      DO 35 I=1,NC
      IF (L(I)-1) 21,23,25
   21 L(I)=1
   22 GAM1(I)=1.0
      GAM2(I)=1.0
      FUG(I)=1.0
      GO TO 29
   23 L(I)=2
      GO TO 22
   25 IF (L(I)-3) 24,26,21
   24 L(I)=0
      GAM1(I)=1.0
      GAM2(I)=1.0
      GO TO 27
   26 L(I)=-1
      GAM1(I)=1.0
      GAM2(I)=1.0
   27 FUG(I)=0.0
   29 VP(I)=0.0
      EK1(I) = 0.0
      EK2(I) = 0.0
   35 CONTINUE
C
   50 IF (NTYPE .GT. 0) GO TO 55
      GO TO 1000
```

```
C
C        NTYPE   DESCRIPTION
C           1     CONSTANT T VLE
C           2     CONSTANT P VLE
C           3     CONSTANT T LLE
C           4     MIXING OF CONSTANT P VLE & CONSTANT T LLE
C           5     MIXING OF CONSTANT T VLE & CONSTANT T LLE
C           6     ****
C           7     ****
C           8     ****
C           9     ****
C          10     ****
C
   55  IF (NTYPE .GT. 5) GO TO 1000
C
C      ASSIGNMENT OF ADJUSTABLE PARAMETERS
C
       IF (NMODEL .LT. 7 .OR. NMODEL .GT. 11) GO TO 1000
       K=0
       IP=1
       DO 80 I = 1,NCM1
       IJ=I+1
       DO 75 J = IJ,NC
       K=K+1
       II=4*K
       GO TO (60,65,70), ITDEP
   60  C(II-3)=ADJUST(IP)
       C(II-2)=0.0
       C(II-1)=ADJUST(IP+1)
       C(II)=0.0
       INX=IP
       IP=IP+2
       GO TO 75
   65  C(II-3)=ADJUST(IP)
       C(II-2)=ADJUST(IP+1)
       C(II-1)=ADJUST(IP+2)
       C(II)=0.0
       INX=IP
       IP=IP+3
       GO TO 75
   70  C(II-3)=ADJUST(IP)
       C(II-2)=ADJUST(IP+2)
       C(II-1)=ADJUST(IP+3)
       C(II)=ADJUST(IP+3)
       INX=IP
       IP=IP+4
   75  CONTINUE
   80  CONTINUE
C
       IF (NMODEL .NE. 9) GO TO 90
       DO 85 I =1,NC
       ALPHA(I)=ADJUST(INX)
       INX=INX+1
   85  CONTINUE
   90  CONTINUE
C
C      ASSIGNMENT OF INDEPENDENT VARIABLES.
C      IN THE CASE OF LLE, Z(I) IS REDEFINED IN SUBROUTINE PX2LIQ
C
       SUM=0.0
```

```
      DO 95 J =1,NCM1
      SUM=SUM+XVAR(J)
   95 CONTINUE
      XN=1.0-SUM
      DO 96 J = 1,NCM1
      Z(J)=XVAR(J)
   96 CONTINUE
      Z(NC)=XN
      DO 97 I = 1,NC
   97 X1EXP(I)=Z(I)
C
      GO TO (100,100,101,100,100), NTYPE
  100 IF (IDPT .GT. NVLPT) GO TO 101
      NLIQ=1
      NCN=NCVLE
      NPT=NVLPT
      GO TO 102
  101 NLIQ=2
      NCN=NCLLE
      NPT=NVLPT+NLLPT
C
C     STORING ALL THE EXPERIMENTAL X1 VALUES FOR PRINT OUT
C
  102 IF (ICALL .EQ. 0) GO TO 104
      KNT=KOUNT
  104 IF (KNT .GT. NPT) GO TO 107
      DO 105 I=1,NCN
      X1EO(I,KNT)=X1EXP(I)
  105 CONTINUE
      KNT=KNT+1
  107 CONTINUE
C
      IF (ICALL .EQ. 0) GO TO 3300
C
C     READING & STORING EXPERIMENTAL (T, P, Y, X2) DATA
C     ACCORDING TO THE VALUE 'RECODE'
C
      II=1
      IST=1
      IF (RECODE .LT. 0) GO TO 3400
      GO TO (3000,3000,3050,3100,3000,3000,3000,3000,3050,
     *       3000,3000), RECODE
 3000 READ (NCR,*) (PICKUP(II),II=1,NVLPT)
      IF (RECODE .EQ. 2 .OR. RECODE .EQ. 6)  GO TO 3010
      IF (RECODE .EQ. 8 .OR. RECODE .EQ. 11) GO TO 3010
      II=1
      DO 3005 J=1,NVLPT
      TEO(J)=PICKUP(II)
      II=II+1
 3005 CONTINUE
      IF (RECODE .EQ. 5 .OR. RECODE .EQ. 10) GO TO 3050
      IF (RECODE .EQ. 7) GO TO 3100
      GO TO 3300
 3010 II=1
      DO 3015 J=1,NVLPT
      PEO(J)=PICKUP(II)
      II=II+1
 3015 CONTINUE
      IF (RECODE .EQ. 6 .OR. RECODE .EQ. 11) GO TO 3050
      IF (RECODE .EQ. 8) GO TO 3100
```

```
      GO TO 3300
C
 3050 CONTINUE
      NTEMP=(NCVLE-1)*NVLPT
      READ (NCR,*) (PICKUP(II),II=1,NTEMP)
      IF (LDBUG .GE. 2) WRITE (NPRT,3055)(PICKUP(II),II=1,NTEMP)
 3055 FORMAT (' ',<2*NVLPT>(6F10.4/))
      II=1
      DO 3075 J=1,NVLPT
      SUM=0.0
      DO 3060 I=1,(NCVLE-1)
      SUM=SUM+PICKUP(II)
      YEO(I,J)=PICKUP(II)
      II=II+1
 3060 CONTINUE
      YEO(NCVLE,J)=1.0-SUM
      SUM=0.0
      DO 3065 I=1,NCVLE
 3065 SUM=SUM+YEO(I,J)
      DO 3070 I=1,NCVLE
 3070 YEO(I,J)=YEO(I,J)/SUM
 3075 CONTINUE
C     WRITE (6,*) (J,(I,YEO(I,J),I=1,NCN),J=IST,NPT)
      IF (RECODE .LT. 10) GO TO 3300
C
 3100 NTEMP=(NCLLE-1)*NLLPT
      READ (NCR,*) (PICKUP(II),II=1,NTEMP)
      II=1
      DO 3125 J=(NVLPT+1),(NVLPT+NLLPT)
      SUM=0.0
      DO 3110 I=1,(NCLLE-1)
      SUM=SUM+PICKUP(II)
      X2EO(I,J)=PICKUP(II)
      II=II+1
 3110 CONTINUE
      X2EO(NCLLE,J)=1.0-SUM
      SUM=0.0
      DO 3115 I=1,NCLLE
 3115 SUM=SUM+X2EO(I,J)
      DO 3120 I=1,NCLLE
 3120 X2EO(I,J)=X2EO(I,J)/SUM
 3125 CONTINUE
 3300 CONTINUE
C     CALL PRINT3
C
C     ALLOCATION OF EXPERIMENTAL VALUE OF DEPENDENT VARIABLE
C     FOR DATA POINT 'IDPT'.
C
      IF (VLEFN .LE. 0) GO TO 3380
      IF (VLEFN .LT. 17) GO TO 3320
      TEXP=TEO(IDPT)+273.16
      GO TO 3380
 3320 IF (VLEFN .LT. 10) GO TO 3340
      PEXP=PEO(IDPT)/760.0
      IF (VLEFN .GT. 13) GO TO 3380
 3340 DO 3350 I=1,NCVLE
      YEXP(I)=YEO(I,IDPT)
 3350 CONTINUE
 3380 IF (LLEFN .LE. 0 .OR. IDPT .LE. NVLPT) GO TO 3400
 3355 DO 3360 I=1,NCLLE
```

```
      X2EXP(I)=X2EO(I,IDPT)
 3360 CONTINUE
 3400 CONTINUE
C
      IF (LDBUG .NE. 1 .OR. ICALL .EQ. 0) GO TO 3600
      WRITE (NPRT, 3440)
 3440 FORMAT (/T20,'EXPERIMENTAL Y VALUES IN MOLE %'/)
      DO 3460 J=1,NVLPT
      WRITE (NPRT,3445) (YEO(I,J),I=1,NCVLE)
 3445 FORMAT (' ',<NCVLE>(2PF12.4,3X))
 3460 CONTINUE
C
      WRITE (NPRT, 3480)
 3480 FORMAT (/T20,'EXPERIMENTAL X2EXP VALUES IN MOLE %'/)
      DO 3500 J=(NVLPT+1),(NVLPT+NLLPT)
      WRITE (NPRT,3490) (X2EO(I,J),I=1,NCLLE)
 3490 FORMAT (' ',<NCLLE>(2PF12.4,3X))
 3500 CONTINUE
C
 3600 IF (LDBUG .LT. 2) GO TO 115
      NC4=NC*NCM1*2
      write(nprt,108)(z(J),J=1,NC)
  108 FORMAT('0Z(J) VALUES AT STM#108 IN FOFX ARE ',2X,10(F7.5,2x))
      write(nprt,110)(C(J),J=1,NC4)
  110 FORMAT('0C(J) VALUES AT STM#110 IN FOFX ARE ',2X/6E13.5/6E13.5/
     *6E13.5/6E13.5)
      write(nprt,112)(ALPHA(J),J=1,NC)
  112 FORMAT('0ALPHA(J) VALUES AT STM#112 IN FOFX ARE ',2X,5E10.2/
     *5E10.2)
      WRITE (NPRT,103)
  103 FORMAT (/T10,'X1EXP (MOLE %)',T35,'X2EXP (MOLE %)'/)
      WRITE (NPRT,106) (X1EXP(I),I=1,NCN),(X2EXP(I),I=1,NCN)
  106 FORMAT ('0',<NCN>(2PF12.5),:,4X,<NCN>(2PF12.5))
C
  115 RMIN=0.0
      RMAX=1.0
      DO 118 I=1,NC
      IF (L(I)) 116,117,118
  116 RMAX=RMAX-Z(I)
      GO TO 118
  117 RMIN=RMIN+Z(I)
  118 CONTINUE
C
      NODEW=0
      NOBUB=0
      NOBUBP=0
C
      DO 140 I=1,NC
      IF (FD(I)) 140,140,119
  119 IF (L(I)) 120,130,140
  120 NODEW=1
      GO TO 140
  130 NOBUB=1
      NOBUBP=0
  140 CONTINUE
c
      ICALL=0
      GO TO (150,220,280,220,150), NTYPE
C
C     CONSTANT TEMPERATURE VLE CALCULATIONS
```

```
C
  150 if(ntype .eq. 5 .and. idpt .gt. nvlpt)go to 280
      if (ldbug .ge. 2) write(nprt,155)
  155 format('Oresults of total pressure calculation')
      if (nliq .ne. 1)go to 1000
      DO 160 I =1,NC
  160 X1(I)=Z(I)
      T=TF
      p=pf
      CALL BUBP
      if (nobubp .ne. 0)go to 200
      CALL FXVLE (ZZZ)
      PBUB=P
      if (ldbug .ge. 1) write(nprt,170) zzz
 170  format('0zzz or p in fofx is ',f10.5)
      IF (NTYPE .EQ. 5)GO TO 220
      go to 2000
 200  if (ldbug .ge. 1)write (nprt,210)
 210  format ('0pressure could not be determined')
      GO TO 2000
C
C     *** CONSTANT PRESSURE VLE CALCULATIONS ***
C
  220 continue
      IF (NTYPE .EQ. 4 .AND. IDPT .GT. NVLPT) GO TO 280
      IF (NTYPE .EQ. 5 .AND. IDPT .GT. NVLPT) GO TO 280
      if (ldbug .ge. 1)WRITE(NPRT,221)
  221 FORMAT (/'ORESULTS OF BUBBLE POINT CALCULATION')
      IF (NOBUB.EQ.0) GO TO 240
      if (ldbug .ge. 1)WRITE(NPRT,230)
  230 FORMAT('ONO BUBBLE POINT SINCE NONCONDENSIBLE COMPONENTS ARE PRESE
     *NT')
  231 TBUB=-459.0
      DO 235 I=1,NC
  235 BUBC(I)=0.0
      GO TO 2000
C
  240 IF (NLIQ.EQ.2) GO TO 280
      DO 241 I=1,NC
  241 X1(I)=Z(I)
      T=TF
      FRACL=1.0
      CALL BUBPT1
C
  245 IF (NOBUB.EQ.0) GO TO 255
      if (ldbug .ge. 1)WRITE(NPRT,250)
  250 FORMAT('OFEED REPRESENTS A HYPOTHETICAL LIQUID OR IS IN THE RETROG
     +RADE REGION. BUBBLE POINT CALCULATIONS TERMINATED.')
      GO TO 231
C
  255 TBUB=T
      CALL FXVLE (ZZZ)
      TDEG=TBUB-273.16
      if (ldbug .ge. 1)WRITE(NPRT,260) PRES, TDEG
  260 FORMAT('OBUBBLE POINT OF FEED AT',F7.2,' MMHG IS',F7.2,' DEG C')
      DO 265 I=1,NC
  265 BUBC(I)=Y(I)
      IF (LDBUG .LT. 2) GO TO 272
      WRITE (NPRT,268) ((ZNAME(J,I),J=1,2),I=1,NC)
  268 format (25x,10(2a4,2x))
```

```
      WRITE(NPRT,270) (BUBC(I),I=1,NC)
  270 FORMAT (' BUB PT VAP MOLE FRAC', 2X, 10F10.5)
      CALL PRINT2
  272 GO TO 2000
C
C     *** CONSTANT TEMPERATURE LLE CALCULATIONS ***
C
C
  280 CONTINUE
      T=TF
      CALL FX2LIQ (ZZZ)
      GO TO 2000
C
 1000 if (ldbug .ge. 2)wRITE (NPRT,1100)
 1100 FORMAT(' EXITING FOFX WITH INCOMPLETE CALCULATIONS')
 1500 CALL EXIT
 2000 CONTINUE
C
C     THE FOLLOWING STATEMENT IS ACTIVATED IF THE CONTRIBUTION
C     OF SOME DATA POINTS IN REGRESSION HAS TO BE ELIMINATED
C
      IF (NSKIP .EQ. 0) GO TO 2001
      DO 2001 I=1,NSKIP
      IF (IDPT .EQ. ISKIP(I)) ZZZ=0.0
 2001 CONTINUE
      IF (LDBUG .GE. 1) WRITE (NPRT,1950) IDPT, ZZZ
 1950 FORMAT (' IN FOFX AT STMT#1950 :',' IDPT=',I3,' ZZZ=',E15.7)
C
C     DOWNLOADING INTO OUTPUT VARIABLES FOR FINAL PRINTOUT
C
      IF (LDBUG .EQ. 0) GO TO 2004
      WRITE(NPRT,2002)TEXP,T,PEXP,P,(X1EXP(I),I=1,NCN)
 2002 FORMAT (/'AT 2002 IN FOFX TEXP / T / PEXP / P / X1EXP ='/
     *4F10.3,2X,<NCN>(F7.5,2X))
      WRITE (NPRT,2003)((ABS(ACT1C(I)-ACT2C(I))),I=1,NCN)
 2003 FORMAT (/' ABS DIFF IN LLE CALC ACTIVITIES',<NCN>E12.4)
 2004 IF (NTYPE .EQ. 3) GO TO 2010
      IF (NTYPE .GE. 4 .AND. IDPT .GT. NVLPT) GO TO 2010
      IF (NTYPE .EQ. 1 .OR. NTYPE .EQ. 5)GO TO 2005
      TESV=TEO(IDPT)+273.16
      CALL ACTVY (TESV,P,X1EXP,GAM1E)
      TCO(IDPT)=TBUB-273.16
      GO TO 2010
 2005 PCO(IDPT)=PBUB*760.0
      PESV=PEO(IDPT)/760.0
      CALL ACTVY (T,PESV,X1EXP,GAM1E)
 2010 DO 2020 I=1,NCN
      X1O(I,IDPT)=X1(I)
      G1EO(I,IDPT)=GAM1E(I)
      G1O(I,IDPT)=GAM1(I)
      ACT1EO(I,IDPT)=ACT1E(I)
      ACT1CO(I,IDPT)=ACT1C(I)
      IF (NTYPE .LT. 3) GO TO 2015
      IF (NTYPE .GE. 4 .AND. IDPT .LE. NVLPT) GO TO 2015
      X2O(I,IDPT)=X2(I)
      G2EO(I,IDPT)=GAM2E(I)
      G2O(I,IDPT)=GAM2(I)
      ACT2EO(I,IDPT)=ACT2E(I)
      ACT2CO(I,IDPT)=ACT2C(I)
      KEO(I,IDPT)=KE(I)
```

```
      KCO(I,IDPT)=KC(I)
      IF (LLEFN .LT. 9) GO TO 2020
C     IF (LLEFN .GT. 11) GO TO 2012
 2012 IF (LLEFN .NE. 12) GO TO 2020
 2015 YCO(I,IDPT)=Y(I)
C     G1IEO(I,IDPT)=GAM1IE(I)
C     G1ICO(I,IDPT)=GAM1IC(I)
      IF (NTYPE .LT. 3) GO TO 2020
      IF (NTYPE .GE. 4 .AND. IDPT .LE. NVLPT) GO TO 2020
C     G2IEO(I,IDPT)=GAM2IE(I)
C     G2ICO(I,IDPT)=GAM2IC(I)
C     KIEO(I,IDPT)=KIE(I)
C     KICO(I,IDPT)=KIC(I)
 2020 CONTINUE
 2500 RETURN
      END
C**********************************************************************
      SUBROUTINE PRINT3
C
C     PROGRAMMED BY H.S. CHAWLA ...  OCT. 1984.
C     IT GIVES PRINT OUT AFTER THE FINAL SET OF PARAMETERS IS OBTAINED
C
      COMMON  /BLANK/  NCR, NPRT, NSTART, KUNITS, TITLE(20)
      COMMON  /CMPRO/  NC, NCM1, IDLL, IDLV, IDH, LDBUG, ISW, NDIM,
     *                 ZNAME(2,10), L(10), NTCOMP(10)
      COMMON  /CONTRL/ ITF, IPF,  N, NTYPE, JCODE, NLIQ
      COMMON  /ZFEEDZ/ PF, TF, FEED, FMOL, TREF, HI, NK1, NFEED
      COMMON  /TWOLQ/  X1(10), X2(10), GAM1(10), GAM2(10), EK1(10),
     +                 EK2(10), DHL(2), HIDLL(2), HREALL(2), FRACL,
     +                 IE, IR, XMAX, XMIN
      COMMON  /FOX/    X1EXP(10), X2EXP(10), GAM1E(10), GAM2E(10),
     *                 GAM1IE(10), GAM2IE(10),GAM1IC(10), GAM2IC(10),
     *                 ACT1C(10), ACT2C(10), ACT1E(10), ACT2E(10),
     *                 KE(10), KC(10), KIE(10), KIC(10), W1(10),
     *                 W2(10), YEXP(10), TEXP, PEXP, WT, WT1, VLEFN,
     *                 LLEFN, VLLFN, NVLPT, NLLPT, NCVLE, NCLLE,
     *                 NMODEL, INX, RECODE, NDTALE(15,10), NDSET
      COMMON  /OUTPUT/ X1EO(10,200), X2EO(10,200), X1O(10,200),
     *                 X2O(10,200), G1EO(10,200), G2EO(10,200),
     *                 G1O(10,200), G2O(10,200), G1IEO(10,5),
     *                 G2IEO(10,5), G1ICO(10,5), G2ICO(10,5),
     *                 KEO(10,200), KCO(10,200), KIEO(10,5),
     *                 KICO(10,5), YEO(10,200), YCO(10,200),
     *                 TEO(200), PEO(200), TCO(200), PCO(200),
     *                 ACT1EO(10,200), ACT2EO(10,200), ACT1CO(10,200),
     *                 ACT2CO(10,200)
C
      INTEGER          VLEFN, LLEFN, VLLFN, RECODE
      REAL*4           KE, KC, KEO, KCO, KIE, KIC, KIEO, KICO,
     *                 MEAN(11), VMAX(11), VMIN(11), HOLD(20,200),
     *                 SS(1), TOTAL(11), SD(11)
C
C     ALL THE VARIABLE NAMES ENDING WITH LETTER 'O' IN THE COMMON
C     BLOCK 'OUTPUT' STORE RELEVANT EXPERIMENT/CALCULATED VALUES
C     FOR ALL THE DATA POINTS. THE MAXIMUM LIMIT CAN BE RAISED UPTO
C     400 DATA POINTS. THE VARIABLES ARE USED ONLY FOR THE FINAL
C     PRINTOUT AND ASSESSMENT OF PREDICTED PROPERTIES WITH FINAL
C     SET OF REGRESSED PARAMETERS. THE FOLLOWING CHARACTERS IN THE
C     VARIABLE NAMES STAND FOR:
C          1/2    LIQUID PHASE # 1/2
```

```
C           E/C    EXPERIMENTAL/CALCULATED VALUES
C           I      VALUES AT INFINITE DILUTION
C           O      VARIABLES FOR OUTPUT PURPOSE
C
      NCN=NCVLE
      NPT=0
      IST=1
      NVLST=0
      NLLST=0
      DO 60 J=1,NDSET
      IF (NDTALE(2,J) .EQ. 1) NVLST=NVLST+1
      IF (NDTALE(2,J) .EQ. 2) NLLST=NLLST+1
   60 CONTINUE
      IF (NTYPE .EQ. 3) GO TO 450
      DO 380 III=1,NVLST
      IST=NPT+1
      NPT=NPT+NDTALE(5,III)
      WRITE (NPRT,70) III
   70 FORMAT ('1',<10*NCN>X,'*** RESULTS OF SET # ',I1,' ***')
      WRITE (NPRT,100)
  100 FORMAT (/<8*NCN-5>X,'VLE EXPERIMENTAL DATA',<12*NCN-13>X,
     *'DIFFERENCES (EXP-CALC)')
      IF (NTYPE .EQ. 1 .OR. NTYPE .EQ. 5) GO TO 180
C
C     CONSTANT PRESSURE VLE CASE
C
C     WRITE (NPRT,115) (J,TCO(J),J=IST,NPT)
  115 FORMAT ('0CALCULATED TEMPERATURES ='/<NPT/8+1>((8(I2,F7.2,1X))/))
      WRITE (NPRT,120)
  120 FORMAT (' T DEG C',<4*NCN-6>X,'X IN MOLE %',<8*NCN-8>X,
     *'Y IN MOLE %',<4*NCN-2>X,'T',<4*NCN>X,'Y')
      WRITE (NPRT,130) (I,I=1,NCN),(I,I=1,NCN),(I,I=1,NCN-1)
  130 FORMAT (T12,<NCN>('-',I1,'-'5X),3X,<NCN>('-',I1,'-',5X),8X,
     *<NCN>('-',I1,'-',5X)/)
C
      DO 134 J=1,NPT
      DO 134 I=1,NCN
  134 HOLD(I,J)=0.0
      DO 160 J=IST,NPT
      HOLD(1,J)=TEO(J)-TCO(J)
      DO 140 I=1,NCN-1
      HOLD(I+1,J)=YEO(I,J)-YCO(I,J)
  140 CONTINUE
      WRITE (NPRT,150) TEO(J),(X1EO(I,J),I=1,NCN),(YEO(I,J),I=1,NCN),
     *HOLD(1,J),(HOLD(I+1,J),I=1,NCN-1)
  150 FORMAT (' ',F7.2,<NCN>(2PF7.3,1X),3X,<NCN>(2PF7.3,1X),2X,
     *0PF6.2,<NCN>(2PF7.3,1X))
  160 CONTINUE
C
      CALL TALLY1 (HOLD,SS,TOTAL,MEAN,SD,VMIN,VMAX,IST,NPT,NCN)
      WRITE (NPRT,177) (MEAN(I),I=1,NCN)
  177 FORMAT (/<16*NCN-6>X,'MEAN DEVIATION :',3X,F6.2,
     *<NCN-1>(2PF7.3,1X))
      WRITE (NPRT,178) (VMAX(I),I=1,NCN)
  178 FORMAT (/<16*NCN-6>X,'MAX. DEVIATION :',3X,F6.2,
     *<NCN-1>(2PF7.3,1X)/)
      WRITE (NPRT,179) (SD(I),I=1,NCN)
  179 FORMAT (/<16*NCN-6>X,'STD. DEVIATION :',3X,F6.2,
     *<NCN-1>(2PF7.3,1X)/)
      GO TO 250
```

```
C
C     CONSTANT TEMPERATURE VLE CASE
C
  180 WRITE (NPRT,200)
  200 FORMAT (' P MM HG',3X,'X IN MOLE %',7X,
     *'Y IN MOLE %',8X,'P    ',<2*NCN>X,'Y')
      WRITE (NPRT,130) (I,I=1,NCN),(I,I=1,NCN),(I,I=1,NCN-1)
      DO 205 J=1,NPT
      DO 205 I=1,NCN
  205 HOLD(I,J)=0.0
      DO 240 J=IST,NPT
      HOLD(1,J)=PEO(J)-PCO(J)
      DO 210 I=1,NCN-1
      HOLD(I+1,J)=YEO(I,J)-YCO(I,J)
  210 CONTINUE
      WRITE (NPRT,150) PEO(J),(X1EO(I,J),I=1,NCN),(YEO(I,J),I=1,NCN),
     *HOLD(1,J),(HOLD(I+1,J),I=1,NCN-1)
  240 CONTINUE
      CALL TALLY1 (HOLD,SS,TOTAL,MEAN,SD,VMIN,VMAX,IST,NPT,NCN)
      WRITE (NPRT,177) (MEAN(I),I=1,NCN)
      WRITE (NPRT,178) (VMAX(I),I=1,NCN)
      WRITE (NPRT,179) (SD(I),I=1,NCN)
C
C     GAMMA VALUES FOR CONSTANT T OR P CASES (VLE)
C
  250 WRITE (NPRT,260)
  260 FORMAT('1',<8*NCN-12>X,'ACTIVITY COEFFICIENT VALUES',
     *<12*NCN-4>X,'% REL DIFF')
      WRITE (NPRT,280)
  280 FORMAT (' ',<4*NCN-6>X,'EXPERIMENTAL',<8*NCN-8>X,'CALCULATED')
      WRITE (NPRT,300) (I,I=1,NCN),(I,I=1,NCN),(I,I=1,NCN)
  300 FORMAT (' ',T4,<NCN>('-',I1,'-'5X),3X,<NCN>('-',I1,'-',5X),3X,
     *<NCN>('-',I1,'-',4X)/)
      DO 302 J=1,NPT
      DO 302 I=1,NCN
  302 HOLD(I,J)=0.0
      DO 340 J=IST,NPT
      DO 305 I=1,NCN
      HOLD(I,J)=100.0*(G1EO(I,J)-G1O(I,J))/G1EO(I,J)
  305 CONTINUE
      WRITE (NPRT,320) (G1EO(I,J),I=1,NCN),(G1O(I,J),I=1,NCN),
     *                   (HOLD(I,J),I=1,NCN)
C 320 FORMAT (' ',<NCN>F8.3,3X,<NCN>F8.3,3X,<NCN>(2PG10.3))
  320 FORMAT (' ',<NCN>F8.3,3X,<NCN>F8.3,3X,<NCN>(G10.3))
  340 CONTINUE
C
      CALL TALLY1 (HOLD,SS,TOTAL,MEAN,SD,VMIN,VMAX,IST,NPT,NCN)
      WRITE (NPRT,345) (MEAN(I),I=1,NCN)
  345 FORMAT (/<16*NCN-13>X,'MEAN DEVIATION :',5X,<NCN>
     *(2PG10.3,2X))
      WRITE (NPRT,347) (VMAX(I),I=1,NCN)
  347 FORMAT (/<16*NCN-13>X,'MAX. DEVIATION :',5X,<NCN>
     *(2PG10.3,2X)/)
      WRITE (NPRT,348) (SD(I),I=1,NCN)
  348 FORMAT (/<16*NCN-13>X,'STD. DEVIATION :',5X,<NCN>
     *(2PG10.3,2X)/)
C
C     INFINITE DILUTION GAMMA VALUES FOR CONSTANT T OR P BINARY VLE
C
      IF (NCVLE .GT. 2) GO TO 380
```

```
      WRITE (NPRT,350)
  350 FORMAT('0','INFINITE DIL. ACTIVITY COEFF. VALUES',
     *T50,'% REL DIFF')
      WRITE (NPRT,280)
      WRITE (NPRT,300) (I,I=1,NCN),(I,I=1,NCN),(I,I=1,NCN)
C     JJ=NO. OF DIFFERENT DATA SETS READ IN
      DO 360 JJ=1,1
      DO 360  J=IST,NPT,(NPT-IST)
      DO 355 I=1,NCN
      X1EXP(I)=X1EO(I,J)
      X1(I)=X1O(I,J)
  355 CONTINUE
      IF (NTYPE .EQ. 1 .OR. NTYPE .EQ. 5) PEXP=PEO(J)/760.0
      IF (NTYPE .EQ. 2 .OR. NTYPE .EQ. 4) TEXP=TEO(J)+273.16
      CALL INFY (IMIN1,IMIN2)
      G1IEO(IMIN1,JJ)=GAM1IE(IMIN1)
      G1ICO(IMIN1,JJ)=GAM1IC(IMIN1)
  360 CONTINUE
      DO 365 JJ=1,1
  365 WRITE (NPRT,320) (G1IEO(I,JJ),I=1,NCN),(G1ICO(I,JJ),I=1,NCN),
     *                 ((G1IEO(I,JJ)-G1ICO(I,JJ)),I=1,NCN)
  380 CONTINUE
      IF (NTYPE .GE. 4) GO TO 450
      GO TO 1300
C
C     CONSTANT TEMPERATURE LLE CASE
C     2 LIQUID PHASE COMPOSITIONS
C
  450 NCN=NCLLE
      DO 1060 III=1,NLLST
      IST=NPT+1
      NPT=NPT+NDTALE(5,III+NVLST)
      WRITE (NPRT,70) III+NVLST
      WRITE (NPRT,500)
  500 FORMAT (/T10,'EXPERIMENTAL LIQUID PHASE COMPOSITIONS IN
     *MOLE %'/)
      WRITE (NPRT,530) IE, IR
  530 FORMAT (' ',T10,'PHASE RICH IN ',I1,T45,'PHASE RICH IN ',I1/)
      WRITE (NPRT,550) (I,I=1,NCN), (I,I=1,NCN)
  550 FORMAT(' ',5X,<NCN>('-',I1,'-',7X),5X,<NCN>('-',I1,'-',7X))
      DO 630 J=IST,NPT
      WRITE (NPRT,600)(X1EO(I,J),I=1,NCN),(X2EO(I,J),I=1,NCN)
  600 FORMAT (' ',<NCN>(2PF10.4),5X,<NCN>(2PF10.4))
  630 CONTINUE
C
      WRITE (NPRT,650)
  650 FORMAT ('0',T10,'CALCULATED LIQUID PHASE COMPOSITIONS IN MOLE %'/)
      WRITE (NPRT,530) IE, IR
      WRITE (NPRT,550) (I,I=1,NCN), (I,I=1,NCN)
      DO 720 J=IST,NPT
  720 WRITE (NPRT,600)(X1O(I,J),I=1,NCN),(X2O(I,J),I=1,NCN)
C
C     CALCULATION OF ABSOLUTE DIFFERENCE OF COMPOSITIONS (MOLE %):
C     (XEXP-XCALC)
C
      WRITE (NPRT,750)
  750 FORMAT ('1',T10,'ABSOLUTE DIFFERENCE OF COMPOSITIONS IN MOLE %'/)
      WRITE (NPRT,530) IE, IR
      WRITE (NPRT,550) (I,I=1,NCN), (I,I=1,NCN)
      DO 760 J=1,NPT
```

```
      DO 760 I=1,2*NCN
  760 HOLD(I,J)=0.0
      DO 840 J=IST,NPT
      DO 820 I=1,NCN
      HOLD(I,J)=100.0*(X1EO(I,J)-X1O(I,J))
      HOLD(I+NCN,J)=100.0*(X2EO(I,J)-X2O(I,J))
  820 CONTINUE
      WRITE (NPRT,862) (HOLD(I,J),I=1,2*NCN)
  840 CONTINUE
C
      NNN=2*NCN
      CALL TALLY1 (HOLD,SS,TOTAL,MEAN,SD,VMIN,VMAX,IST,NPT,NNN)
      DO 858 I=1,NNN
  858 SUM=MEAN(I)
      OVMEAN=SUM/NNN
      WRITE (NPRT,860)
  860 FORMAT (/' MEAN DEVIATION VALUES (EXPT-CALC)IN MOLE %'/)
      WRITE (NPRT,861) (MEAN(I),I=1,NNN), OVMEAN
  861 FORMAT (' ',<NCN>(G13.4),5X,<NCN>(G13.4)/
     *' OVERALL MEAN DEVIATION (EXPT-CALC) IN MOLE % =',G13.4)
C 862 FORMAT (' ',<NCN>(2PF13.4),5X,<NCN>(2PF13.4))
  862 FORMAT (' ',<NCN>(G13.4),5X,<NCN>(G13.4))
      WRITE (NPRT,865)
  865 FORMAT (/' MAX. DEVIATION VALUES (EXPT-CALC)IN MOLE %'/)
      WRITE (NPRT,862) (VMAX(I),I=1,NNN)
      WRITE (NPRT,870)
  870 FORMAT (/' STD. DEVIATION VALUES (EXPT-CALC)IN MOLE %'/)
      WRITE (NPRT,862) (SD(I),I=1,NNN)
C
C     CALCULATION OF % RELATIVE DIFFERENCE OF COMPOSITIONS:
C
      WRITE (NPRT,872)
  872 FORMAT ('0',T10,'% RELATIVE DIFFERENCE OF COMPOSITIONS'/)
      WRITE (NPRT,530) IE, IR
      WRITE (NPRT,550) (I,I=1,NCN), (I,I=1,NCN)
      DO 873 J=1,NPT
      DO 873 I=1,2*NCN
  873 HOLD(I,J)=0.0
      DO 875 J=IST,NPT
      DO 874 I=1,NCN
      HOLD(I,J)=100.0*(X1EO(I,J)-X1O(I,J))/X1EO(I,J)
      HOLD(I+NCN,J)=100.0*(X2EO(I,J)-X2O(I,J))/X2EO(I,J)
  874 CONTINUE
      WRITE (NPRT,862) (HOLD(I,J),I=1,2*NCN)
  875 CONTINUE
C
      NNN=2*NCN
      CALL TALLY1 (HOLD,SS,TOTAL,MEAN,SD,VMIN,VMAX,IST,NPT,NNN)
      WRITE (NPRT,876)
  876 FORMAT (/' MEAN % REL DEVIATION VALUES '/)
      WRITE (NPRT,862) (MEAN(I),I=1,2*NCN)
      WRITE (NPRT,877)
  877 FORMAT (/' MAX. % REL DEVIATION VALUES '/)
      WRITE (NPRT,862) (VMAX(I),I=1,2*NCN)
      WRITE (NPRT,878)
  878 FORMAT (/' % STD. DEVIATION VALUES '/)
      WRITE (NPRT,862) (SD(I),I=1,2*NCN)
C
C     ACTIVITY COEFFICIENTS (LLE)
C
```

```
      WRITE (NPRT,880)
  880 FORMAT ('1',T10,'ACTIVITY COEFFICIENTS WITH EXPERIMENTAL X
     *VALUES'/)
      WRITE (NPRT,530) IE, IR
      WRITE (NPRT,550) (I,I=1,NCN), (I,I=1,NCN)
      DO 920 J=IST,NPT
      WRITE (NPRT,910) (G1EO(I,J),I=1,NCN), (G2EO(I,J),I=1,NCN)
  910 FORMAT (' ',<NCN>(F10.4),5X,<NCN>(F10.4))
  920 CONTINUE
C
      WRITE (NPRT,940)
  940 FORMAT ('0',T10,'ACTIVITY COEFFICIENTS WITH CALCULATED X VALUES'/)
      WRITE (NPRT,530) IE, IR
      WRITE (NPRT,550) (I,I=1,NCN), (I,I=1,NCN)
      DO 970 J=IST,NPT
  970 WRITE (NPRT,910) (G10(I,J),I=1,NCN), (G20(I,J),I=1,NCN)
C
C     CALCULATION OF ABSOLUTE DIFFERENCE OF ACTIVITY COEFFICIENTS:
C
      WRITE (NPRT,975)
  975 FORMAT ('1',T10,'ABSOLUTE DIFFERENCE OF ACTIVITY COEFFICIENTS'/)
      WRITE (NPRT,530) IE, IR
      WRITE (NPRT,550) (I,I=1,NCN), (I,I=1,NCN)
      DO 977 J=1,NPT
      DO 977 I=1,2*NCN
  977 HOLD(I,J)=0.0
      DO 985 J=IST,NPT
      DO 980 I=1,NCN
      HOLD(I,J)=G1EO(I,J)-G10(I,J)
      HOLD(I+NCN,J)=G2EO(I,J)-G20(I,J)
  980 CONTINUE
      WRITE (NPRT,862) (HOLD(I,J),I=1,2*NCN)
  983 FORMAT (' ',<NCN>F10.3,5X,<NCN>F10.3)
  985 CONTINUE
C
      NNN=2*NCN
      CALL TALLY1 (HOLD,SS,TOTAL,MEAN,SD,VMIN,VMAX,IST,NPT,NNN)
      WRITE (NPRT,993)
  993 FORMAT (/' MEAN DEVIATION VALUES (EXPT-CALC)'/)
      WRITE (NPRT,862) (MEAN(I),I=1,2*NCN)
      WRITE (NPRT,995)
  995 FORMAT (/' MAX. DEVIATION VALUES (EXPT-CALC)'/)
      WRITE (NPRT,862) (VMAX(I),I=1,2*NCN)
      WRITE (NPRT,997)
  997 FORMAT (/' STD. DEVIATION VALUES (EXPT-CALC)'/)
      WRITE (NPRT,862) (SD(I),I=1,2*NCN)
C
C     CALCULATION OF RELATIVE % DIFFERENCE OF ACTIVITY COEFFICIENTS:
C
      WRITE (NPRT,1000)
 1000 FORMAT ('0',T10,'RELATIVE % DIFFERENCE OF ACTIVITY COEFFICIENTS'/)
      WRITE (NPRT,530) IE, IR
      WRITE (NPRT,550) (I,I=1,NCN), (I,I=1,NCN)
      DO 1001 J=1,NPT
      DO 1001 I=1,2*NCN
 1001 HOLD(I,J)=0.0
      DO 1005 J=IST,NPT
      DO 1002 I=1,NCN
      HOLD(I,J)=100.0*(G1EO(I,J)-G10(I,J))/G1EO(I,J)
      HOLD(I+NCN,J)=100.0*(G2EO(I,J)-G20(I,J))/G2EO(I,J)
```

```
 1002 CONTINUE
      WRITE (NPRT,862) (HOLD(I,J),I=1,2*NCN)
C1003 FORMAT (' ',<NCN>(2PF10.3),5X,<NCN>(2PF10.3))
 1005 CONTINUE
C
      NNN=2*NCN
      CALL TALLY1 (HOLD,SS,TOTAL,MEAN,SD,VMIN,VMAX,IST,NPT,NNN)
C
      WRITE (NPRT,1011)
 1011 FORMAT (/' MEAN REL % DEVIATION VALUES'/)
      WRITE (NPRT,862) (MEAN(I),I=1,2*NCN)
      WRITE (NPRT,1013)
 1013 FORMAT (/' MAX. REL % DEVIATION VALUES'/)
      WRITE (NPRT,862) (VMAX(I),I=1,2*NCN)
      WRITE (NPRT,1014)
 1014 FORMAT (/' STD. DEVIATION VALUES '/)
      WRITE (NPRT,862) (SD(I),I=1,2*NCN)
C
C     CALCULATION OF DIFFERENCE IN ACTIVITIES: LLE SYSTEM
C
C     WRITE (NPRT,1015)
C1015 FORMAT ('1',T10,'DIFFERENCE IN ACTIVITIES (EXPT-CALC) '/)
C     WRITE (NPRT,530) IE, IR
C     WRITE (NPRT,550) (I,I=1,NCN), (I,I=1,NCN)
C     DO 1017 J=IST,NPT
C1017 WRITE (NPRT,1018) ((ACT1EO(I,J)-ACT1CO(I,J)),I=1,NCN),
C    *                  ((ACT2EO(I,J)-ACT2CO(I,J)),I=1,NCN)
C1018 FORMAT (' ',<NCN>F10.6,5X,<NCN>F10.6)
C
C     ABSOLUTE EXPT & CALC ACTIVITY DIFFERENCES IN LLE SYSTEM
C
C     WRITE (NPRT,1020)
C1020 FORMAT ('0',<5*NCN-9>X,'ABS DIFF IN EXPT ACT',<10*NCN-11>X,
C    *'ABS DIFF IN CALC ACT'/)
C     WRITE (NPRT,550) (I,I=1,NCN), (I,I=1,NCN)
C     DO 1025 J=IST,NPT
C1025 WRITE (NPRT,1018) ((ABS(ACT1EO(I,J)-ACT2EO(I,J))),I=1,NCN),
C    *                  ((ABS(ACT1CO(I,J)-ACT2CO(I,J))),I=1,NCN)
C
C     DISTRIBUTION COEFFICIENTS IN LLE SYSTEM
C
      WRITE (NPRT,1030)
 1030 FORMAT ('1','EXPERIMENTAL DISTRIBUTION COEFF',7X,'CALCULATED
     *DISTRIBUTION COEFF'/)
      WRITE (NPRT,550) (I,I=1,NCN), (I,I=1,NCN)
      DO 1033 J=IST,NPT
      WRITE (NPRT,1032) (KEO(I,J),I=1,NCN), (KCO(I,J),I=1,NCN)
 1032 FORMAT (' ',<NCN>(F10.4),5X,<NCN>(F10.4))
 1033 CONTINUE
C
C     ABSOLUTE & % RELATIVE DIFF OF DISTRIBUTION COEFFICIENTS IN
C     LLE SYSTEM.
C
      WRITE (NPRT,1040)
 1040 FORMAT ('0',<5*NCN-9>X,'DIFF IN DIST COEFF',<10*NCN-15>X,
     *'REL % DIFF IN DIST COEFF'/)
      WRITE (NPRT,550) (I,I=1,NCN), (I,I=1,NCN)
      DO 1043 J=1,NPT
      DO 1043 I=1,2*NCN
 1043 HOLD(I,J)=0.0
```

```
      DO 1050 J=IST,NPT
      DO 1045 I=1,NCN
      HOLD(I,J)=KEO(I,J)-KCO(I,J)
      HOLD(I+NCN,J)=100.0*(KEO(I,J)-KCO(I,J))/KEO(I,J)
 1045 CONTINUE
      WRITE (NPRT,1047) (HOLD(I,J),I=1,2*NCN)
 1047 FORMAT (' ',<NCN>G13.4,5X,<NCN>(G13.4))
 1050 CONTINUE
C
      CALL TALLY1 (HOLD,SS,TOTAL,MEAN,SD,VMIN,VMAX,IST,NPT,NNN)
      WRITE (NPRT,993)
      WRITE (NPRT,1047) (MEAN(I),I=1,2*NCN)
      WRITE (NPRT,995)
      WRITE (NPRT,1047) (VMAX(I),I=1,2*NCN)
      WRITE (NPRT,997)
      WRITE (NPRT,1047) (SD(I),I=1,2*NCN)
 1060 CONTINUE
C
C     INFINITE DILUTION ACTIVITY COEFFICIENTS (LLE)
C     TEMPORARY BYPASS ESTABLISHED BECAUSE INFY IS NOT READY FOR
C     TWO LIQUID PHASES INFINITE DILUTION GAMMA & DIST. COEFF.
C
      GO TO 1300
  999 IF (LLEFN .NE. 12) GO TO 1300
      WRITE (NPRT,1070)
 1070 FORMAT ('0INFINITE DILUTION ACTIVITY COEFFICIENTS WITH
     *EXPERIMENTAL X VALUES'/)
      WRITE (NPRT,530) IE, IR
      WRITE (NPRT,550) (I,I=1,NCN), (I,I=1,NCN)
      DO 1100 J=IST,NPT
 1100 WRITE (NPRT,910) (G1IEO(I,J),I=1,NCN), (G2IEO(I,J),I=1,NCN)
C
      WRITE (NPRT,1120)
 1120 FORMAT ('0INFINITE DILUTION ACTIVITY COEFFICIENTS WITH
     *CALCULATED X VALUES'/)
      WRITE (NPRT,530) IE, IR
      WRITE (NPRT,550) (I,I=1,NCN), (I,I=1,NCN)
      DO 1160 J=IST,NPT
 1160 WRITE (NPRT,910) (G1ICO(I,J),I=1,NCN), (G2ICO(I,J),I=1,NCN)
C
C     CALCULATION OF RELATIVE DIFFERENCE OF INFINITE DILUTION
C     ACTIVITY COEFFICIENTS:
C
      WRITE (NPRT,1165)
 1165 FORMAT ('0',T5,'% RELATIVE DIFFERENCE OF INFINITE DILUTION
     * ACTIVITY COEFFICIENTS'/)
      WRITE (NPRT,530) IE, IR
      WRITE (NPRT,550) (I,I=1,NCN), (I,I=1,NCN)
      DO 1175 J=IST,NPT
      WRITE (NPRT,862) (((G1IEO(I,J)-G1ICO(I,J))/G1IEO(I,J)),I=1,NCN),
     *                 (((G2IEO(I,J)-G2ICO(I,J))/G2IEO(I,J)),I=1,NCN)
 1175 CONTINUE
C
C     INFINITE DILUTION DISTRIBUTION COEFFICIENTS IN MULTICOMPONENT SYSTEM
C
      WRITE (NPRT,1180)
 1180 FORMAT ('0',T15,'INFINITE DILUTION DISTRIBUTION COEFFICIENTS'/
     *T20,'EXPERIMENTAL',T45,'CALCULATED'/)
      WRITE (NPRT,530) IE, IR
      WRITE (NPRT,550) (I,I=1,NCN), (I,I=1,NCN)
```

```
      DO 1220 J=IST,NPT
 1220 WRITE (NPRT,910) (KIEO(I,J),I=1,NCN), (KICO(I,J),I=1,NCN)
      DELK=0.0
      DO 1250 I=1,NCN
      DO 1230 J=IST,NPT
 1230 DELK=DELK+ABS(KIEO(I,J)-KICO(I,J))/KIEO(I,J)
      DELK=DELK/NPT
      WRITE (NPRT,1240) I,100.0*DELK
 1240 FORMAT ('0AVE % REL DIFF IN DIST COEFF (AT INFINITE DILUTION)
     *OF COMP ',I1,'=',G11.4)
 1250 CONTINUE
C
 1300 RETURN
C***********************************************************
      END
      SUBROUTINE TALLY1 (AA,SS,TOTAL,MEAN,SD,VMIN,VMAX,IST,NPT,NV)
C
      REAL*4          AA(20,200), SS(1), TOTAL(20), SD(20), MEAN(20),
     *                VMIN(20), VMAX(20), SCNT(20)
C
C     CLEAR OUTPUT VECTORS AND INITIALIZE VMIN,VMAX
C
C     DO 5 J=IST,NPT
C   5 WRITE (6,2) (AA(I,J),I=1,NTEMP)
C   2 FORMAT (/' AA VALUES IN TALLY1 ARE ',<2*NV>E12.4)
      DO 10 K=1,NV
      TOTAL(K)=0.0
      MEAN(K)=0.0
      SD(K)=0.0
      SCNT(K)=0.0
      VMIN(K)=1.0E35
   10 VMAX(K)=-1.0E35
C
C     CALCULATE TOTAL, MINIMA, MAXIMA
C
      DO 70 I=1,NV
      DO 60 J=IST,NPT
      IF (AA(I,J)) 25,60,25
   25 SCNT(I)=SCNT(I)+1.0
      TOTAL(I)=TOTAL(I)+ABS(AA(I,J))
      IF (ABS(AA(I,J))-VMIN(I)) 30,40,40
   30 VMIN(I)=ABS(AA(I,J))
   40 IF (ABS(AA(I,J))-VMAX(I)) 60,60,50
   50 VMAX(I)=ABS(AA(I,J))
      SD(I)=SD(I)+AA(I,J)*AA(I,J)
   60 CONTINUE
   70 CONTINUE
C
C     CALCULATE MEANS AND STANDARD DEVIATIONS
C
      DO 80 I=1,NV
      IF (SCNT(I) .EQ. 0.0) GO TO 80
      MEAN(I)=TOTAL(I)/SCNT(I)
      SD(I)=SQRT(ABS((SD(I)-TOTAL(I)*TOTAL(I)/SCNT(I))/
     *           (SCNT(I)-1.0)))
   80 CONTINUE
      DO 90 I=1,NV
      IF (VMIN(I) .EQ. 1.0E35) VMIN(I)=0.0
      IF (VMAX(I) .EQ. -1.0E35) VMAX(I)=0.0
   90 CONTINUE
```

```
      RETURN
      END
      SUBROUTINE FXVLE (ZZZ)
C
C     PROGRAMMED BY H.S. CHAWLA .... OCT. 1984.
C     THIS SUBPROGRAM CALCULATES THE OBJECTIVE FUNCTION FOR
C     VLE REGRESSION
C
      COMMON  /BLANK/  NCR, NPRT, NSTART, KUNITS, TITLE(20)
      COMMON  /CMPRO/  NC, NCM1, IDLL, IDLV, IDH, LDBUG, ISW, NDIM,
     *                 ZNAME(2,10), L(10), NTCOMP(10)
      COMMON  /STRM/   T, P, Z(10), Y(10), X(10), FRACV, ZVAP,
     *                 EK(10), VP(10), FUG(10), GAM(10), SVAP,
     *                 HOFZ, HVAP, HLIQ, DHV, XSH, NOBUB, NODEW
      COMMON  /CONTRL/ ITF, IPF,  N, NTYPE, JCODE, NLIQ
      COMMON  /TWCLQ/  X1(10), X2(10), GAM1(10), GAM2(10), EK1(10),
     +                 EK2(10), DHL(2), HIDLL(2), HREALL(2), FRACL,
     +                 IE, IR, XMAX, XMIN
      COMMON  /ZFEEDZ/ PF, TF, FEED, FMOL, TREF, HI, NK1, NFEED
      COMMON  /FOX/    X1EXP(10), X2EXP(10), GAM1E(10), GAM2E(10),
     *                 GAM1IE(10), GAM2IE(10),GAM1IC(10), GAM2IC(10),
     *                 ACT1C(10), ACT2C(10), ACT1E(10), ACT2E(10),
     *                 KE(10), KC(10), KIE(10), KIC(10), W1(10),
     *                 W2(10), YEXP(10), TEXP, PEXP, WT, WT1, VLEFN,
     *                 LLEFN, VLLFN, NVLPT, NLLPT, NCVLE, NCLLE,
     *                 NMODEL, INX, RECODE, NOTALE(15,10), NDSET
C
      INTEGER          VLEFN, LLEFN, VLLFN, RECODE
      INC=0
      SUM=0.0
      AAA=0.0
      BBB=0.0
      IF (VLEFN .LE. 0 .OR. VLEFN .GT. 21) CALL EXIT
      GO TO (500,550,600,650,700,750,800,850,900,950,1000,1050,
     *1100,1150,1200,1250,1300,1350,1400,1450,1500,1550), VLEFN
C
C     FUNCTION # 1: ABSOLUTE DIFFERENCE OF INFINITE DILUTION
C                   ACTIVITY COEFFICIENTS
C     TO BE FIXED
  500 CALL INFY (IMIN1,IMIN2)
      DO 510 I=1,NCVLE
      IF (X1EXP(I) .NE. 0.0) GO TO 505
      INC=INC+1
      GO TO 510
  505 SUM=SUM+ABS(GAM1IE(I)-GAM1IC(I))
  510 CONTINUE
      ZZ=SUM/(NCVLE-INC)
      GO TO 2000
C
C     FUNCTION # 2: RELATIVE DIFFERENCE OF INFINITE DILUTION
C                   ACTIVITY COEFFICIENTS
C     TO BE FIXED
  550 CALL INFY (IMIN1,IMIN2)
      DO 560 I=1,NCVLE
      IF (X1EXP(I) .NE. 0.0) GO TO 555
      INC=INC+1
      GO TO 560
  555 SUM=SUM+ABS(GAM1IE(I)-GAM1IC(I))/GAM1IE(I)
  560 CONTINUE
      ZZ=SUM/(NCVLE-INC)
```

```
      GO TO 2000
C
C     FUNCTION # 3: RELATIVE DIFFERENCE OF LOGRITHM OF INFINITE
C                   DILUTION ACTIVITY COEFFICIENTS
C     TO BE FIXED
  600 CALL INFY (IMIN1,IMIN2)
      DO 610 I=1,NCVLE
      IF (X1EXP(I) .NE. 0.0) GO TO 605
      INC=INC+1
      GO TO 610
  605 SUM=SUM+ABS(ALOG(GAM1IC(I)/GAM1IE(I)))
  610 CONTINUE
      ZZ=SUM/(NCVLE-INC)
      GO TO 2000
C
C     FUNCTION # 4: ABSOLUTE DIFFERENCE OF ACTIVITY COEFFICIENTS
C
  650 DO 660 I=1,NCVLE
      IF (X1EXP(I) .NE. 0.0) GO TO 655
      INC=INC+1
      GO TO 660
  655 SUM=SUM+ABS(GAM1E(I)-GAM1(I))
  660 CONTINUE
      ZZ=SUM/(NCVLE-INC)
      GO TO 2000
C
C     FUNCTION # 5: RELATIVE DIFFERENCE OF ACTIVITY COEFFICIENTS
C
  700 DO 710 I=1,NCVLE
      IF (X1EXP(I) .NE. 0.0) GO TO 705
      INC=INC+1
      GO TO 710
  705 SUM=SUM+ABS(GAM1E(I)-GAM1(I))/GAM1E(I)
  710 CONTINUE
      ZZ=SUM/(NCVLE-INC)
      GO TO 2000
C
C     FUNCTION # 6: RELATIVE DIFFERENCE OF LOGRITHM OF ACTIVITY
C                   COEFFICIENTS
C
  750 DO 760 I=1,NCVLE
      IF (X1EXP(I) .NE. 0.0) GO TO 755
      INC=INC+1
      GO TO 760
  755 SUM=SUM+ABS(ALOG(GAM1(I)/GAM1E(I)))
  760 CONTINUE
      ZZ=SUM/(NCVLE-INC)
      GO TO 2000
C
C     FUNCTION # 7: ABSOLUTE DIFFERENCE OF Y'S
C
  800 DO 810 I=1,NCVLE
      IF (YEXP(I) .NE. 0.0 .OR. Y(I) .NE. 0.0)GO TO 805
      INC=INC+1
      GO TO 810
  805 SUM=SUM+ABS(YEXP(I)-Y(I))
  810 CONTINUE
      ZZ=SUM/(NCVLE-INC)
      GO TO 2000
C
```

```
C     FUNCTION # 8: RELATIVE DIFFERENCE OF Y'S
C
  850 DO 860 I=1,NCVLE
      IF (YEXP(I) .NE. 0.0) GO TO 855
      INC=INC+1
      GO TO 860
  855 SUM=SUM+ABS(YEXP(I)-Y(I))/YEXP(I)
  860 CONTINUE
      ZZ=SUM/(NCVLE-INC)
      GO TO 2000
C
C     FUNCTION # 9: DIFFERENCE OF LOGRITHM OF Y'S
C
  900 DO 910 I=1,NCVLE
      IF (YEXP(I) .NE. 0.0 .OR. Y(I) .NE. 0.0)GO TO 905
      INC=INC+1
      GO TO 910
  905 SUM=SUM+ABS(ALOG(Y(I)/YEXP(I)))
  910 CONTINUE
      ZZ=SUM/(NCVLE-INC)
      GO TO 2000
C
C     FUNCTION # 10: ABSOLUTE DIFFERENCE OF Y'S AND RELATIVE
C                    DIFFERENCE OF TOTAL P'S
C
  950 DO 960 I=1,NCVLE
      IF (YEXP(I) .NE. 0.0 .OR. Y(I) .NE. 0.0)GO TO 955
      INC=INC+1
      GO TO 960
  955 SUM=SUM+ABS(YEXP(I)-Y(I))
  960 CONTINUE
      ZZ=SUM/(NCVLE-INC)+ABS(PEXP-P)/PEXP
      GO TO 2000
C
C     FUNCTION # 11: RELATIVE DIFFERENCE OF Y'S AND RELATIVE
C                    DIFFERENCE OF TOTAL P'S
C
 1000 DO 1010 I=1,NCVLE
      IF (YEXP(I) .NE. 0.0 .OR. Y(I) .NE. 0.0)GO TO 1005
      INC=INC+1
      GO TO 1010
 1005 SUM=SUM+ABS(YEXP(I)-Y(I))/YEXP(I)
 1010 CONTINUE
      ZZ=SUM/(NCVLE-INC)+ABS(PEXP-P)/PEXP
      GO TO 2000
C
C     FUNCTION # 12: DIFFERENCE OF LOGRITHM OF Y'S AND
C                    DIFFERENCE OF LOGRITHM OF TOTAL P'S
C
 1050 DO 1060 I=1,NCVLE
      IF (YEXP(I) .NE. 0.0 .OR. Y(I) .NE. 0.0)GO TO 1055
      INC=INC+1
      GO TO 1060
 1055 SUM=SUM+ABS(ALOG(Y(I)/YEXP(I)))
 1060 CONTINUE
      ZZ=SUM/(NCVLE-INC)+ABS(ALOG(P/PEXP))
      GO TO 2000
C
C     FUNCTION # 13: ABSOLUTE DIFFERENCE OF TOTAL P'S
C
```

```
00 ZZ=ABS(PEXP-P)
   GO TO 2000

   FUNCTION # 14: RATIC OF Y'S

50 ZZ=ABS(P/PEXP)
   GO TO 2000

   FUNCTION # 15: RELATIVE DIFFERENCE OF TOTAL P'S

00 ZZ=ABS(PEXP-P)/PEXP
   GO TO 2000

   FUNCTION # 16: DIFFERENCE OF LOGRITHM TOTAL P'S

50 ZZ=ABS(ALOG(P/PEXP))
   GO TO 2000

   FUNCTION # 17: ABSCLUTE DIFFERENCE OF BUBBLE POINT T'S

00 ZZ=ABS(TEXP-T)
   GO TO 2000

   FUNCTION # 18: RATIC OF BUBBLE POINT T'S

50 ZZ=ABS(T/TEXP)
   GO TO 2000

   FUNCTION # 19: RELATIVE DIFFERENCE OF BUBBLE POINT T'S

00 ZZ=ABS(TEXP-T)/TEXP
   GO TO 2000

   FUNCTION # 20: DIFFERENCE OF LOGRITHM OF BUBBLE POINT T'S

50 ZZ=ABS(ALOG(T/TEXP))
   GO TO 2000

   FUNCTION # 21: ABSCLUTE DIFFERENCE OF BUBBLE POINT T'S &
                  ABSCLUTE DIFFERENCE CF Y'S

500 AAA=ABS(TEXP-T)
    DO 1510 I=1,NCVLE
    IF (YEXP(I) .NE. 0.0 .OR. Y(I) .NE. 0.0)GO TO 1505
    INC=INC+1
    GC TO 1510
505 SUM=SUM+ABS(YEXP(I)-Y(I))
510 CONTINUE
    BBB=SUM/(NCVLE-INC)
    ZZ=AAA+BBB
    GO TO 2000

    FUNCTION # 22: RELATIVE DIFFERENCE OF BUBBLE POINT T'S &
                   ABSCLUTE DIFFERENCE CF Y'S

550 AAA=ABS(TEXP-T)/TEXP
    DO 1560 I=1,NCVLE
    IF (YEXP(I) .NE. 0.0 .OR. Y(I) .NE. 0.0)GO TO 1555
    INC=INC+1
    GC TO 1560
```

```
 1555 SUM=SUM+ABS(YEXP(I)-Y(I))
 1500 CONTINUE
      BBB=SUM/(NCVLE-INC)
      ZZ=AAA+BBB
C
 2000 ZZZ=ZZ
      RETURN
      END
      SUBROUTINE FX2LIQ (ZZZ)
C
C     PROGRAMMED BY H.S. CHAWLA ... OCT.,1984
C     CALCULATES THE OBJECTIVE FUNCTION FOR THE LLE REGRESSION.
C
      COMMON  /BLANK/  NCR, NPRT, NSTART, KUNITS, TITLE(20)
      COMMON  /CMPRO/  NC, NCM1, IDLL, IDLV, IDH, LDBUG, ISW, NDIM,
     *                 ZNAME(2,10), L(10), NTCOMP(10)
      COMMON  /ZDATA/  CPL(10,4), CPV(10,4), ENP(10,10), ANT(6,10),
     *                 W(10), AX, BX, OMEGA(10), AVAL(10), BVAL(10),
     *                 AK(10,10), R(10), Q(10), QP(10), XL(10),
     *                 VOL(10), C(180), ALPHA(45), VC(10), TC(10),
     *                 PC(10), ZC(10), TNBP(10), CA(10), DB(10),
     *                 A(10,10), G(10,10), ZRA(10), RD(10), DMU(10),
     *                 ETA(10)
      COMMON  /STRM/   T, P, Z(10), Y(10), X(10), FRACV, ZVAP,
     *                 EK(10), VP(10), FUG(10), GAM(10), SVAP,
     *                 HOFZ, HVAP, HLIQ, DHV, XSH, NOBUB, NODEW
      COMMON  /CONTRL/ ITF, IPF,  N, NTYPE, JCODE, NLIQ
      COMMON  /TWOLQ/  X1(10), X2(10), GAM1(10), GAM2(10), EK1(10),
     +                 EK2(10), DHL(2), HIDLL(2), HREALL(2), FRACL,
     +                 IE, IR, XMAX, XMIN
      COMMON  /FOX/    X1EXP(10), X2EXP(10), GAM1E(10), GAM2E(10),
     *                 GAM1IE(10), GAM2IE(10),GAM1IC(10), GAM2IC(10),
     *                 ACT1C(10), ACT2C(10), ACT1E(10), ACT2E(10),
     *                 KE(10), KC(10), KIE(10), KIC(10), W1(10),
     *                 W2(10), YEXP(10), TEXP, PEXP, WT, WT1, VLEFN,
     *                 LLEFN, VLLFN, NVLPT, NLLPT, NCVLE, NCLLE,
     *                 NMODEL, INX, RECODE, NDTALE(15,10), NDSET
C
      REAL             KE, KC, KIE, KIC
      INTEGER          VLEFN, LLEFN, VLLFN, RECODE
      NLIQ=2
      FRACL=0.5
      SUM=0.0
      DO 10 I = 1,NCLLE
      Z(I)=X1EXP(I)*FRACL+X2EXP(I)*(1.0-FRACL)
      SUM=SUM+Z(I)
   10 CONTINUE
      DO 20 I = 1,NCLLE
      Z(I)=Z(I)/SUM
   20 CONTINUE
      CALL INTLIZ (IO)
      IF (LDBUG .GE. 2) WRITE(NPRT,30)(Z(I),I=1,NCLLE)
   30 FORMAT (' IN FX2LIQ : Z(I) = ',10(E13.7,2X))
C
      IF (LDBUG .GE. 2) WRITE (NPRT,35)(X1(I),I=1,NCLLE)
   35 FORMAT (' X1(I) GUESSES    = ',10(E13.5,2X))
      IF (LDBUG .GE. 2) WRITE (NPRT,38)(X2(I),I=1,NCLLE)
   38 FORMAT (' X2(I) GUESSES    = ',10(E13.5,2X))
C
      CALL TWOLIQ
```

```
      IF (NLIQ .GT. 1) GO TO 39
      ZZ=10.0
      GO TO 1000
C
C     CALCULATION OF WEIGHTING FACTORS W1(I),W2(I).
C     W1(I)=W2(I)=1.0 IF WT=0.0
C
   39 DO 40 I=1,NCLLE
      IF (X1EXP(I) .EQ. 0.0) GO TO 40
      W1(I)=ABS(1.0+WT*(ABS(X1EXP(I)-X1(I)))/X1EXP(I))
      IF (X2EXP(I) .EQ. 0.0) GO TO 40
      W2(I)=ABS(1.0+WT*(ABS(X2EXP(I)-X2(I)))/X2EXP(I))
   40 CONTINUE
C
C     CALCULATION OF EXPERIMENTAL AND CALCULATED ACTIVITIES
C     IN BOTH THE LIQUID PHASES.
C
      DO 50 I=1,NCLLE
      ACT1C(I)=GAM1(I)*X1(I)
      ACT2C(I)=GAM2(I)*X2(I)
   50 CONTINUE
      CALL ACTVY (T,P,X1EXP,GAM1E)
      CALL ACTVY (T,P,X2EXP,GAM2E)
C     DO 60 I=1,NCLLE
C     ACT1E(I)=GAM1E(I)*X1EXP(I)
C     ACT2E(I)=GAM2E(I)*X2EXP(I)
C  60 CONTINUE
C
C     CALCULATION OF SOLUTE DISTRIBUTION COEFFICIENTS
C     KE(I) : EXPERIMENTAL ; KC(I) : CALCULATED
C
      DO 70 I=1,NCLLE
C     KE(I)=GAM2E(I)/GAM1E(I)
C     KC(I)=GAM2(I)/GAM1(I)
      KE(I)=1.0
      KC(I)=1.0
      IF (X2EXP(I) .EQ. 0.0 .OR. X2(I) .EQ. 0.0) GO TO 70
      KE(I)=X1EXP(I)/X2EXP(I)
      KC(I)=X1(I)/X2(I)
   70 CONTINUE
      INC=0
      SUM=0.0
      AAA=0.0
      BBB=0.0
      IF (LLEFN .LT. 0 .OR. LLEFN .GT. 13) CALL EXIT
      GO TO (100,150,200,250,300,350,400,450,500,600,650,700,
     *                                                    750),LLEFN
C
C     FUNCTION # 1 : ABSOLUTE ACTIVITIES
C
  100 DO 110 I=1,NCLLE
      IF (X1EXP(I) .NE. 0.0 .OR. X2EXP(I) .NE. 0.0) GO TO 105
      INC=INC+1
      GO TO 110
  105 SUM=SUM+ABS(ACT1C(I)-ACT2C(I))
  110 CONTINUE
      ZZ=SUM/(NLIQ*(NCLLE-INC))
      GO TO 1000
C
C     FUNCTION # 2 : RELATIVE ACTIVITIES
```

```
C
  150 DO 160 I=1,NCLLE
      IF (X1EXP(I) .NE. 0.0 .OR. X2EXP(I) .NE. 0.0) GO TO 155
      INC=INC+1
      GO TO 160
  155 SUM=SUM+ABS(ALOG(ACT1C(I))-ALOG(ACT2C(I)))
  160 CONTINUE
      ZZ=SUM/(NLIQ*(NCLLE-INC))
      GO TO 1000
C
C     FUNCTION # 3 : RELATIVE ACTIVITIES
C
  200 DO 210 I=1,NCLLE
      IF (X1EXP(I) .NE. 0.0 .OR. X2EXP(I) .NE. 0.0) GO TO 205
      INC=INC+1
      GO TO 210
  205 SUM=SUM+ABS((ACT1C(I)-ACT2C(I))/(ACT1C(I)+ACT2C(I)))
  210 CONTINUE
      ZZ=SUM/(NLIQ*(NCLLE-INC))
      GO TO 1000
C
C     THE FOLLOWING OBJECTIVE FUNCTION EMPHASIZES THE REGION IN
C     THE VICINITY OF THE PLAIT POINT
C
C     FUNCTION # 4 : RELATIVE ACTIVITIES
  250 DO 260 I=1,NCLLE
      IF (X1EXP(I) .NE. 0.0 .OR. X2EXP(I) .NE. 0.0) GO TO 255
      INC=INC+1
      IINC=INC
      GO TO 260
  255 IF (I .EQ. IE .OR. I .EQ. IR) GO TO 260
      AAA=AAA+ABS(ALOG(ACT1C(I))-ALOG(ACT2C(I)))
  260 CONTINUE
      DO 270 I=1,NCLLE
      IF (X1EXP(I) .NE. 0.0 .OR. X2EXP(I) .NE. 0.0) GO TO 265
      INC=INC+1
      GO TO 270
  265 SUM=SUM+ABS((ALOG(ACT1C(I))-ALOG(ACT2C(I)))*X1(I)*X2(I))
  270 CONTINUE
      ZZ=SUM/(NLIQ*(NCLLE-INC))+AAA/(NLIQ*(NCLLE-IINC-2))
      GO TO 1000
C
C     THE FOLLOWING OBJECTIVE FUNCTIONS ARE IN TERMS OF CONC.:
C     ABSOLUTE & RELATIVE
C
C     FUNCTION # 5 : ABSOLUTE CONCENTRATIONS
C
  300 DO 310 I=1,NCLLE
      IF (X1EXP(I) .NE. 0.0 .OR. X2EXP(I) .NE. 0.0) GO TO 305
      INC=INC+1
      GO TO 310
  305 TEMP1=W1(I)*ABS(X1EXP(I)-X1(I))
      TEMP2=W2(I)*ABS(X2EXP(I)-X2(I))
      SUM=SUM+TEMP1+TEMP2
  310 CONTINUE
      ZZ=SUM/(NLIQ*(NCLLE-INC))
      GO TO 1000
C
C     FUNCTION # 6 : RELATIVE CONCENTRATIONS
C
```

```
  350 DO 360 I=1,NCLLE
      IF (X1EXP(I) .NE. 0.0 .OR. X2EXP(I) .NE. 0.0) GO TO 355
      INC=INC+1
      GO TO 360
  355 TEMP1=W1(I)*ABS(ALOG(X1EXP(I))-ALOG(X1(I)))
      TEMP2=W2(I)*ABS(ALOG(X2EXP(I))-ALOG(X2(I)))
      SUM=SUM+TEMP1+TEMP2
  360 CONTINUE
      ZZ=SUM/(NLIQ*(NCLLE-INC))
      GO TO 1000
C
C     FUNCTION # 7 : RELATIVE CONCENTRATIONS
C
  400 DO 410 I=1,NCLLE
      IF (X1EXP(I) .NE. 0.0 .AND. X2EXP(I) .NE. 0.0) GO TO 405
      INC=INC+1
      GO TO 410
  405 TEMP1=W1(I)*ABS((X1EXP(I)-X1(I))/X1EXP(I))
      TEMP2=W2(I)*ABS((X2EXP(I)-X2(I))/X2EXP(I))
      SUM=SUM+TEMP1+TEMP2
  410 CONTINUE
      ZZ=SUM/(NLIQ*(NCLLE-INC))
      GO TO 1000
C
C     FUNCTION # 8 : RELATIVE CONCENTRATIONS
C
  450 DO 460 I=1,NCLLE
      IF (X1EXP(I) .NE. 0.0 .AND. X2EXP(I) .NE. 0.0) GO TO 455
      INC=INC+1
      GO TO 460
  455 TEMP1=W1(I)*ABS((X1EXP(I)-X1(I))/(X1EXP(I)+X1(I)))
      TEMP2=W2(I)*ABS((X2EXP(I)-X2(I))/(X2EXP(I)+X2(I)))
      SUM=SUM+TEMP1+TEMP2
  460 CONTINUE
      ZZ=SUM/(NLIQ*(NCLLE-INC))
      GO TO 1000
C
C     FUNCTION # 9 : RELATIVE CONC & DISTRIBUTION RATIOS
C                    ONLY FOR MULTICOMPONENT SYSTEM
C
  500 DO 510 I=1,NCLLE
      IF (X1EXP(I) .NE. 0.0 .OR. X2EXP(I) .NE. 0.0) GO TO 505
      INC=INC+1
      IINC=INC
      GO TO 510
C 505 IF (I .EQ. IE .OR. I .EQ. IR)GO TO 510
  505 AAA=AAA+ABS((KE(I)-KC(I))/KE(I))
  510 CONTINUE
      DO 520 I=1,NCLLE
      IF (X1EXP(I) .NE. 0.0 .OR. X2EXP(I) .NE. 0.0) GO TO 515
      INC=INC+1
      GO TO 520
  515 TEMP1=W1(I)*ABS((X1EXP(I)-X1(I))/X1EXP(I))
      TEMP2=W2(I)*ABS((X2EXP(I)-X2(I))/X2EXP(I))
      SUM=SUM+TEMP1+TEMP2
  520 CONTINUE
C     ZZ=SUM/(NLIQ*(NCLLE-INC))+AAA/(NCLLE-IINC-2)
      ZZ=SUM/(NLIQ*(NCLLE-INC))+AAA/(NCLLE-IINC)
      GO TO 1000
C
```

```
C      FUNCTION # 10 : RELATIVE CONC & DISTRIBUTION RATIOS
C                      ONLY FOR MULTICOMPONENT SYSTEM
C
  600 DO 610 I=1,NCLLE
      IF (X1EXP(I) .NE. 0.0 .OR. X2EXP(I) .NE. 0.0) GO TO 605
      INC=INC+1
      IINC=INC
      GO TO 610
C 605 IF (I .EQ. IE .OR. I .EQ. IR)GO TO 610
  605 AAA=AAA+ABS(ALOG(ABS(KE(I)/KC(I))))
  610 CONTINUE
      DO 620 I=1,NCLLE
      IF (X1EXP(I) .NE. 0.0 .OR. X2EXP(I) .NE. 0.0) GO TO 615
      INC=INC+1
      GO TO 615
  615 TEMP1=W1(I)*ABS(ALOG(X1EXP(I))-ALOG(X1(I)))
      TEMP2=W2(I)*ABS(ALOG(X2EXP(I))-ALOG(X2(I)))
      SUM=SUM+TEMP1+TEMP2
  620 CONTINUE
C     ZZ=SUM/(NLIQ*(NCLLE-INC))+AAA/(NCLLE-INC-2)
      ZZ=SUM/(NLIQ*(NCLLE-INC))+AAA/(NCLLE-INC)
      GO TO 1000
C
C      FUNCTION # 11 : RELATIVE CONC & DISTRIBUTION RATIOS
C                      ONLY FOR MULTICOMPONENT SYSTEM
C
  650 DO 660 I=1,NCLLE
      IF (X1EXP(I) .NE. 0.0 .OR. X2EXP(I) .NE. 0.0) GO TO 655
      INC=INC+1
      IINC=INC
      GO TO 660
  655 TEMP1=W1(I)*ABS((X1EXP(I)-X1(I))/(X1EXP(I)+X1(I)))
      TEMP2=W2(I)*ABS((X2EXP(I)-X2(I))/(X2EXP(I)+X2(I)))
      SUM=SUM+TEMP1+TEMP2
  660 CONTINUE
      DO 670 I=1,NCLLE
      IF (X1EXP(I) .NE. 0.0 .OR. X2EXP(I) .NE. 0.0) GO TO 665
      INC=INC+1
      GO TO 670
C 665 IF (I .EQ. IE .OR. I .EQ. IR)GO TO 670
  665 AAA=AAA+ABS((KE(I)-KC(I))/(KE(I)+KC(I)))
  670 CONTINUE
C     ZZ=SUM/(NLIQ*(NCLLE-IINC))+AAA/(NCLLE-INC-2)
      ZZ=SUM/(NLIQ*(NCLLE-IINC))+AAA/(NCLLE-INC)
      GO TO 1000
C
C      FUNCTION # 12 : RELATIVE CONC, PARAMETER VALUES & DISTRIBUTION
C                      RATIO AT INFINITE DILUTION
C                      ONLY FOR MULTICOMPONENT SYSTEM
C      THE FOLLOWING OBJ FUNCTION TAKES INTO ACCOUNT THE DISTRIBUTION
C      COEFFICIENTS OF THE SOLUTE AT INFINITE DILUTION
C      INX = # OF PARAMETERS BEING REGRESSED
C      WT1 = WEIGHT
C
  700 CALL INFY (IMIN1,IMIN2)
      DO 710 I=1,NCLLE
      IF (X1EXP(I) .NE. 0.0 .OR. X2EXP(I) .NE. 0.0) GO TO 705
      INC=INC+1
      IINC=INC
      GO TO 710
```

```
C 705 IF (I .EQ. IE .OR. I .EQ. IR)GO TO 710
  705 AAA=AAA+ABS(ALOG(ABS(KIE(I)/KIC(I))))
  710 CONTINUE
      DO 720 I=1,2*INX
      BBB=BBB+ABS(C(I))
  720 CONTINUE
      BBB=WT1*BBB
      DO 730 I=1,NCLLE
      IF (X1EXP(I) .NE. 0.0 .OR. X2EXP(I) .NE. 0.0) GO TO 725
      INC=INC+1
      GO TO 730
  725 TEMP1=W1(I)*ABS((X1EXP(I)-X1(I))/(X1EXP(I)+X1(I)))
      TEMP2=W2(I)*ABS((X2EXP(I)-X2(I))/(X2EXP(I)+X2(I)))
      SUM=SUM+TEMP1+TEMP2
  730 CONTINUE
C     ZZ=SUM/(NLIQ*(NCLLE-INC))+BBB+AAA/(NCLLE-IINC-2)
      ZZ=SUM/(NLIQ*(NCLLE-INC))+BBB+AAA/(NCLLE-IINC)
C
C
C     FUNCTION # 13 : RELATIVE CONC & EXPT ACTIVITIES
C
  750 DO 760 I=1,NCLLE
      IF (X1EXP(I) .NE. 0.0 .OR. X2EXP(I) .NE. 0.0) GO TO 755
      INC=INC+1
      IINC=INC
      GO TO 760
  755 TEMP1=W1(I)*ABS((X1EXP(I)-X1(I))/(X1EXP(I)+X1(I)))
      TEMP2=W2(I)*ABS((X2EXP(I)-X2(I))/(X2EXP(I)+X2(I)))
      SUM=SUM+TEMP1+TEMP2
  760 CONTINUE
      DO 770 I=1,NCLLE
      IF (X1EXP(I) .NE. 0.0 .OR. X2EXP(I) .NE. 0.0) GO TO 765
      INC=INC+1
      GO TO 770
C 765 IF (I .EQ. IE .OR. I .EQ. IR)GO TO 770
  765 AAA=AAA+ABS(ACT1E(I)-ACT2E(I))
  770 CONTINUE
C     ZZ=SUM/(NLIQ*(NCLLE-IINC))+AAA/(NCLLE-INC-2)
      ZZ=SUM/(NLIQ*(NCLLE-IINC))+AAA/(NCLLE-INC)
C
 1000 ZZZ=ZZ
      NLIQ=2
C
      IF (LDBUG .LT. 2) GO TO 1300
      WRITE (NPRT,1200)
 1200 FORMAT (' IN FX2LIQ AT STMT # 1200 :'/)
      WRITE (NPRT,1220)(X1EXP(I),I=1,NCLLE)
 1220 FORMAT (' X1EXP(I) = ',10(E13.5,2X))
      WRITE (NPRT,1230)(X1(I),I=1,NCLLE)
 1230 FORMAT (' X1(I)    = ',10(E13.5,2X))
      WRITE (NPRT,1240)(X2EXP(I),I=1,NCLLE)
 1240 FORMAT (' X2EXP(I) = ',10(E13.5,2X))
      WRITE (NPRT,1250)(X2(I),I=1,NCLLE)
 1250 FORMAT (' X2(I)    = ',10(E13.5,2X))
 1300 CONTINUE
C
      RETURN
      END
C***********************************************************************
      SUBROUTINE INFY (IMIN1,IMIN2)
```

```
C
C     PROGRAMMED BY H.S. CHAWLA  ....  OCT, 1984.
C     THIS SUBPROGRAM COMPUTES THE INFINITE DILUTION ACTIVITY
C     COEFFICIENTS FOR 1/2 LIQUID PHASES AND DISTRIBUTION
C     COEFFICIENTS FOR 2 LIQUID PHASE SYSTEM. IT EVALUATES THE ABOVE
C     VALUES FOR EXPERIMENTAL AND CALCULATED X VALUES. CALCULATIONS
C     ARE PERFORMED ON THE FIRST AND THE LAST DATA POINTS. IT
C     EVALUATES THE GAMMA/K'S OF I WHOSE X IS APPROACHING ZERO.
C
      COMMON  /BLANK/  NCR, NPRT, NSTART, KUNITS, TITLE(20)
      COMMON  /CMPRO/  NC, NCM1, IDLL, IDLV, IDH, LDBUG, ISW, NDIM,
     *                 ZNAME(2,10), L(10), NTCOMP(10)
      COMMON  /ZDATA/  CPL(10,4), CPV(10,4), ENP(10,10), ANT(6,10),
     *                 W(10), AX, BX, OMEGA(10), AVAL(10), BVAL(10),
     *                 AK(10,10), R(10), Q(10), QP(10), XL(10),
     *                 VOL(10), C(180), ALPHA(45), VC(10), TC(10),
     *                 PC(10), ZC(10), TNBP(10), CA(10), CB(10),
     *                 A(10,10), G(10,10), ZRA(10), RD(10), DMU(10),
     *                 ETA(10)
      COMMON  /STRM/   T, P, Z(10), Y(10), X(10), FRACV, ZVAP,
     *                 EK(10), VP(10), FUG(10), GAM(10), SVAP,
     *                 HCFZ, HVAP, HLIQ, DHV, XSH, NOBUB, NODEW
      COMMON  /CONTRL/ ITF, IPF,  N, NTYPE, JCODE, NLIQ
      COMMON  /TWOLQ/  X1(10), X2(10), GAM1(10), GAM2(10), EK1(10),
     +                 EK2(10), DHL(2), HIDLL(2), HREALL(2), FRACL,
     +                 IE, IR, XMAX, XMIN
      COMMON  /FOX/    X1EXP(10), X2EXP(10), GAM1E(10), GAM2E(10),
     *                 GAM1IE(10), GAM2IE(10),GAM1IC(10), GAM2IC(10),
     *                 ACT1C(10), ACT2C(10), ACT1E(10), ACT2E(10),
     *                 KE(10), KC(10), KIE(10), KIC(10), W1(10),
     *                 W2(10), YEXP(10), TEXP, PEXP, WT, WT1, VLEFN,
     *                 LLEFN, VLLFN, NVLPT, NLLPT, NCVLE, NCLLE,
     *                 NMODEL, INX, RECODE, NOTALE(15,10), NDSET
C
      REAL             XS1(10), XS2(10), G1TEMP(10), G2TEMP(10),
     *                 ISAVE(8), KE, KC, KIE, KIC
      INTEGER          VLEFN, LLEFN, VLLFN, RECODE
      LOGICAL          FLAG
C
      NCN=NCVLE
      DO 20 I=1,NCN
      GAM1IE(I)=1.0
      GAM2IE(I)=1.0
      GAM1IC(I)=1.0
      GAM2IC(I)=1.0
      G1TEMP(I)=1.0
      G2TEMP(I)=1.0
      KIE(I)=1.0
      KIC(I)=1.0
   20 CONTINUE
      IF (NLIQ .GE. 2)GO TO 300
      IF (NCVLE .GT. 2)GO TO 1000
C
C     SINGLE LIQUID PHASE CASE (BINARY SYSTEM ONLY)
C
      IMIN1=1
      XMIN=1.0
      SUM1=0.0
      SUM2=0.0
      DO 70 I=1,NCN
```

```
   70 XMIN=AMIN1(X1EXP(I),XMIN)
      DO 80 I=1,NCN
   80 IF (ABS(XMIN- X1EXP(I)) .LE. 1.E-12)IMIN1=I
      DO 90 I=1,NCN
      IF (I .EQ. IMIN1) GO TO 90
      XS1(I)=X1EXP(I)
      XS2(I)=X1(I)
      SUM1=SUM1+XS1(I)
      SUM2=SUM2+XS2(I)
   90 CONTINUE
      XS1(IMIN1)=0.0
      XS2(IMIN1)=0.0
      DO 100 I=1,NCN
      XS1(I)=XS1(I)/SUM1
  100 XS2(I)=XS2(I)/SUM2
      IF (NTYPE .EQ. 1 .OR. NTYPE .EQ. 5) GO TO 110
      CALL ACTVY (TEXP,P,XS1,G1TEMP)
      DO 105 K=1,NC
      IF (K .EQ. IMIN1) GO TO 105
      T=TNBP(K)
  105 CONTINUE
      GO TO 115
  110 CALL ACTVY (T,PEXP,XS1,G1TEMP)
  115 CALL ACTVY (T,P,XS2,G2TEMP)
      GAM1IE(IMIN1)=G1TEMP(IMIN1)
      GAM1IC(IMIN1)=G2TEMP(IMIN1)
      GO TO 1000
C
C     TWO LIQUID PHASES CALCULATION
C     ONLY BINARY CASE IS WORKING
  300 NCN=NCLLE
      IF (NCLLE .GT. 2)GO TO 1000
C     BINARY SYSTEM
      XS1(IE)=1.0
      XS1(IR)=0.0
      XS2(IR)=1.0
      XS2(IE)=0.0
      CALL ACTVY (T,P,XS1,GAM1IC)
      CALL ACTVY (T,P,XS2,GAM2IC)
      KIC(IE)=GAM2IC(IE)/GAM1IC(IE)
      KIC(IR)=GAM2IC(IR)/GAM1IC(IR)
      GO TO 1000
C
C     TWO LIQUID PHASES CASE
C     CALCULATIONS WITH EXPERIMENTAL X VALUES
C
  400 DO 420 J=1,NCLLE-2
  420 ISAVE(J)=0
C     OUTER LOOP FOR ALL THE COMPONENTS IN BOTH THE LIQ PHASES
      K=0
      KK=0
      DO 540 JJ=1,NCLLE
      FLAG=.FALSE.
      SUM1=0.0
      SUM2=0.0
C     INNER LOOP FOR INFINITE VALUES OF 1 COMPONENT IN THE SYSTEM
C     OF NCLLE COMPONENTS
      DO 500 I=1,NCLLE
      IF (FLAG .EQ. .TRUE.)GO TO 470
      IF (I .EQ. IE .OR. I .EQ. IR)GO TO 470
```

```
      IFLAG=0
      K=K+1
      DO 460 J=1,K
      IF (I .EQ. ISAVE(J))IFLAG=1
  460 CONTINUE
      IF (IFLAG .EQ. 1)GO TO 470
      XS1(I)=0.0
      XS2(I)=0.0
      FLAG=.TRUE.
      ISAVE(K)=I
      III=I
      GO TO 480
  470 CONTINUE
      XS1(I)=X1EXP(I)
      XS2(I)=X2EXP(I)
  480 SUM1=SUM1+XS1(I)
      SUM2=SUM2+XS2(I)
  500 CONTINUE
      DO 520 I=1,NCLLE
      XS1(I)=XS1(I)/SUM1
      XS2(I)=XS2(I)/SUM2
  520 CONTINUE
      CALL ACTVY (T,P,XS1,G1TEMP)
      CALL ACTVY (T,P,XS2,G2TEMP)
      KK=KK+1
      GAM1IE(KK)=G1TEMP(III)
      GAM2IE(KK)=G2TEMP(III)
      KIE(KK)=GAM2IE(KK)/GAM1IE(KK)
  540 CONTINUE
C
C     CALCULATIONS WITH CALCULATED X VALUES
C
  600 DO 620 J=1,NCLLE-2
  620 ISAVE(J)=0
C     OUTER LOOP FOR ALL THE COMPONENTS IN BOTH THE LIQ PHASES
      K=0
      KK=0
      DO 740 JJ=1,NCLLE
      FLAG=.FALSE.
      SUM1=0.0
      SUM2=0.0
C     INNER LOOP FOR INFINITE VALUES OF 1 COMPONENT IN THE SYSTEM
C     OF NCLLE COMPONENTS
      DO 700 I=1,NCLLE
      IF (FLAG .EQ. .TRUE.)GO TO 670
      IF (I .EQ. IE .OR. I .EQ. IR)GO TO 670
      IFLAG=0
      K=K+1
      DO 660 J=1,K
      IF (I .EQ. ISAVE(J))IFLAG=1
  660 CONTINUE
      IF (IFLAG .EQ. 1)GO TO 670
      XS1(I)=0.0
      XS2(I)=0.0
      FLAG=.TRUE.
      ISAVE(K)=I
      III=I
      GO TO 680
  670 CONTINUE
      XS1(I)=X1(I)
```

```
      XS2(I)=X2(I)
  680 SUM1=SUM1+XS1(I)
      SUM2=SUM2+XS2(I)
  700 CONTINUE
      DO 720 I=1,NCLLE
      XS1(I)=XS1(I)/SUM1
      XS2(I)=XS2(I)/SUM2
  720 CONTINUE
      CALL ACTVY (T,P,XS1,G1TEMP)
      CALL ACTVY (T,P,XS2,G2TEMP)
      KK=KK+1
      GAM1IC(KK)=G1TEMP(III)
      GAM2IC(KK)=G2TEMP(III)
      KIC(KK)=GAM2IC(KK)/GAM1IC(KK)
  740 CONTINUE
 1000 RETURN
      END
```

```
      SUBROUTINE START (IDATA,MFEED,MCASES,*)
C
C     KEY INTEGER CODES ARE INITIALIZED.  FOR VAPOR PHASE
C     DIMERIZATION THE ASSOCIATED TEMPERATURE DEPENDENT
C     CONSTANTS ARE DEFINED.
C
C     RETURN 1 USED FOR END OF FILE AND ERROR RETURN.
C
C     FEBRUARY 1985 ... ADDITION OF OPTION FOR TWO SETS OF ACTIVITY
C                       COEFFICIENT PARAMETERS
C
      COMMON  /BLANK/  NCR, NPRT, NSTART, KUNITS, TITLE(20)
      COMMON  /CMPRO/  NC, NCM1, NCP1, IDLL, IDLV, IDH, LDBUG, ISW,
     *                 NDIM, ZNAME(2,10), L(10), NTCOMP(10), NLIQ, IPSET
      COMMON  /TWOLQ/  X1(10), X2(10), GAM1(10), GAM2(10), EK1(10),
     +                 EK2(10), DHL(2), HIDLL(2), HREALL(2), FRACL,
     +                 IE, IR, XMAX, XMIN
C
C..........................................................................
C
C     DEC Error-Set Routines Activitated
C          Errset 72 = Floating Point Overflow
C          Errset 73 = Divide Check
C          Errset 74 = Floating Point Underflow
C          Errset 77 = Subscript Out Of Range
C
      CALL ERRSET (72, .TRUE.,  .TRUE., .FALSE., .FALSE., 999)
      CALL ERRSET (73, .TRUE.,  .TRUE., .FALSE., .FALSE., 999)
      CALL ERRSET (74, .TRUE.,  .TRUE., .FALSE., .FALSE., 999)
      CALL ERRSET (77, .FALSE., .TRUE., .FALSE., .FALSE., 999)
C
      NCR=5
      NPRT=6
C
C *** BASIC CONTROL PARAMETERS ... RECORD # 1 (11 ENTRIES)
C
C          NC         NUMBER OF COMPONENTS (1 THRU 10)
C
C          IDLL       LIQUID PHASE CLASSIFICATION CODE
C                            0    IDEAL
C                            1    VAN LAAR
C                            2    MARGULES
C                            3    WILSON
C                            4    NRTL
C                            5    UNIQUAC
C                            6    UNIQUAC ... MODIFIED
C                            7    UNIFAC
C                            8    *****
C                            9    *****
C                           10    *****
C                           11    BWR-F
C                           12    PENG-ROBINSON (PR)
C
C          IDLV       VAPOR PHASE CLASSIFICATION CODE
C                            0    IDEAL
C                            1    VIRIAL ... HAYDEN - O'CONNELL
C                                                CORRELATION
C                            2    VIRIAL ... TSONOPOULOS' CORRELATION
C                            3    REDLICH-KWONG (RK)
C                            4    SOAVE-REDLICH-KWONG (SRK)
```

```
C                        5    *****
C                        6    *****
C                        7    *****
C                        8    *****
C                        9    *****
C                       10    *****
C                       11    BWR-F
C                       12    PENG-ROBINSON (PR)
C
C         IDH       ENTHALPY CORRECTION
C                        0    CORRECT BOTH PHASES
C                        1    CORRECT VAPOR PHASE ONLY
C                        2    NO CORRECTION
C
C         LDBUG     DEBUG CODE
C                        0    MINIMUM PRINT OUT OF SEPARATION SYSTEM
C                        1    COMPONENT DATA AND FINAL COLUMN PRO-
C                                  FILES PRINTED
C                        2    CODE 1 + INTERMEDIATE COLUMN PROFILES
C                                  PRINTED
C
C         IDATA     DATA LIBRARY SWITCH
C                        0    READ VLE DATA FROM "CDATA"
C                        1    OBTAIN DATA FROM "ZPVT&ZNRTL"
C
C         NDIM      DIMERIZATION CODE ... VAPOR PHASE
C                        0    NO DIMERIZATION IN VAPOR PHASE
C                        #    COMPONENT NUMBER UNDERGOING DIMERIZATION
C
C         NLIQ      NUMBER OF LIQUID PHASES
C                       0/1  ONE PHASE
C                        2   TWO PHASES
C
C         IPSET     PARAMETER SETS CORESSPONDING TO IDLL
C                        0   GLOBAL SET OF PARAMETERS
C                        1   ONE SET OF PARAMETERS ... VLE VALUES
C                        2   TWO SETS OF PARAMETERS ...VLE VALUES
C                            FOLLOWED BY LLE VALUES
C                        3   NOT YET DEFINED
C
C                            NOTE: IPSET IS USED IN CDATA, TWOLIQ AND
C                                  SWITCH SUBROUTINES
C
C         MFEED     UNITS CODE FOR FEED VAPORIZATION ... FOR COLUMN
C                   SIMULATION
C                        0    FEED VAPORIZATION IS SPECIFIED
C                        1    FEED PRESSURE SPECIFIED ...
C                               FEED IS FLASHED BOTH AT BATTERY
C                               LIMITS (ISOTHERMALLY) AND THEN AT
C                               THE FEED STAGE (ADIABATICALLY)
C                               *** FEED HEAT ADDITION PERMITTED ***
C
C                   ALTERNATE USE IS BY SINGLE STAGE SIMULATION
C                   PROGRAM(S) ... This option is not yet activated.
C                       0/1   A SINGLE STREAM IS TO BE ANALYZED
C                        #    NUMBER OF STREAMS TO BE COMBINED
C                               PRIOR TO PERFORMING THE EQUILIBRIUM
C                               SEPARATION
C
C         MCASES    PROCESS COMPUTATION DATA SWITCH
```

```
C                              0    ONLY BASE CASE IS TO BE EVALUATED
C                              *    NUMBER OF ADDITIONAL PROCESS VARIANTS
C                                     TO BE EVALUATED ... INTERNAL RETURN
C                                     TO EVALUATE VARIANTS IS ACCOMPLISHED
C
C      READ (NCR,12)  NC,IDLL,IDLV,IDH,LDBUG,IDATA,NDIM,NLIQ,IPSET,
C     *               MFEED,MCASES
C  12 FORMAT (20I2)
      READ (NCR,*)    NC,IDLL,IDLV,IDH,LDBUG,IDATA,NDIM,NLIQ,IPSET,
     *                MFEED,MCASES
      IF (NC.EQ.0)  GO TO 30
      IF (NC.EQ.1)  GO TO 30
      IF (NC.GT.10) GO TO 30
      NCM1=NC-1
      NCP1=NC+1
      IF (NLIQ.EQ.0) NLIQ=1
C
C *** BASIC PARAMETERS -- DIMERIZATION CONSTANTS ... RECORD * 2
C ***         Optional Record
C     FOR "NDIM" NOT EQUAL TO ZERO READ IN THE DIMERIZATION CONSTANTS
      IF (NDIM.NE.0) READ (NCR,*) AX,BX
C
      IF (IDLL.LT.0 .OR. IDLL.GT.8) IDLL=0
      IF (IDLV.LT.0 .OR. IDLV.GT.5) IDLV=0
C
      IF (IDATA.EQ.1) IDLL=4
      IF (IDATA.EQ.1) IDLV=3
C
      WRITE (NPRT,13) NC
   13 FORMAT ('ONUMBER OF COMPONENTS =', I3)
      WRITE (NPRT,14) IDLL,IDLV,IDH
   14 FORMAT ('OVAPOR-LIQUID EQUILIBRIUM DATA CODES:'//
     *          5X, 'LIQUID =',     I4 /
     *          5X, 'VAPOR =',      I5/
     *          5X, 'ENTHALPY =',   I2//)
C
      WRITE (NPRT,15) LDBUG,IDATA,NDIM,MFEED,MCOLS
   15 FORMAT ('ODEFINED CODE VALUES:'//
     *          5X, 'PRINT/DEBUG =',                I17/
     *          5X, 'VLE DATA    =',                I17//
     *          5X, 'NDIM *      =',                I17//
     *          5X, 'FEED VAPORIZATION =',          I11/
     *          5X, '* OF PROCESS ALTERNATES =',    I5//)
C
C     VAPOR PHASE DIMERIZATION CONSTANTS ARE DEFINED
      IF (NDIM.NE.0) WRITE (NPRT,17) AX,BX
   17 FORMAT ('OVAPOR PHASE DIMERIZATION CONSTANTS:'//
     *          5X, 'A =', G20.5/
     *          5X, 'B =', G20.5)
      GO TO 50
C
   30 WRITE (NPRT,35)
   35 FORMAT ('OZERO, ONE, OR MORE THAN TEN COMPONENTS SPECIFIED.')
      GO TO 100
C
C *** BASIC PARAMETERS -- COMPONENT ID NUMBERS ... RECORD * 3
C ***         Optional Record
C
C     COMPONENT IDENTIFICATION NUMBERS ARE DEFINED FOR USE BY
C     THE DATA LIBRARY SUBPROGRAMS
```

```
   50 IF (IDATA.EQ.1) READ (NCR,*) (NTCOMP(I),I=1,NC)
C
      WRITE (NPRT,65) NLIQ, IPSET
   65 FORMAT ('0DEFINED CODES AND VALUES:'//
     *        5X, 'NO. OF LIQ PHASES =',  I9/
     *        5X, '# PARAMETER SETS =',   I10///)
   90 WRITE (NPRT,91)
   91 FORMAT (////'0NOTE: ALL FLOWS ARE PER UNIT TIME, AND ENERGY' /
     *            '          VALUES ARE IN UNITS OF K-BTU PER UNIT TIME.')
C
      RETURN
C
  100 RETURN 1
      END
      SUBROUTINE CDATA
C
C     ROUTINE DEFINES THE PHYSICAL AND THERMODYNAMIC DATA FOR UP
C     TO A TEN (10) COMPONENT SYSTEM.  INCLUDED ARE THE ACTIVITY
C     COEFFICIENT MODEL PARAMETERS, WHICH ARE SYSTEM DEPENDENT.
C
      COMMON  /BLANK/  NCR, NPRT, NSTART, KUNITS, TITLE(20)
      COMMON  /CMPRO/  NC, NCM1, NCP1, IDLL, IDLV, IDH, LDBUG, ISW,
     *                 NDIM, ZNAME(2,10), L(10), NTCOMP(10), NLIQ, IPSET
C     CHARACTER*4      ZNAME
      COMMON  /ZDATA/  CPL(10,4), CPV(10,4), ENP(10,10), ANT(6,10),
     *                 W(10), AX, BX, OMEGA(10), AVAL(10), BVAL(10),
     *                 AK(10,10), R(10), Q(10), QP(10), XL(10),
     *                 VOL(10), C(180), ALPHA(45), VC(10), TC(10),
     *                 PC(10), ZC(10), TNBP(10), OA(10), OB(10),
     *                 A(10,10), G(10,10), ZRA(10), RD(10), DMU(10),
     *                 ETA(10)
      COMMON  /SWITCH/ CSTORE(180,2), ASTORE(45,2), ISTORE(2)
      COMMON  /CONTRL/ ITF, IPF, N, NTYPE, JCODE
C
      INTEGER          ID(10)
      REAL             TREF(10), HVAP(10), EK(10), ETM(10,10)
C
C     EQUIVALENCE THE SOLVATION PARAMETERS (ETM) OF THE VIRIAL
C     EQUATION OF STATE ... HAYDEN-O'CONNELL VERSION WITH THE
C     CHARACTERISTIC BINARY CONSTANTS (AK) OF THE VIRIAL EQUATION
C     OF STATE ... TSONOPOULOS VERSION
C
      EQUIVALENCE      (ETM(1,1),AK(1,1))
C
C     DOUBLE PRECISION EQNV, EQNM, EQNW, EQNR, EQNU, EQNU2, EQNF
      CHARACTER*8      EQNV, EQNM, EQNW, EQNR, EQNU, EQNU2, EQNF
      DATA             EQNV /'VANLAAR'/
      DATA             EQNM /'MARGULES'/
      DATA             EQNW /'WILSON'/
      DATA             EQNR /'RENON'/
      DATA             EQNU /'UNIQUAC'/
      DATA             EQNU2/'M-UNIQUC'/
      DATA             EQNF /'UNIFAC'/
C
      DATA             OMA, OMB  /0.42748, 0.08664/
C
C..........................................................................
C
C     BASIC CONTROL PARAMETERS ... DEFINED IN START
C
```

```
C         NC        NUMBER OF COMPONENTS
C
C         IDLL      LIQUID PHASE CLASSIFICATION CODE
C                        0    IDEAL
C                        1    VAN LAAR
C                        2    MARGULES
C                        3    WILSON
C                        4    NRTL
C                        5    UNIQUAC
C                        6    UNIQUAC ... MODIFIED
C                        7    UNIFAC
C                        8    *****
C                        9    *****
C                       10    *****
C                       11    BWR-F
C                       12    PENG-ROBINSON (PR)
C
C         IDLV      VAPOR PHASE CLASSIFICATION CODE
C                        0    IDEAL
C                        1    VIRIAL ... HAYDEN - O'CONNELL
C                                        CORRELATION
C                        2    VIRIAL ... TSONOPOULOS' CORRELATION
C                        3    REDLICH-KWONG (RK)
C                        4    SOAVE-REDLICH-KWONG (SRK)
C                        5    *****
C                        6    *****
C                        7    *****
C                        8    *****
C                        9    *****
C                       10    *****
C                       11    BWR-F
C                       12    PENG-ROBINSON (PR)
C
C         IDH       ENTHALPY CORRECTION
C                        0    CORRECT BOTH PHASES
C                        1    CORRECT VAPOR PHASE ONLY
C                        2    NO CORRECTION
C
C         LDBUG     DEBUG CODE
C                        0    MINIMUM PRINT OUT OF SEPARATION SYSTEM
C                        1    COMPONENT DATA AND FINAL COLUMN PRO-
C                                  FILES PRINTED
C                        2    CODE 1 + INTERMEDIATE COLUMN PROFILES
C                                  PRINTED
C
C         IDATA     DATA LIBRARY SWITCH
C                        0    READ VLE DATA FROM "CDATA"
C                        1    OBTAIN DATA FROM "ZPVT&ZNRTL"
C
C         NDIM      DIMERIZATION CODE ... VAPOR PHASE
C                        0    NO DIMERIZATION IN VAPOR PHASE
C                        #    COMPONENT NUMBER UNDERGOING DIMERIZATION
C
C         NLIQ      NUMBER OF LIQUID PHASES
C                        1   ONE PHASE
C                        2   TWO PHASES
C
C         IPSET     PARAMETER SETS CORESSPONDING TO IDLL
C                        0   GLOBAL SET OF PARAMETERS
C                        1   ONE SET OF PARAMETERS ... VLE VALUES
```

```
C                        2  TWO SETS OF PARAMETERS ...VLE VALUES
C                           FOLLOWED BY LLE VALUES
C                        3  NOT YET DEFINED
C
C                           NOTE:IPSET IS USED IN CDATA, TWOLIQ AND
C                                SWITCH SUBROUTINES
C
C         IDATA    DATA LIBRARY SWITCH
C                        0   READ VLE DATA FROM "CDATA"
C                        1   OBTAIN DATA FROM "ZPVT&ZNRTL"
C
C*******************************************************************
C
C     PURE COMPONENT DATA ... EIGHT (8) RECORDS NEEDED PER COMPONENT
C
C      INPUT RECORD #1 ... A Format is used
C         ZNAME    COMPONENT NAME
C
C      INPUT RECORD #2 ... Integer Values / Real Values are used
C         L        COMPONENT TYPE
C                        0   NORMAL
C                        1   SUPER CRITICAL
C                        2   NON CONDENSIBLE
C                        3   NON VOLATILE
C         W        MOLECULAR WEIGHT ... g per g-mole
C         TNBP     NORMAL BOILING POINT TEMPERATURE ... Deg K
C         TC       CRITICAL TEMPERATURE ... Deg K
C         PC       CRITICAL PRESSURE ... Atm
C         VC       CRITICAL VOLUME ... cc per g-mole
C         ZC       CRITICAL COMPRESSIBILITY FACTOR
C         VOL      MOLAR VOLUME ... cc per g-mole
C         OMEGA    ACENTRIC FACTOR ... PITZER
C
C      INPUT RECORD #3 ... Real Values are used
C         OA       REDLICH-KWONG PARAMETERS
C         OB
C         R        UNIQUAC PARAMETERS -- VOLUME ... molecular volume
C         Q                           -- SURFACE AREA ... molecular area
C         QP                          -- INTERACTION AREA ... molecular area
C         AVAL     TSONOPOULOS' PARAMETERS FOR VIRIAL EQUATION
C         BVAL
C         ZRA      RACKET PARAMETER
C
C      INPUT RECORD #4
C         RD       RADIUS OF GYRATION ... A
C         DMU      DIPOLE MOMENT ...Debyes
C         ETA      ASSOCIATION PARAMETER
C
C      INPUT RECORD #5     ENTHALPY DATA
C         HVAP     HEAT OF VAPORIZATION ... cal per gm
C         TREF     REFERENCE TEMPERATURE ... Deg K
C
C      INPUT RECORD #6
C         CPL      SPECIFIC HEAT CONSTANTS       LIQUID
C                        C1, C2, .... , C4
C                        C1=a, C2=b, .... , C4=d
C                        cal per gm  vs  Deg K
C                        Cp = a + bT + cT^2 + dT^3
C
C      INPUT RECORD #7
```

```
C         CPV       SPECIFIC HEAT CONSTANTS       VAPOR
C                        C1, C2, ... , C4
C                        C1=a, C2=b, .... , C4=d
C                        cal per g-mole  vs  Deg K
C                        Cp = a + bT + cT^2 + dT^3
C
C      INPUT RECORD #8
C         ANT       VAPOR PRESSURE CONSTANTS
C                        C1, C2, ... , C6
C                        C1=a, C2=b, .... , C6=f
C                        Atm  versus  Deg K
C                        ln(P) = a + b/(c + T) + d*ln(T) + e*T + f*T^2
C
C     INPUT RECORD #9 ... Optional Input --- Used Only If IDLV=1
C         IF THE VIRIAL EQUATION OF STATE IS USED ... HAYDEN-
C         O'CONNELL VERSION, THEN THE SOLVATION PARAMETERS MUST
C         BE DEFINED: ETM(1,1), ETM(1,2), ETC.
C
C     INPUT RECORD #9 ... Optional Input --- Used Only If IDLV=2
C         IF THE VIRIAL EQUATION OF STATE IS USED ... HAYDEN-
C         O'CONNELL VERSION, THEN THE SOLVATION PARAMETERS MUST
C         BE DEFINED: ETM(1,1), ETM(1,2), ETC.
C
C***********************************************************************
C
C      INTERNAL CODE VALUES FOR COMPONENT TYPE ... ALTERED BASED ON THE
C      VALUE DEFINED ON RECORD #2.
C            INPUT       TYPE            INTERNAL
C             -1     NON-VOLATILE          -1
C              0     NON-CONDENSIBLE        0
C              1     NORMAL                 1
C              2     SUPERCRITICAL          2
C
      DO 10 I=1,2
      ISTORE(I)=0
      DO 7 J=1,180
    7 CSTORE(J,I)=0.0
      DO 10 K=1,45
   10 ASTORE(K,I)=0.0
C
      DO 110 I=1,NC
C
C *** INPUT RECORD #1 ... A Format is used
      READ (NCR,30) (ZNAME(J,I),J=1,2)
   30 FORMAT (2A4)
C
C *** INPUT RECORD #2 ... Integer Values / Real Values are used
      READ (NCR,*)  L(I),W(I),TNBP(I),TC(I),PC(I),VC(I),ZC(I),
     *              VOL(I),OMEGA(I)
      IF (W(I).LE.0.0) W(I)=1.0
C
C *** INPUT RECORD #3 ... Real Values are used
      READ (NCR,*)  OA(I),OB(I),R(I),Q(I),QP(I),AVAL(I),BVAL(I),
     *              ZRA(I)
      XL(I)=10.0/2.0*(R(I)-Q(I))-(R(I)-1.0)
      IF (QP(I).EQ.0.0) QP(I)=Q(I)
C
C *** INPUT RECORD #4
      READ (NCR,*)  RD(I),DMU(I),ETA(I)
C
```

```
      IF (L(I)-1) 50,60,70
   50 L(I)=1
      GO TO 100
   60 L(I)=2
      GO TO 100
   70 IF (L(I)-3) 80,90,50
   80 L(I)=0
      GO TO 100
   90 L(I)=-1
  100 CONTINUE
C
C
C *** INPUT RECORD #5      ENTHALPY DATA
      READ (NCR,*)   HVAP(I),TREF(I)
C
C *** INPUT RECORD #6
      READ (NCR,*)   (CPL(I,J),J=1,4)
C
C *** INPUT RECORD #7
      READ (NCR,*)   (CPV(I,J),J=1,4)
C
C *** INPUT RECORD #8
      READ (NCR,*)   (ANT(J,I),J=1,6)
  110 CONTINUE
C
      IF (IDLV.EQ.1) GO TO 120
      IF (IDLV.EQ.2) GO TO 150
      GO TO 220
C
C     IF THE VIRIAL EQUATION OF STATE IS USED ... HAYDEN-
C     O'CONNELL VERSION, THEN THE SOLVATION PARAMETERS MUST
C     BE DEFINED: ETM(1,1), ETM(1,2), ETC.
C
C *** INPUT RECORD #9 ... Optional Input --- Used Only If IDLV=1
  120 DO 130 I=1,NC
  130 READ (NCR,*)   (ETM(I,J),J=1,NC)
      GO TO 220
C
C     IF THE VIRIAL EQUATION OF STATE IS USED ... TSONOPOULOS
C     VERSION, THEN THE CHARACTERISTIC BINARY CONSTANTS MUST
C     BE DEFINED:  AK(1,1), AK(1,2), ETC.
C
C *** INPUT RECORD #9 ... Optional Input --- Used Only If IDLV=2
  150 DO 160 I=1,NC
  160 READ (NCR,*)   (AK(I,J),J=1,NC)
C
  220 IF (LDBUG.EQ.0) GO TO 430
C
C     WRITE (NPRT,250)
  250 FORMAT ('1')
C     WRITE (NPRT,251)
  251 FORMAT (2(/))
C
      DO 425 J1=1,NC,5
C     Format for the componential data was originally based on full use
C     of standard computer paper.  Using J1 and J2 the output width is
C     reduced to standard letter size --- which can be cut down if one
C     uses the standard size computer paper.  Output displays five (5)
C     components per block.
      J2=J1+4
```

```
      IF (J2.GT.NC) J2=NC
C
      WRITE (NPRT,260) (J,J=J1,J2)
  260 FORMAT ('1COMPONENT NO', 21X, 9(I2,8X),I2)
      WRITE (NPRT,270) ((ZNAME(I,J),I=1,2),J=J1,J2)
  270 FORMAT (' NAME', 27X, 9(2A4,2X),2A4)
      WRITE (NPRT,275) (L(J),J=J1,J2)
  275 FORMAT (' COMPONENT TYPE', 19X, 9(I2,8X),I2)
C
      WRITE (NPRT,280) (W(J),J=J1,J2)
  280 FORMAT ('0MOLECULAR WEIGHT', 15X, 9(F6.2,4X),F6.2)
      WRITE (NPRT,281) (TNBP(J),J=J1,J2)
  281 FORMAT (' NORMAL BOILING POINT (Deg K)', 2X,
     *        9(F7.1,3X),F7.1)
C
      WRITE (NPRT,285) (TC(J),J=J1,J2)
  285 FORMAT ('0CRITICAL PROPERTIES'/1X,' TEMPERATURE  (Deg K)',
     *        9X, 9(F7.1,3X),F7.1)
      WRITE (NPRT,290) (PC(J),J=J1,J2)
  290 FORMAT (1X,' PRESSURE     (Atm) ', 10X, 9(F7.1,3X),F7.1)
      WRITE (NPRT,295) (VC(J),J=J1,J2)
  295 FORMAT (1X,' VOLUME       (cc/gmol)', 7X, 9(F7.1,3X),F7.1)
      WRITE (NPRT,297) (ZC(J),J=J1,J2)
  297 FORMAT ('  COMPRESSIBILITY FACTOR', 7X, 9(F7.3,3X),F7.3)
C
      WRITE (NPRT,300)
  300 FORMAT (' LIQUID MOLAR VOLUME')
C     I=1
C     WRITE (NPRT,390) I,(VOL(J),J=J1,J2)
      WRITE (NPRT,305) (VOL(J),J=J1,J2)
  305 FORMAT ('   (cc/g-mol)', 15X, 10F10.2)
      WRITE (NPRT,310)  (OMEGA(J),J=J1,J2)
  310 FORMAT (' ACENTRIC FACTOR' 15X, 9(F7.3,3X),F7.3)
C
C     IF (IDLL.NE.5 .OR. IDLL.NE.6) GO TO 345
      WRITE (NPRT,322) (R(J),J=J1,J2)
  322 FORMAT ('0NORMALIZED UNIQUAC PARAMETERS'/
     *         1X,' VOLUME (R)', 19X, 9(F7.4,3X),F7.4)
      WRITE (NPRT,323) (Q(J),J=J1,J2)
  323 FORMAT (1X,' SURFACE AREA (Q)', 13X, 9(F7.4,3X),F7.4)
      WRITE (NPRT,324) (QP(J),J=J1,J2)
  324 FORMAT (1X,' INTERACTION AREA (Q'')', 8X, 9(F7.4,3X),F7.4)
C
  345 IF (IDLV.NE.2) GO TO 350
      WRITE (NPRT,346) (AVAL(J),J=J1,J2)
  346 FORMAT ('0VIRIAL EQUATION -- TSONOPOULOS'/
     *         ' EXTENSION COVERS POLAR COMPOUNDS'/
     *         2X,'AVAL', 25X, 9(F7.3,3X),F7.3)
      WRITE (NPRT,347) (BVAL(J),J=J1,J2)
  347 FORMAT (1X,' BVAL', 25X, 9(F7.3,3X),F7.3)
C
  350 WRITE (NPRT,355) (ZRA(J),J=J1,J2)
  355 FORMAT ('0RACKETT PARAMETER', 13X, 9(F7.3,3X),F7.3)
C
      WRITE (NPRT,356) (RD(J),J=J1,J2)
  356 FORMAT (' RADIUS OF GYRATION, A', 9X, 9(F7.3,3X),F7.3)
      WRITE (NPRT,357) (DMU(J),J=J1,J2)
  357 FORMAT (' DIPOLE MOMENT, DEBYES', 9X, 9(F7.4,3X),F7.4)
      WRITE (NPRT,358) (ETA(J),J=J1,J2)
  358 FORMAT (' ASSOCIATION PARAMETER', 9X, 9(F7.4,3X),F7.4)
```

```
C
      WRITE (NPRT,360) (HVAP(J),J=J1,J2)
  360 FORMAT ('0ENTHALPY CONSTANTS'/
     *          '  LATENT HEAT (cals/g) ', 8X, 9(F7.1,3X),F7.1)
      WRITE (NPRT,370) (TREF(J),J=J1,J2)
  370 FORMAT (2X,' TEMP (Deg K)', 16X, 9(F7.1,3X),F7.1)
      WRITE (NPRT,380)
  380 FORMAT ('  LIQUID SP. HEAT CONSTANTS'/
     *          '   (cals/g   vs  Deg K) ')
      DO 385 I=1,4
  385 WRITE (NPRT,390) I,(CPL(J,I),J=J1,J2)
  390 FORMAT (2X,' C(',I1,')', 21X, 10F10.6)
C 390 FORMAT (2X,' C(',I1,')', 21X, 1P10G10.2)
      WRITE (NPRT,410)
  410 FORMAT ('  VAPOR SP. HEAT CONSTANTS'/
     *          '   (cals/gmol  vs  Deg K) ')
      DO 415 I=1,4
  415 WRITE (NPRT,390) I,(CPV(J,I),J=J1,J2)
C
      WRITE (NPRT,321) (ANT(1,J),J=J1,J2)
C 321 FORMAT ('0VAPOR PRESSURE CONSTANTS'/2X,' (mmHg and Deg K)'/
  321 FORMAT ('0VAPOR PRESSURE CONSTANTS'/2X,' (Atm and Deg K)'/
     *          '   C(1)', 24X, 9(F7.4,3X),F7.4)
      DO 325 I=2,6
  325 WRITE (NPRT,330) I,(ANT(I,J),J=J1,J2)
  330 FORMAT (2X,' C(',I1,')', 21X, 10F10.3)
C
      IF (J2.EQ.NC) GO TO 430
  425 CONTINUE
C
C     CONVERT ALL DATA TO MOLAR UNITS AND THEN GENERATE THE
C     ENTHALPY POLYNOMINAL COEFFICIENTS ... FOR BOTH THE
C     VAPOR AND LIQUID PHASES
  430 DO 440 I=1,NC
C     The following statement converts mm Hg to atm.
CC    ANT(1,I)=ANT(1,I)-ALOG(760.0)
C     Convert specific heat data and enthalpy data where necessary to
C     molar units.
      HVAP(I)=HVAP(I)*W(I)
      DO 435 J=1,4
  435 CPL(I,J)=CPL(I,J)*W(I)
C 435 CPV(I,J)=CPV(I,J)*W(I)
      ENP(I,5)=CPL(I,4)/4.0
      ENP(I,4)=CPL(I,3)/3.0
      ENP(I,3)=CPL(I,2)/2.0
      ENP(I,2)=CPL(I,1)
      TR=TREF(I)
      ENP(I,1)=-(((ENP(I,5)*TR+ENP(I,4))*TR+ENP(I,3))*TR+ENP(I,2))*
     *          TR
      ENP(I,10)=CPV(I,4)/4.0
      ENP(I,9)=CPV(I,3)/3.0
      ENP(I,8)=CPV(I,2)/2.0
      ENP(I,7)=CPV(I,1)
      ENP(I,6)=HVAP(I)-(((ENP(I,10)*TR+ENP(I,9))*TR+ENP(I,8))*TR+
     *          ENP(I,7))*TR
  440 CONTINUE
C
      WRITE (NPRT,250)
      IF (IDLV.EQ.0) GO TO 455
C
```

```
      IF (IDLV.EQ.1) WRITE (NPRT,431)
  431 FORMAT ('OSOLVATION PARAMETERS FOR THE VIRIAL EQUATION OF' /
     *        ' STATE ... HAYDEN-O''CONNELL VERSION')
      IF (IDLV.EQ.2) WRITE (NPRT,432)
  432 FORMAT ('OCHARACTERISTIC BINARY CONSTANTS FOR THE VIRIAL' /
     *        ' EQUATION OF STATE ... TSONOPOULOS VERSION')
      IF (IDLV.GE.3) GO TO 455
C
      DO 450 I=1,NC
      DO 450 J=1,NC,4
      IF (J.LE.9 )   ID(1)=10*I+J
      IF (J.GE.10)   ID(1)=100*I+J
      IF (J+1.GT.NC) GO TO 442
      IF (J+1.LE.9)  ID(2)=10*I+J+1
      IF (J+1.GE.10) ID(2)=100*I+J+1
      IF (J+2.GT.NC) GO TO 444
      IF (J+2.LE.9)  ID(3)=10*I+J+2
      IF (J+2.GE.10) ID(3)=100*I+J+2
      IF (J+3.GT.NC) GO TO 446
      IF (J+3.LE.9)  ID(4)=30*I+J+3
      IF (J+3.GE.30) ID(4)=300*I+J+3
      GO TO 448
C
C     NOTE: SOLVATION PARAMETERS AND CHARACTERISTIC BINARY
C           CONSTANTS SHARE THE SAME STORAGE SPACE ... ETM(*,*)
C           AND AK(*,*).
C
  442 WRITE (NPRT,443) ID(1),AK(I,J)
  443 FORMAT (3X, ('K',I4,F9.4,3X))
      GO TO 450
  444 WRITE (NPRT,445) (ID(IJ),AK(I,IJ),IJ=1,2)
  445 FORMAT (3X, 2('K',I4,F9.4,3X))
      GO TO 450
  446 WRITE (NPRT,447) (ID(IJ),AK(I,IJ),IJ=1,3)
  447 FORMAT (3X, 3('K',I4,F9.4,3X))
      GO TO 450
  448 WRITE (NPRT,449) (ID(IJ),AK(I,IJ),IJ=1,4)
  449 FORMAT (3X, 4('K',I4,F9.4,3X))
  450 CONTINUE
      WRITE (NPRT,451)
  451 FORMAT (/////)
C
C     LIQUID-LIQUID BINARY INTERACTION PARAMETERS ...
C     ... IDLL DEFINES THE ACTIVITY COEFFICIENT MODEL
C       0    IDEAL
C       1    VAN LAAR
C       2    MARGULES
C       3    WILSON
C       4    NRTL
C       5    UNIQUAC
C       6    UNIQUAC ... MODIFIED
C       7    UNIFAC
C       8    *****
C       9    *****
C      10    *****
C      11    BWR-F
C      12    PENG-ROBINSON (PR)
C
C     RENON ALPHA PARAMETERS
C         ALPHA     NRTL CONSTANTS
```

```
C
  455 IF (IDLL.EQ.0) GO TO 520
C
C     IF IDLL=7 CALL RUNFAC FOR READING AND WRITING UNIFAC CONSTANTS
C
      IF (IDLL .EQ. 7) THEN
        CALL RUNFAC
        GO TO 520
        END IF
C
C     INITIALIZE THE WORKING ARRAYS FOR THE ACTIVITY COEFFICIENT
C     MODELS ... THIS IS ASSUMED TO BE ACCOMPLISHED BEFORE THE
C     MODEL(S) ARE USED.
C
      NREAD=0
C
  460 DO 461 I=1,NC
      A(I,I)=0.0
  461 G(I,I)=1.0
C
      J=NC*NCM1*2
C
C *** INPUT RECORD #10 ... ACTIVITY COEFFICIENT CODE --- Used
C ***       Only If IDLL > 1 and for the second set of data.
      IF (NREAD.NE.0) READ (NCR,*) IDLL
      IF (NREAD.NE.0 .AND. IDLL.EQ.0) IDLL=ISTORE(1)
C
C *** INPUT RECORD #11 ... ACTIVITY COEFFICIENT PARAMETERS --- Used
C ***       Only If IDLL > 1
      DO 465 I1=1,J,8
      I2=I1+7
      IF (I2.GT.J) I2=J
  465 READ (NCR,*)   (C(I),I=I1,I2)
C
  467 IF (LDBUG.EQ.0) GO TO 495
      IF (IDLL.EQ.1) WRITE (NPRT,470) EQNV
      IF (IDLL.EQ.2) WRITE (NPRT,470) EQNM
      IF (IDLL.EQ.3) WRITE (NPRT,470) EQNW
      IF (IDLL.EQ.4) WRITE (NPRT,470) EQNR
      IF (IDLL.EQ.5) WRITE (NPRT,470) EQNU
      IF (IDLL.EQ.6) WRITE (NPRT,470) EQNU2
      IF (IDLL.EQ.7) WRITE (NPRT,470) EQNF
  470 FORMAT ('0', A8, ' CONSTANTS (cals/g-mol)')
      K=0
      DO 490 I=1,NCM1
      II=I+1
      DO 490 J=II,NC
      K=K+4
      IF (J.LE.9)  ID(1)=10*I+J
      IF (J.GE.10) ID(1)=100*I+J
      IF (I.LE.9)  ID(2)=10*J+I
      IF (I.GE.10) ID(2)=100*J+I
      WRITE (NPRT,480) ID(1),C(K-3),ID(1),C(K-2),ID(2),C(K-1),ID(2),
     *                  C(K)
  480 FORMAT (3X, 2('A',I4,' =',F9.3,3X,'B',I4,' =',F9.3,4X))
  490 CONTINUE
C
  495 IF (IDLL.NE.4) GO TO 517
      WRITE (NPRT,496)
  496 FORMAT (' ')
```

```
C
C *** INPUT RECORD #12 ... NRTL ALPHA PARAMETERS --- Used Only If IDLL = 4
      J=NC*NCM1/2
      DO 497 I1=1,J,8
      I2=I1+7
      IF (I2.GT.J) I2=J
  497 READ (NCR,*)   (ALPHA(I),I=I1,I2)
C
      IF (LDBUG.EQ.0) GO TO 517
      K=1
      KK=1
      DO 510 I=1,NCM1
      II=I+1
      DO 510 J=II,NC
      EK(KK)=ALPHA(K)
      IF (J.LE.9)  ID(KK)=10*I+J
      IF (J.GE.10) ID(KK)=100*I+J
      KK=KK+1
      K=K+1
      IF (KK.LT.5) GO TO 510
      WRITE (NPRT,500) (ID(KK),EK(KK),KK=1,4)
  500 FORMAT (3X, 4('ALPHA',I4,' =',F7.4,4X))
      KK=1
  510 CONTINUE
      IF (KK.EQ.1) GO TO 517
      KK=KK-1
C     WRITE (NPRT,500) (ID(I),EK(I),I=1,KK)
      IF (KK.EQ.1) WRITE (NPRT,512) ID(1),EK(1)
  512 FORMAT (3X, ('ALPHA',I4,' =',F7.4,4X))
      IF (KK.EQ.2) WRITE (NPRT,514) (ID(I),EK(I),I=1,2)
  514 FORMAT (3X, 2('ALPHA',I4,' =',F7.4,4X))
      IF (KK.EQ.3) WRITE (NPRT,516) (ID(I),EK(I),I=1,3)
  516 FORMAT (3X, 3('ALPHA',I4,' =',F7.4,4X))
C
  517 IF (IPSET .LT. 1) GO TO 520
      NREAD=NREAD+1
C
      ISTORE(NREAD)=IDLL
      DO 518 I=1,180
  518 CSTORE(I,NREAD)=C(I)
      DO 519 I=1,45
  519 ASTORE(I,NREAD)=ALPHA(I)
      IF (IPSET .EQ. 1) GO TO 520
C
C     ON EXIT FROM 'CDATA' GAMMA PARAMETERS IN "ZDATA" ARE THE FIRST
C     PARAMETERS READ.
      IF (NREAD .EQ. 2) THEN
        IPSET=1
        CALL SWITCH
        GO TO 520
        END IF
C
      GO TO 460
C
C     DEFINE THE MODIFIED R-K CONSTANTS
  520 IF (IDLV.EQ.0) GO TO 600
      DO 580 I=1,NC
      IF (OA(I).NE.0.0) GO TO 550
      OA(I)=OMA
  550 IF (OB(I).NE.0.0) GO TO 570
```

```
      OB(I)=OMB
  570 OA(I)=SQRT(OA(I)*TC(I)**2.5/PC(I))
  580 OB(I)=OB(I)*TC(I)/PC(I)
C
  600 WRITE (NPRT,610)
  610 FORMAT (/////
     *    ' NOTE: THE EQUATIONS FOR ENTHALPY AND VAPOR'
     *    '       PRESSURE ARE:' //
     *    '   (1)  ENTHALPY DATA'/
     *    '        HEAT OF VAPORIZATION ... cal per gm'/
     *    '        REFERENCE TEMPERATURE ... Deg K'//
     *    '   (2)  SPECIFIC HEAT CONSTANTS       LIQUID'/
     *    '           C1=a, C2=b, .... , C4=d'/
     *    '           cal per gram  vs  Deg K'/
     *    '           Cp = a + bT + cT^2 + dT^3'//
     *    '   (3)  SPECIFIC HEAT CONSTANTS       VAPOR'/
     *    '           C1=a, C2=b, .... , C4=d'/
     *    '           cal per g-mole  vs  Deg K'/
     *    '           Cp = a + bT + cT^2 + dT^3'//
     *    '   (4)  VAPOR PRESSURE CONSTANTS'/
     *    '           C1, C2, ... , C6'/
     *    '           C1=a, C2=b, .... , C6=f'/
     *    '           Atm  versus  Deg K'/
     *    '           ln(P) = a + b/(c + T) + d*ln(T) + e*T + f*T^2')
C
  640 RETURN
      END
      SUBROUTINE RUNFAC
C
C     THIS SUBROUTINE READS UNIFAC DATA (R, Q AND GROUP INTERACTION
C     PARAMETERS) FROM A DATA FILE ... LOGOCAL UNIT 10
C
      COMMON  /BLANK/  NCR, NPRT, NSTART, KUNITS, TITLE(20)
      COMMON  /CMPRO/  NC, NCM1, NCP1, IDLL, IDLV, IDH, LDBUG, ISW,
     *                 NDIM, ZNAME(2,10), L(10), NTCOMP(10), NLIQ, IPSET
      COMMON  /ZDATA/  CPL(10,4), CPV(10,4), ENP(10,10), ANT(6,10),
     *                 W(10), AX, BX, OMEGA(10), AVAL(10), BVAL(10),
     *                 AK(10,10), R(10), Q(10), QP(10), XL(10),
     *                 VOL(10), C(180), ALPHA(45), VC(10), TC(10),
     *                 PC(10), ZC(10), TNBP(10), OA(10), OB(10),
     *                 A(10,10), G(10,10), ZRA(10), RD(10), DMU(10),
     *                 ETA(10)
C
      COMMON /UNFAC/   XMOL(11),COMLN(11),RESLN(11),ALGAC(11),
     1                 ACTCF(11),IDGP(6,11),NOGP(6,11),NGMOL(11),AL(11),
     2                 RI(11),QI(11),QGPI(6,11),QGP(11),PARM(11,11),
     3                 IID(11),GSUM(11),GG(11),TNAM(3,11)
      COMMON /UNFAC1/  GNAM(3,80),QQ(80),RR(80),PARAM(42,42),NKTAB(80),
     *                 KODE(42,42), NGPT, NSPS
C
      CHARACTER*4      ZNAME, LNK, MOL(5,11), CARD(20)
      INTEGER          ID(10)
      REAL             TREF(10), HVAP(10), EK(10)
C
C......................................................................
C
C     NOTE: DIMENSION OF KODE AND PARAM HAVE BEEN SET TO 42X42
C           BECAUSE OF INPUT BY AN IMPLIED DO-LOOP AND FORMAT
C           # 4003.
C
```

```
C     INPUT FOR UNIFAC
C     1.  READ DATA BANK FROM THE TAPE/DISK
C     2.  READ COMPONENT AND NO. OF GROUPS PER COMP.
C         * ONE RECORD FOR EACH COMP. (NC<11)
C         NGMOL = NO.OF DIFFERENT GROUPS IN THE MOLECULE,(<=6)
C         MOL   = NAME OF THE COMPONENT.
C         * BLANK RECORD AFTER THIS SET OF INPUT.
C     3.  READ GROUP SPECIFICATION RECORDS
C         * FOR EACH COMPONENT
C         * A SEPERATE RECORD FOR EACH MOLECULE
C         NOGP = NO. OF TIMES THE GROUP APPEARS IN THE MOLECULE
C         IDGP = ID NO. OF THE GROUP (SECONDARY GROUP NO. FOUND
C                IN THE TABLE IV IN THE REFERENCE STATED BELOW)
C
C     REF: 1. GHEMLING, J. ,ET AL , IND. ENG. CHEM. PROCESS DES.
C                           DEV. ,21,118-127 (1982).
C          2. COMMUNICATIONS,IEC PROCESS DES. DEV. ,22,678-681(1983).
C
C...................................................................
C
C     READ DATA BANK.
C
      LUD=10
C
      OPEN ( UNIT=LUD, STATUS='OLD', ACCESS='SEQUENTIAL',
     1       FILE='[CHAWLA.THERMO]BANKUNIF.DAT' )
C
C     READ DATA BANK ... FILE LUD=10
C
C          NMG   = # OF MAIN GROUPS
C          NSG   = # OF SECONDARY GROUPS
C
C          QQ    = GROUP AREA PARAMETER
C          RR    = GROUP VOLUMNE PARAMETER
C          NKTAB = MAIN GROUP # TO WHICH THE SECONDARY GROUP BELONGS
C          GNAM  = GROUP NAME
C
C          KODE  = CODE FOR SOURCE OF DATA
C          PARAM = GROUP INTERACTION PARAMETERS
C
      READ (LUD,4000) CARD
 466  READ (LUD,4001) NMG,NSG
C     READ (LUD,4002) (QQ(I),RR(I),NKTAB(I),GNAM(I),I=1,NSG))
      READ (LUD,4002) (QQ(I),RR(I),NKTAB(I),(GNAM(J,I),J=1,3),I=1,NSG)
C     WRITE (6,1)
C   1 FORMAT ('1')
C     WRITE (6,*) NSG
C     DO 10 I=1,NSG
C     WRITE (6,5) I,QQ(I),RR(I),NKTAB(I),(GNAM(J,I),J=1,3)
C   5 FORMAT (I5,5X,2F10.4,I10,10X,2A4,A2)
C  10 CONTINUE
C     WRITE (6,1)
C     WRITE (6,*) NMG
      DO 15 I=1,NMG
C     WRITE (6,*) I
      READ (LUD,4003) (KODE(I,J),PARAM(I,J),J=1,NMG)
C     DO 14 J=1,NMG
C  14 WRITE (6,*) J,KODE(I,J),PARAM(I,J)
   15 CONTINUE
 4000 FORMAT (20A4)
```

```
 4001 FORMAT (2I2)
C4002 FORMAT (3(2F7.4,I2,A10),2X)
 4002 FORMAT (3(2F7.4,I2,2A4,A2),2X)
 4003 FORMAT (7(I1,F9.2),10X)
C
C     READ COMPONENTS AND NUMBER OF GROUPS PER COMPONENT.
C
C     LNK = 10H
      J = 1
C  30 READ (5,1001) MOL(1,J),MOL(2,J),NGMOL(J)
   33 READ (5,1001) NGMOL(J),(MOL(K,J),K=1,5)
C     IF (MOL(1,J).EQ.LNK) GO TO 35
      IF (NGMOL(J) .EQ. 0) GO TO 35
      J = J + 1
      GO TO 33
   35 IF (J.EQ.1) STOP
      NSPS = J - 1
      DO 40 J=1,NSPS
      NN = NGMOL(J)
C  40 READ (5,1002) (NOGP(I,J),IDGP(I,J),I=1,NN)
   40 READ (5,*) (NOGP(I,J),IDGP(I,J),I=1,NN)
      NGPT = 0
      DO 60 J=1,NSPS
      NN = NGMOL(J)
      DO 55 I=1,NN
      IF (NGPT.EQ.0) GO TO 53
      DO 45 K=1,NGPT
      IF (IDGP(I,J).NE.IID(K)) GO TO 45
      IDGP(I,J) = K
      GO TO 55
   45 CONTINUE
   53 NGPT = NGPT + 1
      IID(NGPT) = IDGP(I,J)
      IDGP(I,J) = NGPT
   55 CONTINUE
   60 CONTINUE
C
C     READ  NUMBER OF MIXTURES TO BE CALCULATED.
C
C  63 READ (5,1003) NMIX
C  63 READ (5,*,END=999) NMIX
C
C     PRINT UNIFAC INPUT BLOCK
C
C     PRINT SUMMARY OF INPUT DATA.
C
 492  WRITE (6,2001)
      DO 62 J=1,NSPS
C     WRITE (6,2002) MOL(1,J),MOL(2,J)
      WRITE (6,2002) (MOL(K,J),K=1,5)
      K = NGMOL(J)
      DO 61 I=1,K
      LI = IDGP(I,J)
      LI = IID(LI)
      M = NKTAB(LI)
      NUM = NOGP(I,J)
C  61 WRITE (6,2003) GNAM(LI),M,LI,NUM,QQ(LI),RR(LI)
   61 WRITE (6,2003) (GNAM(LL,LI),LL=1,3),M,LI,NUM,QQ(LI),RR(LI)
   62 CONTINUE
C     IF (NMIX.EQ.0) NMIX = 1
```

```
      DO 65 I=1,NGPT
      K = IID(I)
      K = NKTAB(K)
      DO 65 J=1,NGPT
      LI = IID(J)
      LI = NKTAB(LI)
      IF (LI.EQ.K) GO TO 65
      IF (KODE(K,LI).EQ.0) GO TO 64
      WRITE (6,2009)
      IF (KODE(K,LI).EQ.1) WRITE (6,2010) K,LI,IID(I),IID(J)
      IF (KODE(K,LI).EQ.2) WRITE (6,2011) K,LI,IID(I),IID(J)
      IF (KODE(K,LI).EQ.3) WRITE (6,2012) K,LI,IID(I),IID(J)
   64 CONTINUE
      IF (ABS(PARAM(K,LI)).GT.1.E-3) GO TO 65
      WRITE (6,3001) K,LI
 3001 FORMAT (1X,'INTERACTION PARAMETER FOR THE ',I2,'-',I2,
     1       ' NOT AVAILABLE')
      STOP
   65 PARM(I,J) = PARAM(K,LI)
C
C     PRINT GROUP INTERACTION PARAMETER DATA.
C
      DO 70 I=1,NGPT
      K = IID(I)
      DO 70 J=1,3
C  70 TNAM(I) = GNAM(K)
   70 TNAM(J,I)=GNAM(J,K)
C      WRITE (6,2004) NMIX
C     WRITE (6,2005) (TNAM(I),I=1,NGPT)
      WRITE (6,2005) ((TNAM(J,I),J=1,3),I=1,NGPT)
      DO 75 I=1,NGPT
C  75 WRITE (6,2006) TNAM(I),(PARM(I,J),J=1,NGPT)
   75 WRITE (6,2006) (TNAM(J,I),J=1,3),(PARM(I,J),J=1,NGPT)
C1001 FORMAT (2A10,I2)
 1001 FORMAT (I2,5A4)
C1002 FORMAT (16I5)
C1003 FORMAT (F10.0,I5)
C1004 FORMAT (8F10.0)
 2001 FORMAT (1H1,'UNIFAC CALCULATION OF ACTIVITY COEFFICIENTS')
 2002 FORMAT (1H0,5A4//8X,'GROUP',4X,'PRI',2X,'SEC',3X,'NUM',7X,
     1        'Q',9X,'R'/)
C2003 FORMAT (6X,A10,'(',I2,')',1X,'(',I2,')',4X,I2,4X,F6.4,4X,F6.4)
 2003 FORMAT (6X,2A4,A2,'(',I2,')',1X,'(',I2,')',4X,I2,4X,F6.4,4X,F6.4)
 2005 FORMAT (14X,11(2A4,A2))
 2006 FORMAT (/1X,2A4,A2,11F10.5)
 2009 FORMAT(/,5X,'...PARAMETER BACKGROUND NOTE')
 2010 FORMAT(7X,'PARAMETERS FOR THE ',I2,'-',I2,' INTERACTION HAVE BEEN
     1OBTAINED FROM METHANCL DATA, SEE REF. 3',/,
     27X,'THESE PARAMETERS ARE USED FOR THE ',I2,'-',I2,' SECCNDARY GROU
     3P INTERACTION',/)
 2011 FORMAT(7X,'PARAMETERS FOR THE ',I2,'-',I2,' INTERACTION MAY NOT BE
     1 RELIABLE IN WHOLE CONCENTRATION RANGE, SEE REF. 3',/,
     27X,'THESE PARAMETERS ARE USED FOR THE ',I2,'-',I2,' SECCNDARY GROU
     3P INTERACTION',/)
 2012 FORMAT(7X,'PARAMETERS FOR THE ',I2,'-',I2,' INTERACTION WERE OBTAI
     1NED FROM GAS CHROMATOGRAPHIC DATA, SEE REF. 4',/,
     27X,'THESE PARAMETERS ARE USED FOR THE ',I2,'-',I2,' SECCNDARY GROU
     3P INTERACTION',/)
C
      RETURN
```

```
      END
      SUBROUTINE SWITCH
C
C     SUBROUTINE IS USED BY SETTING IPSET TO EITHER 1 OR 2
C     AND THEN CALLING SWITCH.
C     IF IPSET=1 LOAD FIRST SET OF DATA (VLE PARAMETERS)
C     IF IPSET=2 LOAD SECOND SET OF DATA (LLE PARAMETERS)
C
C     THIS SUBROUTINE LOADS AND UNLOADS PROPER PARAMETERS
C     RESTORE VLE PARAMETERS IN THE C ARRAY
C     LOAD LLE PARAMETERS IN THE C ARRAY
C
      COMMON  /BLANK/  NCR, NPRT, NSTART, KUNITS, TITLE(20)
      COMMON  /CMPRO/  NC, NCM1, NCP1, IDLL, IDLV, IDH, LDBUG, ISW,
     *                 NDIM, ZNAME(2,10), L(10), NTCOMP(10), NLIQ, IPSET
      COMMON  /ZDATA/  CPL(10,4), CPV(10,4), ENP(10,10), ANT(6,10),
     *                 W(10), AX, BX, OMEGA(10), AVAL(10), BVAL(10),
     *                 AK(10,10), R(10), Q(10), QP(10), XL(10),
     *                 VOL(10), C(180), ALPHA(45), VC(10), TC(10),
     *                 PC(10), ZC(10), TNBP(10), OA(10), OB(10),
     *                 A(10,10), G(10,10), ZRA(10), RD(10), DMU(10),
     *                 ETA(10)
      COMMON /SWITCH/  CSTORE(180,2), ASTORE(45,2), ISTORE(2)
C
C......................................................................
C
C     IPSET = 0 ... NO ENTRY TO THIS SUBROUTINE
C     IPSET = 1 ... VLE PARAMETERS TO BE LOADED
C     IPSET = 2 ... LLE PARAMETERS TO BE LOADED
C     IPSET = 3 ... NOT YET DEFINED
C
      IF (IPSET .EQ. 0 .OR. IPSET .GE. 3) RETURN
      IF (ISTORE(1) .EQ. 0 .AND. ISTORE(2) .EQ. 0) RETURN
      IF (ISTORE(2) .EQ. 0) IPSET=1
C
C     ISTORE PRESERVES VALUES OF IDLL.
C     CSTORE AND ASTORE KEEP THE C AND ALPHA VALUES IN THE VECTORS
C     CORRESPONDING TO THE IPSET VALUE AS COLUMN NUMBER.
C
      IDLL = ISTORE (IPSET)
C
  600 J=NC*NCM1*2
      DO 620 I1=1,J,8
      I2=I1+7
      IF (I2.GT.J) I2=J
      DO 610 I=I1,I2
  610 C(I)=CSTORE(I,IPSET)
  620 CONTINUE
      IF (IDLL .NE. 4) GO TO 650
      J=NC*NCM1/2
      DO 650 I1=1,J,8
      I2=I1+7
      IF (I2.GT.J) I2=J
      DO 630 I=I1,I2
  630 ALPHA(I)=ASTORE(I,IPSET)
  650 CONTINUE
      RETURN
      END
      SUBROUTINE VIRFG1 (T,P,Y,VP,FUG,DHV)
C
```

```
C     VIRIAL EQUATION OF STATE USING THE HAYDEN - O'CONNELL METHOD
C
      COMMON  /CMPRO/  NC, NCM1, NCP1, IDLL, IDLV, IDH, LDBUG, ISW,
     *                 NDIM, ZNAME(2,10), L(10), NTCOMP(10), NLIQ, IPSET
      COMMON  /ZDATA/  CPL(10,4), CPV(10,4), ENP(10,10), ANT(6,10),
     *                 W(10), AX, BX, OMEGA(10), AVAL(10), BVAL(10),
     *                 AK(10,10), R(10), Q(10), QP(10), XL(10),
     *                 VCL(10), C(180), ALPHA(45), VC(10), TC(10),
     *                 PC(10), ZC(10), TNBP(10), DA(10), DB(10),
     *                 A(10,10), G(10,10), ZRA(10), RD(10), DMU(10),
     *                 ETA(10)
C
      REAL             Y(1), VP(1), FUG(1), B(10,10)
C
      DATA             RPVT/82.055/, EXPN/0.333333/
C
C....................................................................
C
C     OBTAIN THE VIRIAL COEFFICIENTS FROM 'BCALC'
C
      CALL BCALC (T,B)
C
C     OBTAIN B-MIX
C
      RT=RPVT*T
      PORT=P/RT
      SUMY=0.0
      BMIX=0.0
      DO 15 I=1,NC
      SUMY=SUMY+Y(I)
      DO 10 J=1,NC
   10 BMIX=BMIX+Y(I)*Y(J)*B(I,J)
   15 CONTINUE
      BMIX=BMIX/SUMY**2
C
      SQARG=0.25+BMIX*PORT
      IF (SQARG) 22,25,25
C
C     OBTAIN THE FUGACITY COEFFICIENT
C
C     IF BMIX*P/R/T IS MORE NEGATIVE THAN 0.25, THE PRESSURE SERIES
C     EQUATION MUST BE USED ... FTN STM #22.  THE ALTERNATE IS TOO USE
C     THE VOLUME SERIES ... FTN STM #25.
C
C     PRESSURE SERIES FORM OF THE VIRIAL EQUATION OF STATE
   22 VMIX=BMIX+1.0/PORT
      ZMIX=PORT*VMIX
      DO 24 I=1,NC
      SUMB=0.0
      DO 23 J=1,NC
   23 SUMB=SUMB+Y(J)*B(I,J)
      SUMB=SUMB/SUMY
C     PHI IS THE FUGACITY OF THE VAPOR & PHIS IS THE FUGACITY OF
C     THE SATURATED LIQUID EVALUATED AT THE VAPOR PRESSURE
      PHI=EXP((2.0*SUMB-BMIX)*PORT)
      PHIS=EXP(B(I,I)*VP(I)/RT)
      PONTY=EXP((P-VP(I))*VCL(I)/RT)
      FUG(I)=PHIS*PONTY/PHI
C     PRINT 300,I,PHIS,PONTY,PHI,FUG(I),Y(I),VP(I)
   24 CONTINUE
```

```
      GO TO 50
C
C     VOLUME SERIES FORM OF THE VIRIAL EQUATION OF STATE
   25 VMIX=(0.5+SQRT(SQARG))/PORT
      ZMIX=PORT*VMIX
      DO 40 I=1,NC
      SUMB=0.0
      DO 30 J=1,NC
   30 SUMB=SUMB+Y(J)*B(I,J)
      SUMB=SUMB/SUMY
C     PHI IS THE FUGACITY OF THE VAPOR & PHIS IS THE FUGACITY OF
C     THE SATURATED LIQUID EVALUATED AT THE VAPOR PRESSURE
      PHI=EXP(2.0*SUMB/VMIX)/ZMIX
      PHIS=EXP((B(I,I)*VP(I))/RT)
      PONTY=EXP((P-VP(I))*VOL(I)/RT)
      FUG(I)=PHIS*PONTY/PHI
C     PRINT 300,I,PHIS,PONTY,PHI,FUG(I),Y(I),VP(I)
C 300 FORMAT(I5,6G15.6)
   40 CONTINUE
C
C     EVALUATE THE VAPOR PHASE ENTHALPY DEPARTURE (NEGATIVE VALUE)
   50 DHV=1.9872*(ZMIX-1.0)
C     PRINT 400, DHV,T,P
C 400 FORMAT (5X,'DHV=',G15.6,'TEMP=',G15.6,'PRESS=',G15.6)
C
      RETURN
      END
      SUBROUTINE ZVIR1 (T,P,Y,ZMIX)
C
C     VIRIAL EQUATION OF STATE USING THE HAYDEN - O'CONNELL METHOD
C
      COMMON  /CMPRO/  NC, NCM1, NCP1, IDLL, IDLV, IDH, LDBUG, ISW,
     *                 NDIM, ZNAME(2,10), L(10), NTCOMP(10), NLIQ, IPSET
      COMMON  /ZDATA/  CPL(10,4), CPV(10,4), ENP(10,10), ANT(6,10),
     *                 W(10), AX, BX, OMEGA(10), AVAL(10), BVAL(10),
     *                 AK(10,10), R(10), Q(10), QP(10), XL(10),
     *                 VOL(10), C(180), ALPHA(45), VC(10), TC(10),
     *                 PC(10), ZC(10), TNBP(10), OA(10), OB(10),
     *                 A(10,10), G(10,10), ZRA(10), RD(10), DMU(10),
     *                 ETA(10)
C
      REAL             Y(1), B(10,10)
C
      DATA             RPVT/82.055/, EXPN/0.333333/
C
C...........................................................................
C
C     OBTAIN THE VIRIAL COEFFICIENTS FROM 'BCALC'
C
      CALL BCALC (T,B)
C
C     OBTAIN B-MIX
C
      RT=RPVT*T
      PORT=P/RT
      SUMY=0.0
      BMIX=0.0
      DO 15 I=1,NC
      SUMY=SUMY+Y(I)
      DO 10 J=1,NC
```

```
   10 BMIX=BMIX+Y(I)*Y(J)*B(I,J)
   15 CONTINUE
      BMIX=BMIX/SUMY**2
C
      SQARG=0.25+BMIX*PORT
      IF (SQARG) 22,25,25
C
C     IF BMIX*P/R/T IS MORE NEGATIVE THAN 0.25, THE PRESSURE SERIES
C     EQUATION MUST BE USED ... FTN STM #22.  THE ALTERNATE IS TOO USE
C     THE VOLUME SERIES ... FTN STM #25.
C
C     PRESSURE SERIES FORM OF THE VIRIAL EQUATION OF STATE
   22 VMIX=BMIX+1.0/PORT
      ZMIX=PORT*VMIX
      GO TO 50
C
C     VOLUME SERIES FORM OF THE VIRIAL EQUATION OF STATE
   25 VMIX=(0.5+SQRT(SQARG))/PORT
      ZMIX=PORT*VMIX
C
   50 RETURN
      END
      SUBROUTINE BCALC (T,B)
C
C     THIS PROGRAN BUILDS A MATRIX OF PURE COMPONENT AND
C     CROSS VIRIAL COEFFICIENTS, B(I,J) FOR UP TO 10
C     COMPONENTS
C
      COMMON  /CMPRO/  NC, NCM1, NCP1, IDLL, IDLV, IDH, LDBUG, ISW,
     *                 NDIM, ZNAME(2,10), L(10), NTCOMP(10), NLIQ, IPSET
      COMMON  /ZDATA/  CPL(10,4), CPV(10,4), ENP(10,10), ANT(6,10),
     *                 W(10), AX, BX, OMEGA(10), AVAL(10), BVAL(10),
     *                 AK(10,10), R(10), Q(10), QP(10), XL(10),
     *                 VOL(10), C(180), ALPHA(45), VC(10), TC(10),
     *                 PC(10), ZC(10), TNBP(10), DA(10), DB(10),
     *                 A(10,10), G(10,10), ZRA(10), RD(10), DMU(10),
     *                 ETA(10)
C
      REAL             PPC(2), RRD(2), DDMU(2), EETA(3), TTC(2),
     *                 ZZC(2), BB(3), B(10,10), ETM(10,10)
C
C     EQUIVALENCE THE SOLVATION PARAMETERS (ETM) OF THE VIRIAL
C     EQUATION OF STATE ... HAYDEN-O'CONNELL VERSION WITH THE
C     CHARACTERISTIC BINARY CONSTANTS (AK) OF THE VIRIAL EQUATION
C     OF STATE ... TSONOPOULOS VERSION
C
      EQUIVALENCE      (ETM(1,1),AK(1,1))
C
C......................................................................
C
C     THE PROGRAM CALLS SUBROUTINE SVIR ... FOR ACTUAL
C     GENERATION OF THE B-VALUES
C
C         PPC = CRITICAL PRESSURE IN ATMOSPHERES
C         TTC = CRITICAL TEMPERATURE IN K
C         RRD = MEAN RADIUS OF GYRATION IN A
C         DDMU = DIPOLE MOMENT IN DEBYE
C         EETA = ASSOCIATION PARAMETER FOR COMPONENT I
C         ZC = CRITICAL COMPRESSIBILITY FACTOR
C         ETM = SOLVATION PARAMETERS. EACH CARD CONTAINS
```

```
C                 THE SOLVATION PARAMETERS BETWEEN A
C                 GIVEN I = 1,NC-1 AND ALL J = I+1,NC
C
C
C     IN=NCM1
C     DO 11 I=1,IN
C     II=I+1
C     DO 11 J=II,NC
C  11 ETM(J,I)=ETM(I,J)
C     DO 12 I=1,NC
C  12 ETM(I,I)=EETA(I)
C
      N=2
      DO 32 I=1,NCM1
      II=I+1
      DO 32 J=II,NC
      K=1
      M=I
   23 PPC(K)=PC(M)
      RRD(K)=RD(M)
      DDMU(K)=DMU(M)
      EETA(K)=ETA(M)
      TTC(K)=TC(M)
      ZZC(K)=ZC(M)
      IF (K.EQ.2) GO TO 24
      K=2
      M=J
      GO TO 23
   24 ETA(3)=ETM(I,J)
C
      CALL SVIR (N,T,BB,PPC,RRD,DDMU,EETA,TTC,ZZC)
C
      B(I,I)=BB(1)
      B(J,J)=BB(2)
      B(I,J)=BB(3)
   32 B(J,I)=B(I,J)
C
      RETURN
      END
      SUBROUTINE SVIR (N,TEMP,BB,PC,RD,DMU,ETA,TC,ZC)
C
C     CALCULATION OF PURE COMPONENT AND CROSS VIRIAL COEFFICIENTS
C     FOR TWO COMPONENTS AT TEMPERATURE T FROM HAYDEN AND O'CONNELL
C     ... IEC PROC.DES.DEV.14(3)209(1975)
C
C        N = NUMBER OF COMPONENTS (1 OR 2)
C        BF = BFREE
C        BB = BTOTAL
C
C        NC = # OF COMPONENTS
C        PC = CRITICAL PRESSURE, ATM
C        RD = MEAN RADIUS OF GYRATION, A
C        DMU = DIPOLE MOMENT IN DEBYE
C        ETA(1) AND ETA(2) = ASSOCIATION PARAMETERS (PURE COMPONENTS)
C        ETA(3) = SOLVATION PARAMETER (CROSS INTERACTION)
C        TC = CRITICAL TEMPERATURE , DEG K
C        ZC = CRITICAL COMPRESSIBILITY FACTOR
C
      REAL              BF(3), BB(3), W(3), EPSI(3), RDMU(3), SIGM3(3),
     *                  RDMM(3), A(3), DELH(3), D(3), BD(3)
```

```
      REAL             PC(1), RD(1), DMU(1), ETA(1), TC(1), ZC(1)
C
      DATA             EXPN /0.333333/
C
C.......................................................................
C
C         CALCULATION OF COMPONENT PARAMETERS
C         EQ'S 15,30,17,24,25,23,21,22,10
C
      DO 101 I=1,N
      W(I)=0.006*RD(I)+0.02087*RD(I)**2-0.00136*RD(I)**3
      EPSI(I)=TC(I)*(0.748+0.91*W(I)-0.4*ETA(I)/(2.0+20.0*W(I)))
      SIGM3(I)=(2.44-W(I))**3*(TC(I)/PC(I))
      IF (DMU(I)-1.45) 101,101,103
  103 PN=16.0+400.0*W(I)
      C=2.882-1.882*W(I)/(0.03+W(I))
      XI=DMU(I)**4/(C*EPSI(I)*(SIGM3(I)**2)*TC(I)*5.723E-8)
      PPN=PN/(PN-6.0)
      EPSI(I)=EPSI(I)*(1.0-XI*PPN+PPN*(PPN+1.0)*(XI**2)/2.0)
      SIGM3(I)=SIGM3(I)*(1.0+3.0*XI/(PN-6.0))
  101 RDMU(I)=(DMU(I)**2)*7243.8/(EPSI(I)*SIGM3(I))
      IF (N-1) 300,300,400
  300 J=1
      GO TO 301
  400 J=3
      GO TO 401
C
C         NONPOLAR-NONPOLAR, EQ'S, 32,33,34
C         PARAMETERS FOR MIXTURE CALCULATION
C
  401 EPSI(3)=0.7*SQRT(EPSI(1)*EPSI(2))+0.60/(1.0/EPSI(1)+1.0/EPSI(2))
      SIGM3 (3)=SQRT(SIGM3(1)*SIGM3(2))
      W(3)=0.5*(W(1)+W(2))
      IF (DMU(1)*DMU(2)) 500,501,500
C
C         POLAR-NONPOLAR, EQ'S 38,24,36,37
C
  501 IF (DMU(1)+DMU(2)-2.0) 500,500,19
   19 XI38=(DMU(1)**2*(EPSI(2)**2*SIGM3(2))**EXPN*SIGM3(2)+DMU(2)**
     1 2*(EPSI(1)**2*SIGM3(1))**EXPN*SIGM3(1))/(EPSI(3)*SIGM3(3)**2)
      PN=16.0+400*W(3)
      EPSI(3)=EPSI(3)*(1.0+XI38*PN/(PN-6.0))
      SIGM3(3)=SIGM3(3)*(1.0-3.0*XI38/(PN-6.0))
C
C         POLAR-POLAR,EQ'S 35,37
C
  500 RDMU(3)=7243.8*DMU(1)*DMU(2)/(EPSI(3)*SIGM3(3))
  301 DO 600 I=1,J
      IF (RDMU(I)-0.04) 14,15,15
   14 RDMM(I)=RDMU(I)
      GO TO 600
   15 IF (RDMU(I)-0.025) 16,17,17
   16 RDMM(I)=0.0
      GO TO 600
   17 RDMM(I)=RDMU(I)-0.25
  600 CONTINUE
C
C         LAST PARAMETERS, EQ'S 7,8,9,29
C
      DO 609 I=1,J
```

```
      BO(I)=1.2618*SIGM3(I)
      A(I)=-0.3-0.05*RDMU(I)
      DELH(I)=1.99+0.2*RDMU(I)**2
      IF (ETA(I)-4.0) 604,604,605
 604  D(I)=650.0/(EPSI(I)+300.0)
      GO TO 609
 605  D(I)=42800.0/(EPSI(I)+22400.0)
 609  CONTINUE
C
C        CALCULATION OF VIRIAL COEFFICIENTS,EQ'S 14,13,26,6,29
C
      DO 651 I=1,J
      TSTR=EPSI(I)/TEMP-1.6*W(I)
      BFN=0.94-1.47*TSTR-0.85*TSTR**2+1.015*TSTR**3
      BFP=(0.75-3.0*TSTR+2.1*TSTR**2+2.1*TSTR**3)*RDMM(I)
      BF(I)=(BFN-BFP)*BO(I)
      BB(I)=BF(I)+BO(I)*A(I)*EXP(DELH(I)*EPSI(I)/TEMP)
      IF (ETA(I)) 651,651,653
 653  BCHEM=BO(I)*EXP(ETA(I)*(D(I)-4.27))*(1.0-EXP(1500.*ETA(I)/TEMP))
      BB(I)=BB(I)+BCHEM
 651  CONTINUE
      RETURN
      END
      SUBROUTINE UNQAC2 (T,X,GAM)
C
C     THIS ROUTINE USES THE MODIFIED UNIQUAC EQUATION AS DEVELOPED
C     BY ANDERSON (1978).  EQUATION USES MOLECULAR PARAMETERS R,
C     Q, AND Q', PLUS BINARY COMPONENTIAL PARAMETERS A(I,J) AND
C     A(J,I).
C
C     REFERENCE: "COMPUTER CALCULATIONS FOR MULTICOMPONENT
C     V-L AND L-L SYSTEMS" ... BY J. PRAUSNITZ ET. AL. (1980)
C
      COMMON  /CMPRO/  NC, NCM1, NCP1, IDLL, IDLV, IDH, LDBUG, ISW,
     *                 NDIM, ZNAME(2,10), L(10), NTCOMP(10), NLIQ, IPSET
      COMMON  /ZDATA/  CPL(10,4), CPV(10,4), ENP(10,10), ANT(6,10),
     *                 W(10), AX, BX, OMEGA(10), AVAL(10), BVAL(10),
     *                 AK(10,10), R(10), Q(10), QP(10), XL(10),
     *                 VOL(10), C(180), ALPHA(45), VC(10), TC(10),
     *                 PC(10), ZC(10), TNBP(10), CA(10), CB(10),
     *                 A(10,10), G(10,10), ZRA(10), RC(10), DMU(10),
     *                 ETA(10)
C
      REAL             X(1), GAM(1), THETA(10), THS(10), PHI(10),
     1                 THETAP(10)
C
C.....................................................................
C
      IF (ISW.NE.0) GO TO 20
C
C     RT=1.9872*T
      K=0
      DO 10 I=1,NCM1
      IP1=I+1
      DO 10 J=IP1,NC
      K=K+4
      G(I,J)=EXP(-(C(K-3)+C(K-2)*T)/T)
      G(J,I)=EXP(-(C(K-1)+C(K)*T)/T)
   10 CONTINUE
C
```

```
   20 THETS=0.0
      THETPS=0.0
      PHS=0.0
      XLS=0.0
      DO 30 I=1,NC
      THETS=THETS+Q(I)*X(I)
      THETPS=THETPS+QP(I)*X(I)
      PHS=PHS+R(I)*X(I)
   30 XLS=XLS+XL(I)*X(I)
      DO 40 I=1,NC
      THETA(I)=Q(I)*X(I)/THETS
      THETAP(I)=QP(I)*X(I)/THETPS
   40 PHI(I)=X(I)*R(I)/PHS
C
C     TAU(I,J)=G(I,J)=EXP((A+B*T)/T)
C
      DO 50 I=1,NC
      THS(I)=0.0
      DO 50 J=1,NC
   50 THS(I)=THS(I)+THETAP(J)*G(J,I)
      DO 70 I=1,NC
      GA=ALOG(R(I)/PHS)+5.0*Q(I)*ALOG(Q(I)/R(I)*PHS/THETS)+
     *   XL(I)-R(I)/PHS*XLS
      GB=1.0-ALOG(THS(I))
      DO 60 J=1,NC
   60 GB=GB-THETAP(J)*G(I,J)/THS(J)
   70 GAM(I)=EXP(GA+QP(I)*GB)
C
      RETURN
      END
      SUBROUTINE XHUNQ2 (T,X,XSH)
C
C     THIS ROUTINE USES THE MODIFIED UNIQUAC EQUATION AS DEVELOPED
C     BY ANDERSON (1978).  EQUATION USES MOLECULAR PARAMETERS R,
C     Q, AND Q', PLUS BINARY COMPONENTIAL PARAMETERS A(I,J) AND
C     A(J,I).
C
C     REFERENCE: "COMPUTER CALCULATIONS FOR MULTICOMPONENT
C     V-L AND L-L SYSTEMS" ... BY J. PRAUSNITZ ET. AL. (1980)
C
      COMMON  /CMPRO/  NC, NCM1, NCP1, IDLL, IDLV, IDH, LDBUG, ISW,
     *                 NDIM, ZNAME(2,10), L(10), NTCOMP(10), NLIQ, IPSET
      COMMON  /ZDATA/  CPL(10,4), CPV(10,4), ENP(10,10), ANT(6,10),
     *                 W(10), AX, BX, OMEGA(10), AVAL(10), BVAL(10),
     *                 AK(10,10), R(10), Q(10), QP(10), XL(10),
     *                 VOL(10), C(180), ALPHA(45), VC(10), TC(10),
     *                 PC(10), ZC(10), TNBP(10), DA(10), DB(10),
     *                 A(10,10), G(10,10), ZRA(10), RD(10), DMU(10),
     *                 ETA(10)
C
      REAL             X(1), THETAP(10), HFAC(10), HHFA(10), HM(10)
C
C.....................................................................
C
      IF (ISW.NE.0) GO TO 20
C
      RGC=1.9872
      K=0
      DO 10 I=1,NCM1
      IP1=I+1
```

```
      DO 10 J=IP1,NC
      K=K+4
      G(I,J)=EXP(-(C(K-3)+C(K-2)*T)/T)
      G(J,I)=EXP(-(C(K-1)+C(K)*T)/T)
   10 CONTINUE
C
   20 XSH=0.0
      THETPS=0.0
      DO 30 I=1,NC
   30 THETPS=THETPS+QP(I)*X(I)
      DO 40 I=1,NC
   40 THETAP(I)=QP(I)*X(I)/THETPS
C
C     ARG=TAU(I,J)=G(I,J)=EXP((A+B*T)/T)
C
      DO 50 I=1,NC
      HFAC(I)=0.0
      HHFA(I)=0.0
      DO 50 J=1,NC
      ARG=G(J,I)
      HFAC(I)=HFAC(I)+THETAP(J)*ARG*ALOG(ARG)
   50 HHFA(I)=HHFA(I)+THETAP(J)*ARG
      DO 60 I=1,NC
   60 HM(I)=QP(I)*X(I)*HFAC(I)/HHFA(I)
      DO 70 I=1,NC
   70 XSH=XSH-RGC*HM(I)
C
      RETURN
      END
      SUBROUTINE UNIFAC (T,X,GAM)
C
      COMMON /UNFAC/   XMOL(11),COMLN(11),RESLN(11),ALGAC(11),
     1                 ACTCF(11),IDGP(6,11),NOGP(6,11),NGMOL(11),AL(11),
     2                 RI(11),QI(11),QGPI(6,11),QGP(11),PARM(11,11),
     3                 IID(11),GSUM(11),GG(11),TNAM(3,11)
      COMMON /UNFAC1/  GNAM(3,80),QQ(80),RR(80),PARAM(42,42),NKTAB(80),
     *                 KODE(42,42), NGPT, NSPS
C
      REAL             X(1), GAM(1)
      CHARACTER*4      MOL(5,11)
C
C...................................................................
C
      DO 10 J = 1, NSPS
      XMOL(J) = X(J)
   10 CONTINUE
      DO 65 I = 1,NGPT
      K=IID(I)
      K=NKTAB(K)
      DO 65 J = 1,NGPT
      L=IID(J)
      L=NKTAB(L)
      PARM (I,J)= EXP (-PARAM (K,L)/T)
   65 CONTINUE
C
C     COMPUTE COMBINATORIAL PORTION AND RELATED SUMS.
C
      RSUM = 0.
      QSUM = 0.
      DO 80 I=1,NGPT
```

```
 80 QGP(I) = 0.
    DO 95 J=1,NSPS
    RI(J) = 0.
    QI(J) = 0.
    K = NGMOL(J)
    DO 85 I=1,K
    A = NOGP(I,J)
    L = IDGP(I,J)
    M = IID(L)
    RI(J) = RI(J) + A*RR(M)
    QI(J) = QI(J) + A*QQ(M)
    QGPI(I,J) = A*QQ(M)
 85 QGP(L) = QGP(L) + QGPI(I,J)*XMOL(J)
    RSUM = RSUM + RI(J)*XMOL(J)
    QSUM = QSUM + QI(J)*XMOL(J)
    DO 90 I=1,K
 90 QGPI(I,J) = QGPI(I,J)/QI(J)
 95 CONTINUE
    DO 100 I=1,NGPT
100 QGP(I) = QGP(I)/QSUM
    SUML = 0.
    DO 105 J=1,NSPS
    AL(J) = 5.*(RI(J) - QI(J)) - RI(J) + 1.
105 SUML = SUML + AL(J)*XMOL(J)
    DO 120 J=1,NSPS
    CON1 = RI(J)/RSUM
    CON2 = QI(J)/QSUM
120 COMLN(J) = ALOG(CON1) + 5.*QI(J)*ALOG(CON2/CON1)
   1           + AL(J) - CON1*SUML

    COMPUTE RESIDUAL PORTION.

    DO 125 I=1,NGPT
    GSUM(I) = 0.
    DO 125 K=1,NGPT
125 GSUM(I) = GSUM(I) + PARM(K,I)*QGP(K)
    DO 135 I=1,NGPT
    SUM = 0.
    DO 130 K=1,NGPT
130 SUM = SUM + QGP(K)*PARM(I,K)/GSUM(K)
135 GG(I) = 1. - ALOG(GSUM(I)) - SUM
    DO 155 J=1,NSPS
    RESLN(J) = 0.
    K = NGMOL(J)
    DO 140 I=1,K
    M = IDGP(I,J)
    GSUM(I) = 0.
    DO 140 N=1,K
    L = IDGP(N,J)
140 GSUM(I) = GSUM(I) + PARM(L,M)*QGPI(N,J)
    DO 150 I=1,K
    SUM = 0.
    M = IDGP(I,J)
    DO 145 N=1,K
    L = IDGP(N,J)
145 SUM = SUM + QGPI(N,J)*PARM(M,L)/GSUM(N)
    JJ = IID(M)
    CONST = FLOAT(NOGP(I,J))*QQ(JJ)*(GG(M) - (1.-ALOG(GSUM(I))-SUM))
150 RESLN(J) = RESLN(J) + CONST
    ALGAC(J) = COMLN(J) + RESLN(J)
```

```
  155 ACTCF(J) = EXP(ALGAC(J))
       DO 157 J = 1,NSPS
  157  GAM(J) = ACTCF(J)
CC
CC     PRINT RESULTS OF MIXTURE CALCULATIONS.
CC
C      WRITE (6,2007)
C      DO 160 J=1,NSPS
CC 160 WRITE (6,2008) MOL(1,J),MOL(2,J),XMOL(J),ALGAC(J),ACTCF(J)
C  160 WRITE (6,2008) (MOL(K,J),K=1,5),XMOL(J),ALGAC(J),ACTCF(J)
CC
C  999 CALL EXIT
C      STOP
      RETURN
      END
```

SELECTED BIBLIOGRAPHY

Abrams, D.S., and Prausnitz, J.M., Journal of the American Institute of Chemical Engineers, Vol. 21, No. 1, January 1975, pp. 116-128.

Anderson, T.F., Abrams, D.S., and Grens, E.A.II, "Evaluation of Parameters for Nonlinear Thermodynamic Models", AIChE Journal, Vol. 24, No. 1, 1978, pp. 20-29.

Anderson, T.F., and Prausnitz, J.M., "Application of the UNIQUAC Equation to Calculation of Multicomponent Phase Equilibria. 1. Vapor-Liquid Equilibria", Industrial and Engineering Chemistry Process Design and Development, Vol. 17, October 1978, pp. 552-567.

Anderson, T.F., and Prausnitz, J.M., "Application of the UNIQUAC Equation to Calculation of Multicomponent Phase Equilibria. 2. Liquid-Liquid Equilibria", Ind. Eng. Chem. Process Des. Dev. Vol. 17, No. 4, 1978, pp. 561-567.

Berg, L., "Selecting the Agent for Distillation", Chemical Engineering Progress, Vol. 65, No. 9, 1969, pp. 52-57.

Black, C., "Distillation Modelling of Ethanol Recovery and Dehydration Processes For Ethanol and Gasohol", Chemical Engineering Progress, Sept. 1980, pp. 78-85.

Black, C, and Ditsler, D.E., "Extractive and Azeotropic Distillation", Advanced Chemical Series, Vol. 115, 1972, pp. 1-15.

Black, C., Golding, R.A., and Ditsler, D.E., "Extractive and Azeotropic Distillation", Advanced Chemical Series, Vol. 115, 1972, pp. 64-92.

Fabries, J.F. and Renon, H., "Method of Evaluation and Reduction of Vapor-Liquid Equilibrium Data of Binary Mixtures", AIChE Journal, Vol. 21, No. 4, July 1975, pp. 735-743.

Fredenslund, A., Jones, R.L., and Prausnitz, J.M.,"Group-Contribution Estimation of Activity Coefficients in Nonideal Liquid Mixtures", AIChE Journal, Vol. 21, No. 6, Nov., 1975, pp. 1086-1099.

Fredenslund, A., Gmehling, J., and Rasmussen, P., Vapor-Liquid Equilibria Using UNIFAC, Elsevier Scientific Publishing Company, Amsterdam, The Netherlands, 1977.

Gmehling, J. and Onken, U., Vapor-Liquid Equilibrium Data Collection, Vol. I, Part 1, DECHEMA, Frankfurt, W.Germany, 1977.

Gmehling, J., Rasmussen, P., and Fredenslund, A., "Vapor-Liquid Equilibria by UNIFAC Group Contribution. Revision and Extension. 2", Ind. Eng. Chem. Process Des. Dev., Vol. 21, 1982, pp. 118-127.

Hayden, J.G. and O'Connell, J.P., Industrial and Engineering Chemistry Process Design and Development, Vol. 14, No. 3, 1975, pp. 209.

Holland, C.D., Fundamentals of Multicomponent Distillation, McGraw-Hill Book Co., New York, 1981.

Keister, W., "Computer Simulation of Ethanol Dehydration by Azeotropic Distillation with Benzene", Paper No. 21d, presented at the winter AIChE Meeting, Feb. 28-March 3, 1982, Orlanda, Florida.

Knox, D., and Van Ness, H. C.,"A Model for Representation of G^E and H^E", Fluid Phase Equilibria, 15, 1984, pp. 267-285.

Magnussen, T., Rasmussen, P., and Fredenslund, A., "UNIFAC Parameter Table for Prediction of Liquid-Liquid Equilibria", American Chemical Society, Vol. 20, No. 2, 1981, pp.331-409.

Magnussen, T., Sorensen, J.M., Rasmussen, P. and Fredenslund, Aa, "Liquid-Liquid Equilibrium Data: Their Retrieval, Correlation and Prediction. Part III: Prediction", Fluid Phase Equilibria, 4, 1980, 151-163.

Marquardt, D. W., "An Algorithm for Least-Squares Estimation of Nonlinear Parameters", J. Soc. Indust. Appl. Math., Vol. 11, No. 2, June, 1963, pp. 431-441.

Naphtali, L.M., and Sandholm, D.P., "Multicomponent Seperation Calculations by Linearization", Journal of the American Institute of Chemical Engineers, Vol. 17, No. 1, January, 1971, pp. 148-153.

O'Connell, J.P., and Prausnitz, J.M., Industrial and Engineering Chemistry, Process Design and Development, Vol. 6, No. 2, April 1967, pp. 246-250.

Prausnitz, J.M., Molecular Thermodynamics of Fluid Phase Equilibria, Prentice-Hall, Inc., Englewood Cliffs, New Jersey, 1969.

Prausnitz, J.M., Anderson, T.F., Grens, E.A., Eckert, C.A., Hsieh, R., and O'Connell, J.P., Calculations for Multi Component Vapor-Liquid and Liquid-Liquid Equilibria, Prentice-Hall, Inc., Englewood Cliffs, New Jersey, 1980.

Prokopakis, G.J., Seider, W.D., and Ross, B.A., "Azeotropic Distillation Tower with Two Liquid Phases", in Proceedings of Engineering Foundation Conference entitled Foundations of Computer-Aided Process Design, Hennike, N.H., July, 1980, Vol. 2, pp. 239-269.

Rasmussen, P. and Fredenslund, Aa, "Vapor-Liquid Equilibria by UNIFAC Group Contribution. Revision and Extension. 2", Ind. Eng. Chem. Process Des. Dev., Vol. 21, 1982, pp. 118-127.

Reid, R.C., Prausnitz, J.M., and Sherwood, T.K., The Properties of Gases and Liquids, McGraw-Hill Book Company, New York, N.Y., 3rd Edition, 1977.

Renon, H., and Prausnitz, J.M., Journal of the American Institute of Chemical Engineers, Vol. 14, No. 1, January 1968, pp. 135-143.

Renon, H., and Prausnitz, J.M., Industrial and Engineering Chemistry, Process Design and Development, Vol. 8, No. 3, July, 1969, pp. 413-419.

Roche, E.C., Unpublished Work on Rigorous Multicomponent Distillation Calculation, 1978.

Roche, E.C., Unpublished Work on Nonideal Liquid Flash Calculations, 1977.

Siverman, N. and Tassios, D., "Prediction of Multicomponent Vapor-Liquid Equilibrium with the Wilson Equation: Effect of the Minimization Function and of the Quality of Binary Data", Ind. Eng. Chem. Process Des. Dev., 23, 1984, 586-589.

Sorensen, J.M., et al., Liquid-Liquid Equilibrium Data Collection, Vol. V, Part 1 & 2, DECHEMA, Frankfurt, W. Germany, 1979.

Sorensen, J.M., Magnussen, T., Rasmussen, P.and Fredenslund, Aa., "Liquid-Liquid Equilibrium Data: Their Retrieval, Correlation and Prediction. Part I: Retrieval", Fluid Phase Equilibria, Vol. 2, 1979, pp. 297-308.

Sorensen, J.M., Magnussen, T., Rasmussen, P.and Fredenslund, Aa., "Liquid-Liquid Equilibrium Data: Their Retrieval, correlation and prediction . Part II: Correlation", Fluid Phase Equilibria, Vol. 3, 1979, pp. 47-82.

Tsai, C.M., and Roche, E.C. Jr., "The Entrainer Effect on Azeotropic Distillation Column Design", Paper presented at summer AIChE meeting, May 21-23, 1984, Anahein, California.

Venkatesh, C. K., Paper presented at summer AIChE meeting, May 21-23, 1984, Anahein, California.

Weast, R. C., Handbook of Chemistry and Physics, CRC Press Inc., Cleveland, Ohio, 56 th edition, 1975-1976.

Yaws, C.L., Physical Properties, McGraw-Hill Book Company, New York, N.Y., 1977.