An industrial ethanol azeotropic distillation process: modeling, analysis, and simulation

Harpreet Singh Chawla

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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

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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 gratitude and extend his profound sense of respect to his faculty advisor, Prof. Edward C. Roche, Jr. for his precise guidance and cooperation. The author is grateful to Dr. Dana Knox of Chemical Engineering Department for his critical suggestions and providing microcomputer facility for text processing.

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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 coefficient 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 is 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. (1973). 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
\[ \ln \gamma_i = \ln \frac{\phi_i}{x_i} + \left( \frac{2}{Z} \right) q \ln \frac{\theta_i}{\hat{\phi}_i} + l_i - \frac{\phi_i}{x_i} \sum_j x_j \tau_{ji} - q_i' \ln \left( \sum_j \theta_j \tau_{ji} \right) + \]

\[ q_i' - q_i' \sum_j \sum_k \theta_j \tau_{kj} \]

(2.1)

Where

\[ \tau_{ji} = \exp \left( - \frac{a_{ji} + b_{ji}}{T} \right) \]

(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

\[ h^E = -RT^2 \sum_i x_i \left( \frac{\partial \ln \gamma_i}{\partial T} \right)_{p,x} \]

(2.2)

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

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

(2.3)

Where

\[ \tau_{ji} = \exp \left( - \frac{a_{ji} + b_{ji}}{T} \right) \]

(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

\[ \ln \gamma_i = \ln \gamma_i^C + \ln \gamma_i^R \]  

(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

\[ \ln \gamma_i^C = \ln \frac{\Theta_i}{x_i} + \left( \frac{Z}{2} \right) q_i \ln \frac{\Theta_i}{\phi_i} + l_i - \frac{\Theta_i}{x_i} \sum_j x_j l_j \]  

(2.5)

The residual part of the activity coefficient is computed as follows

\[ \ln \gamma_i^R = \sum_k v_{ki} (\ln \gamma_k - \ln \gamma_{k,i}) \]  

(2.6)

The activity coefficient \( \gamma_k \) is computed as follows

\[ \ln \gamma_k = Q_k \left[ 1 - \ln \left( \sum_m \beta_m \xi_{mk} \right) - \sum_m \left( \sum_n \frac{\beta_{mn} \xi_{km}}{\xi_{km}} \right) \right] \]  

(2.7)

The activity coefficient \( \ln \gamma_{k,i} \) is computed as follows

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

(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 (POFX2) 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:

\[ F = \sum_{i} \left( \frac{y_{1,i}}{K_{i}} \right) - 1.0 = 0.0 \quad (2.9) \]

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.

\[ F_1 = \sum (x_{1,i} - x_{2,i}) = \sum z_i \frac{1 - \frac{y_{1,i}}{y_{2,i}}}{R + \frac{z_{2,i}}{(1-R)}} = 0 \quad (2.10) \]

\[ F_2 = \sum (x_{1,i} - y_{1}) = \sum z_i \frac{1 - K_{x,i}}{R + \frac{z_{2,i}}{(1-R)}} = 0 \quad (2.11) \]

Where \( R = \frac{L_1}{(L_1+L_2)} \), 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. \( \frac{|x_1, i, y_1, i - x_2, i, y_2, i|}{x_2, i, y_2, i} \leq 1.0E-5 \)  \( (2.12) \)

B. \( \frac{|x_j, i - x_{j-1}, i|}{x_j, i} \leq 1.0E-5 \)  \( (2.13) \)

C. \( \sum |x_1, i, y_1, i - x_2, i, y_2, i| \leq 1.0E-3 \)  \( (2.14) \)

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:

\[
F_1 = \sum (x_1, i - y_1) = \sum \frac{z_i (1 - K_{1, i})}{W_i} = 0 \quad (2.15)
\]

\[
F_2 = \sum (x_1, i - x_2, i) = \sum \frac{z_i (1 - (K_{1, i} / K_{2, i}))}{W_i} = 0 \quad (2.16)
\]

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

\[
x_{1, i} = \frac{z_i}{W_i} \quad (2.18)
\]

\[
x_{2, i} = (z_i / W_i)(K_{1, i} / K_{2, i}) \quad (2.19)
\]

\[
y_i = (z_i / W_i)(K_{1, i}) \quad (2.20)
\]
\[ U = \frac{V}{F} \quad (2.21) \]

\( V, F, \) 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 0 or 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:

\[ H_F = U H_V + (1 - U) R H_{L1} + (1 - U) H_{L2} \quad (2.22) \]

where \( H_V = \sum h_{V,i} y_i + h_d \quad (2.23) \)

\[ H_{L1} = \sum h_{L,i} x_{1,i} + h_{1}^{\text{mix}} \quad (2.24) \]

\[ H_{L2} = \sum h_{L,i} x_{2,i} + h_{2}^{\text{mix}} \quad (2.25) \]
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 (APDTS)

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

\[ F_1(n,i) = (1 + \frac{S_L}{V_n})v_{n,i} + (1 + \frac{S_V}{V_n})v_{n-1,i} - f_{n,i} = 0 \]  \hspace{1cm} (2.26)

Equilibrium Relationship coupled with the Murphree stage efficiency, \( \eta_n \)

\[ F_2(n,i) = \eta_n \left( \frac{K_{n-1,i}V_n}{V_n} \right) v_{n,i} - v_{n,i} + \left( 1 - \eta_n \right) \frac{V_{n-1,i}}{V_n} = 0 \]  \hspace{1cm} (2.27)

Where the Murphree stage efficiency is defined by

\[ \eta_n = \frac{V_{n-1,i} - V_{n,i}}{K_{n-1,i}v_{n-1,i} - V_{n-1,i}} \]  \hspace{1cm} (2.28)
Subscript $n = \text{stage, } n = 1, 2, \ldots, N$

$i = \text{component, } i = 1, 2, \ldots, c$

$H = \text{vapor phase enthalpy}$

$h = \text{liquid phase enthalpy}$

$H_f = \text{feed enthalpy}$

$V = \text{total vapor flow}$

$v = \text{component vapor flow}$

$L = \text{total liquid flow}$

$l = \text{component liquid flow}$

$F = \text{total feed}$

$f = \text{component feed}$

$S^L = \text{liquid sidestream}$

$S^V = \text{vapor sidestream}$

$Q_n = \text{external heat exchanger}$

\textbf{Figure 2.1 Stage Configuration}
and the equilibrium constant is defined by

$$ K_{n,i} = \frac{Y_{i}^{1}}{y_{i}^{1}} = \frac{I_{i}^{f}}{P_{i}^{f}} $$

(2.29)

**Energy Balance**

$$ F_{3}(n) = (1 + \frac{S_{n}^{L}}{L_{n}})h_{n}^{F} + (1 + \frac{S_{n}^{V}}{V_{n}})h_{n}^{V} - h_{n-1}^{F} - h_{n+1}^{V} $$

$$ h_{n}^{F} - Q_{n} + h_{n+1}^{mix} = 0 $$

(2.30)

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

**Liquid Enthalpy**

$$ h_{n} = l_{i} \int_{T_{ref}}^{T} C_{PL}(T)dT + h_{n}^{mix} $$

(2.31)

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

**Vapor Enthalpy**

$$ H_{v} = v_{i} [\lambda_{i} + \int_{T_{ref}}^{T} C_{PV}(T)dT + \Delta H] $$

(2.32)

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

$ \lambda_{ref} $ = the component heat of vaporization
\[ \Delta H \quad = \text{the enthalpy correction due to pressure} \]

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, \(F_n\), 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 tridiagonal sparse matrix. The functions and variables in the form of vector are given below:

\[
\bar{F}(\bar{x}) = \begin{bmatrix} F_1 \\ F_2 \\ F_3 \end{bmatrix} = 0 \quad \bar{x} = \begin{bmatrix} \bar{l} \\ \bar{v} \\ \bar{T} \end{bmatrix}
\]

(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, \(\bar{x}^{m+1}\).

\[
\Delta x^{m+1} = - (\frac{dF}{dx})^{-1} F_m \quad \text{and} \quad \bar{x}^{m+1} = \bar{x}^m + \Delta x^{m+1}
\]

(2.35)

(2.36)

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 super-
critical, 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 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 pre-determined 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 Raoults 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**

<table>
<thead>
<tr>
<th>Serial No.</th>
<th>Entrainer</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Benzene</td>
</tr>
<tr>
<td>2</td>
<td>Cyclohexane</td>
</tr>
<tr>
<td>3</td>
<td>N-pentane</td>
</tr>
<tr>
<td>4</td>
<td>Cyclopentane</td>
</tr>
<tr>
<td>5</td>
<td>Methyl Cyclopentane</td>
</tr>
<tr>
<td>6</td>
<td>Isopentane</td>
</tr>
<tr>
<td>7</td>
<td>N-Hexane</td>
</tr>
<tr>
<td>8</td>
<td>2-Methyl Pentane</td>
</tr>
<tr>
<td>9</td>
<td>1-Hexene</td>
</tr>
<tr>
<td>10</td>
<td>Diethyl Ether</td>
</tr>
<tr>
<td>11</td>
<td>2,2-Dimethyl Pentane</td>
</tr>
<tr>
<td>12</td>
<td>2,2,3-Trimethyl Butane</td>
</tr>
</tbody>
</table>
(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)

<table>
<thead>
<tr>
<th>System</th>
<th>P mm Hg</th>
<th>A&lt;sub&gt;12&lt;/sub&gt;</th>
<th>A&lt;sub&gt;21&lt;/sub&gt;</th>
<th>A&lt;sub&gt;13&lt;/sub&gt;</th>
<th>A&lt;sub&gt;31&lt;/sub&gt;</th>
<th>A&lt;sub&gt;23&lt;/sub&gt;</th>
<th>A&lt;sub&gt;32&lt;/sub&gt;</th>
<th>α&lt;sub&gt;12&lt;/sub&gt;</th>
<th>α&lt;sub&gt;13&lt;/sub&gt;</th>
<th>α&lt;sub&gt;23&lt;/sub&gt;</th>
<th>α&lt;sub&gt;32&lt;/sub&gt;</th>
</tr>
</thead>
<tbody>
<tr>
<td>Benzene</td>
<td>760</td>
<td>-86.763</td>
<td>1289.908</td>
<td>282.332</td>
<td>1096.899</td>
<td>3820.954</td>
<td>2213.355</td>
<td>0.270</td>
<td>0.295</td>
<td>0.267</td>
<td></td>
</tr>
<tr>
<td>Diethyl Ether</td>
<td>3862.9</td>
<td>175.652</td>
<td>1932.235</td>
<td>633.869</td>
<td>-18.524</td>
<td>2022.547</td>
<td>390.447</td>
<td>0.295</td>
<td>0.275</td>
<td>0.283</td>
<td></td>
</tr>
</tbody>
</table>

---

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Table 3.3

**Binary VLE NRTL Interaction Parameters from Binary VLE Data**

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

Reference: Gmehling (1977)

<table>
<thead>
<tr>
<th></th>
<th>T (deg C)</th>
<th>P (mm Hg)</th>
<th>Interaction Parameters</th>
<th>Data Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cyclohexane</td>
<td>760</td>
<td>761.7739</td>
<td>1393.7993 0.4376</td>
<td>Yuan (1963)</td>
</tr>
<tr>
<td>n-Pentane</td>
<td>20</td>
<td>412.7546</td>
<td>1183.3812 0.2886</td>
<td>Ishii (1935)</td>
</tr>
<tr>
<td>Methyl Cyclo-pentane</td>
<td>760</td>
<td>644.0719</td>
<td>1564.8490 0.4320</td>
<td>Sinor (1960)</td>
</tr>
<tr>
<td>n-Hexane</td>
<td>760</td>
<td>603.0883</td>
<td>1179.2617 0.2887</td>
<td>Kudray-avtseva (1963)</td>
</tr>
</tbody>
</table>
Table 3.4

**Binary LLE NRTL Interaction Parameters**

*from Binary LLE Data*

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

Reference: Sorensen (1979)

<table>
<thead>
<tr>
<th>(3)</th>
<th>T (deg C)</th>
<th>Interaction Parameters</th>
<th>a_{13}</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>A_{13}</td>
<td>A_{31}</td>
</tr>
<tr>
<td>Cyclohexane</td>
<td>25</td>
<td>5644.6696</td>
<td>3589.5155</td>
</tr>
<tr>
<td>n-Pentane</td>
<td>25</td>
<td>5759.1208</td>
<td>3766.5572</td>
</tr>
<tr>
<td>Methyl Cyclopentane</td>
<td>25</td>
<td>5798.8608</td>
<td>4345.4580</td>
</tr>
<tr>
<td>n-Hexane</td>
<td>40</td>
<td>6769.9077</td>
<td>3302.3940</td>
</tr>
</tbody>
</table>

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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

<table>
<thead>
<tr>
<th>No. of Stages</th>
<th>NRTL</th>
<th>UNIFAC</th>
</tr>
</thead>
<tbody>
<tr>
<td>EtOH</td>
<td>Wtr</td>
<td>Entr</td>
</tr>
<tr>
<td>50</td>
<td>98.4074</td>
<td>2.4214E-8</td>
</tr>
<tr>
<td>45</td>
<td>98.4074</td>
<td>3.3175E-7</td>
</tr>
<tr>
<td>*</td>
<td>40</td>
<td>98.4075</td>
</tr>
<tr>
<td>35</td>
<td>98.4074</td>
<td>3.2188E-5</td>
</tr>
<tr>
<td>30</td>
<td>98.4072</td>
<td>3.1857E-5</td>
</tr>
<tr>
<td>25</td>
<td>98.4048</td>
<td>3.1485E-3</td>
</tr>
<tr>
<td>20</td>
<td>98.2433</td>
<td>0.0304</td>
</tr>
<tr>
<td>15</td>
<td>98.1628</td>
<td>0.2932</td>
</tr>
<tr>
<td>10</td>
<td>96.3264</td>
<td>2.5008</td>
</tr>
</tbody>
</table>

**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 therefore 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

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

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 $\alpha$ equals to a constant, $-1$. The modified UNIQUAC equation

$$\ln \gamma_i = \ln \frac{\phi_i}{x_i} + \left(\frac{z}{2}\right)q_i \ln \frac{\theta_i}{\phi_i} + l_i - \frac{\phi_i}{x_i} \sum_j x_j l_{ij} - q_i \ln \left(\sum_j \theta_j^i \tau_{ji}\right) +$$

$$q_i^j - q_i \sum_j \sum_k \frac{\theta_i}{\theta_i^k} \tau_{ij}$$

(2.1)

where

$$\tau_{ji} = \exp \left(-\frac{a_{ij} + b_{ij}/T}{T}ight)$$

(2.2)

41
was selected for the study because of the fact that it has two temperature independent parameters per binary embedded in the variable \( \tau \) 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:

- The selection of the main algorithm and the salient features of the developed software.
- 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

\[ \phi = \sum_{j=1}^{n} [Y_j - Z_j]^2 \] (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 FOPX. 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 \(1.0\times10^{-4}\) 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>
<thead>
<tr>
<th>VLE Func (VLEFN)</th>
<th>VLE Objective Function</th>
</tr>
</thead>
<tbody>
<tr>
<td>7</td>
<td>$z_j = \frac{1}{n} \sum_{i=1}^{n}</td>
</tr>
<tr>
<td>8</td>
<td>$z_j = \frac{1}{n} \sum_{i=1}^{n} \frac{</td>
</tr>
<tr>
<td>9</td>
<td>$z_j = \frac{1}{n} \sum_{i=1}^{n}</td>
</tr>
<tr>
<td>10</td>
<td>$z_j = \frac{1}{n} \sum_{i=1}^{n}</td>
</tr>
<tr>
<td>11</td>
<td>$z_j = \frac{1}{n} \sum_{i=1}^{n} \frac{</td>
</tr>
<tr>
<td>12</td>
<td>$z_j = \frac{1}{n} \sum_{i=1}^{n}</td>
</tr>
<tr>
<td>13</td>
<td>$z_j =</td>
</tr>
<tr>
<td>15</td>
<td>$z_j = \frac{</td>
</tr>
<tr>
<td>17</td>
<td>$z_j =</td>
</tr>
<tr>
<td>19</td>
<td>$z_j = \frac{</td>
</tr>
<tr>
<td>20</td>
<td>$z_j =</td>
</tr>
</tbody>
</table>
Table 4.1 (Contd.)

**Selected Objective Functions for VLE Data Regression**

<table>
<thead>
<tr>
<th>VLE Func (VLEPN)</th>
<th>VLE Objective Functions</th>
</tr>
</thead>
<tbody>
<tr>
<td>#</td>
<td></td>
</tr>
</tbody>
</table>

\[
21 \quad z_j = \left| T_e - T_c \right| + \frac{1}{n} \sum_{i=1}^{n} |y_{ei} - y_{ci}|
\]

\[
22 \quad z_j = \frac{\left| T_e - T_c \right|}{T_e} + \frac{1}{n} \sum_{i=1}^{n} |y_{ei} - y_{ci}|
\]

**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 \( \chi_j = 1.0 \times 10^{-8} \) 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

<table>
<thead>
<tr>
<th>LLEFN #</th>
<th>LLE Objective Functions</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>$z_j = \frac{1}{2n} \sum_{i=1}^{n} w_i^I</td>
</tr>
<tr>
<td>6</td>
<td>$z_j = \frac{1}{2n} \sum_{i=1}^{n} w_i^I</td>
</tr>
<tr>
<td>7</td>
<td>$z_j = \frac{1}{2n} \sum_{i=1}^{n} w_i^I \frac{</td>
</tr>
<tr>
<td>8</td>
<td>$z_j = \frac{1}{2n} \sum_{i=1}^{n} w_i^I \frac{</td>
</tr>
<tr>
<td>9</td>
<td>$z_j = \frac{1}{2n} \sum_{i=1}^{n} w_i^I \frac{</td>
</tr>
<tr>
<td>10</td>
<td>$z_j = \frac{1}{2n} \sum_{i=1}^{n} w_i^I</td>
</tr>
</tbody>
</table>
Table 4.2 (Contd.)

**Selected Objective Functions for LLE Data Regression**

<table>
<thead>
<tr>
<th>LLEFN #</th>
<th>LLE Objective Functions</th>
</tr>
</thead>
<tbody>
<tr>
<td>11</td>
<td>( Z_j = \frac{1}{2n} \sum_{i=1}^{n} w_i \frac{</td>
</tr>
</tbody>
</table>

\[
\frac{1}{2(n-2)} \sum_{i=1}^{n} \frac{|\beta^{I}_{ei} - \beta^{I}_{ci}|}{\beta^{I}_{ei} + \beta^{I}_{ci}}
\]

\(i \neq Ie, Ir\)

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

\(w^{I}_i = |1.0 + W \frac{|x^{I}_i - x^{I}_c|}{x^{I}_e}|\) and

\(w^{II}_i = |1.0 + W \frac{|x^{II}_i - x^{II}_c|}{x^{II}_e}|\)

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. \(\beta^{I}_i\) and \(x^{I}_i\) 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 DEHEMA 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**

<table>
<thead>
<tr>
<th>#</th>
<th>Binary Systems</th>
<th>Type</th>
<th>Condition</th>
<th>n</th>
<th>Reference</th>
<th>Case Series</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Ethanol-Water</td>
<td>VLE</td>
<td>760 mm Hg</td>
<td>34</td>
<td>Reider (1949)</td>
<td>04</td>
</tr>
<tr>
<td>2</td>
<td>Ethanol-Water</td>
<td>VLE</td>
<td>40 °C</td>
<td>13</td>
<td>Mertl (1949)</td>
<td>08</td>
</tr>
<tr>
<td>3</td>
<td>Ethanol-Benzene</td>
<td>VLE</td>
<td>750 mm Hg</td>
<td>9</td>
<td>Tyrer (1949)</td>
<td>06</td>
</tr>
<tr>
<td>4</td>
<td>Ethanol-Benzene</td>
<td>VLE</td>
<td>40 °C</td>
<td>11</td>
<td>Udovenko (1962)</td>
<td>09</td>
</tr>
<tr>
<td>5</td>
<td>Water-Benzene</td>
<td>LLE</td>
<td>25 °C</td>
<td>1</td>
<td>Polak (1962)</td>
<td>22</td>
</tr>
<tr>
<td>6</td>
<td>Water-Benzene</td>
<td>LLE</td>
<td>25 °C</td>
<td>1</td>
<td>Sorensen (1979)</td>
<td>23</td>
</tr>
<tr>
<td>7</td>
<td>Water-Benzene</td>
<td>LLE</td>
<td>35 °C</td>
<td>1</td>
<td>Sorensen (1979)</td>
<td>24</td>
</tr>
<tr>
<td>8</td>
<td>Water-Benzene</td>
<td>LLE</td>
<td>70 °C</td>
<td>1</td>
<td>Sorensen (1979)</td>
<td>25</td>
</tr>
</tbody>
</table>
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 4.5) predicts mean deviation in T and $y_i$ of the order of 0.13 °C and 0.88 mole % respectively. Mean deviations in T and $y_i$ are 0.1 °C 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 Isothermal 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

<table>
<thead>
<tr>
<th>Case No.</th>
<th>VLEFN</th>
<th>$T_{exp}$-$T_{calc}$ in deg C</th>
<th>$Y_{1exp}$-$Y_{1calc}$ in mole %</th>
<th>Inf. Dilution Activity Coeff</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Mean</td>
<td>Max</td>
<td>Mean</td>
</tr>
<tr>
<td>04A</td>
<td>7</td>
<td>0.38</td>
<td>0.93</td>
<td>0.534</td>
</tr>
<tr>
<td>04B</td>
<td>8</td>
<td>0.25</td>
<td>0.81</td>
<td>0.623</td>
</tr>
<tr>
<td>04C</td>
<td>9</td>
<td>0.22</td>
<td>0.77</td>
<td>0.655</td>
</tr>
<tr>
<td>04D</td>
<td>17</td>
<td>0.15</td>
<td>0.45</td>
<td>0.897</td>
</tr>
<tr>
<td>04E</td>
<td>19</td>
<td>0.15</td>
<td>0.43</td>
<td>0.902</td>
</tr>
<tr>
<td>04F</td>
<td>20</td>
<td>0.15</td>
<td>0.43</td>
<td>0.903</td>
</tr>
<tr>
<td>04G</td>
<td>21</td>
<td>0.13</td>
<td>0.56</td>
<td>0.883</td>
</tr>
</tbody>
</table>
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

<table>
<thead>
<tr>
<th>Case No.</th>
<th>VLEFN #</th>
<th>( T_{\text{exp}} - T_{\text{cal}} ) in deg C</th>
<th>( Y_{1\text{exp}} - Y_{1\text{cal}} ) in mole %</th>
<th>Inf. Dilution Activity Coeff</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Mean</td>
<td>Max</td>
<td>Mean</td>
</tr>
<tr>
<td>06A</td>
<td>7</td>
<td>0.33</td>
<td>0.68</td>
<td>0.624</td>
</tr>
<tr>
<td>06B</td>
<td>8</td>
<td>0.44</td>
<td>0.75</td>
<td>0.749</td>
</tr>
<tr>
<td>06C</td>
<td>9</td>
<td>0.46</td>
<td>0.76</td>
<td>0.769</td>
</tr>
<tr>
<td>06D</td>
<td>17</td>
<td>0.11</td>
<td>0.26</td>
<td>0.668</td>
</tr>
<tr>
<td>06E</td>
<td>19</td>
<td>0.12</td>
<td>0.26</td>
<td>0.685</td>
</tr>
<tr>
<td>06F</td>
<td>20</td>
<td>0.12</td>
<td>0.26</td>
<td>0.685</td>
</tr>
<tr>
<td>06G</td>
<td>21</td>
<td>0.10</td>
<td>0.36</td>
<td>0.579</td>
</tr>
</tbody>
</table>
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 °C 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 $y_i^*$ 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.  
No. of data points = 13  
(1972)

<table>
<thead>
<tr>
<th>Case No.</th>
<th>VLEFN #</th>
<th>(P_{\text{exp}} - P_{\text{cal}}) in mm Hg</th>
<th>(Y_{1\text{exp}} - Y_{1\text{cal}}) in mole %</th>
<th>Inf. Dilution Activity Coeff</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Mean</td>
<td>Max</td>
<td>Mean</td>
</tr>
<tr>
<td>08A*</td>
<td>7</td>
<td>1.89</td>
<td>8.60</td>
<td>0.529</td>
</tr>
<tr>
<td>08B*</td>
<td>8</td>
<td>1.67</td>
<td>8.69</td>
<td>0.561</td>
</tr>
<tr>
<td>08C</td>
<td>9</td>
<td>1.66</td>
<td>8.72</td>
<td>0.564</td>
</tr>
<tr>
<td>08D*</td>
<td>10</td>
<td>1.85</td>
<td>7.93</td>
<td>0.577</td>
</tr>
<tr>
<td>08E</td>
<td>11</td>
<td>1.74</td>
<td>8.35</td>
<td>0.541</td>
</tr>
<tr>
<td>08F*</td>
<td>12</td>
<td>1.72</td>
<td>8.32</td>
<td>0.560</td>
</tr>
<tr>
<td>08G*</td>
<td>13</td>
<td>1.74</td>
<td>8.24</td>
<td>0.559</td>
</tr>
<tr>
<td>08H*</td>
<td>15</td>
<td>2.09</td>
<td>7.25</td>
<td>0.673</td>
</tr>
</tbody>
</table>

**Note:** '//' means unconverted 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

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

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
Table 4.8

**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**

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

* $(X_{i, \text{exp}} - X_{i, \text{calc}})/X_{i, \text{exp}} \times 100$
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: \( P = 760 \text{ mm Hg} \)

Gamma Model: Modified UNIQUAC  
Phi Model: Virial EOS

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

<table>
<thead>
<tr>
<th>Case</th>
<th>VLE Interaction Parameters, ( 0^\circ \text{K} )</th>
<th>( \Delta T )</th>
<th>( \Delta y_1 )</th>
<th>( \gamma^\infty )</th>
</tr>
</thead>
<tbody>
<tr>
<td>No.</td>
<td>-FN</td>
<td>Initial</td>
<td>Final</td>
<td>( ^{\circ} \text{C} )</td>
</tr>
<tr>
<td>#</td>
<td>( A_{12} )</td>
<td>( A_{21} )</td>
<td>( A_{12} )</td>
<td>( A_{21} )</td>
</tr>
<tr>
<td>04G</td>
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<td>1</td>
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<tr>
<td>04H</td>
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<td>500</td>
<td>500</td>
<td>-54.12</td>
</tr>
<tr>
<td>04I</td>
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</tr>
<tr>
<td>04J</td>
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<td>-500</td>
<td>-55.43</td>
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<tr>
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<td>-500</td>
<td>-500</td>
<td>-50.82</td>
</tr>
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<td>3000</td>
<td>-361.09</td>
</tr>
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<td>-361.09</td>
</tr>
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<td>8070.10</td>
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<td>04O</td>
<td>21</td>
<td>-3000</td>
<td>-3000</td>
<td>-57.02</td>
</tr>
</tbody>
</table>

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

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<th>Parameter</th>
<th>Phase Rich in 1</th>
<th>Phase Rich in 2</th>
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</thead>
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<tr>
<td></td>
<td>No.</td>
<td>Initial</td>
<td>Final</td>
<td>(1)</td>
</tr>
<tr>
<td></td>
<td>A_{12}</td>
<td>A_{21}</td>
<td>A_{12}</td>
<td>A_{21}</td>
</tr>
<tr>
<td>23A</td>
<td>1</td>
<td>1</td>
<td>392.17</td>
<td>424.59</td>
</tr>
<tr>
<td>23B</td>
<td>100</td>
<td>100</td>
<td>1332.69</td>
<td>354.44</td>
</tr>
<tr>
<td>23C</td>
<td>200</td>
<td>200</td>
<td>1335.51</td>
<td>354.21</td>
</tr>
<tr>
<td>23D</td>
<td>200</td>
<td>-200</td>
<td>1216.70</td>
<td>5192.00</td>
</tr>
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<td>23E</td>
<td>-200</td>
<td>-200</td>
<td>-145.93</td>
<td>-286.40</td>
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<tr>
<td>23F</td>
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<td>300</td>
<td>1325.14</td>
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<td>1150.50</td>
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<tr>
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<td>200</td>
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<tr>
<td>23J</td>
<td>1000</td>
<td>1000</td>
<td>1326.61</td>
<td>356.80</td>
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<tr>
<td>23K</td>
<td>1000</td>
<td>200</td>
<td>1326.94</td>
<td>356.69</td>
</tr>
<tr>
<td>23L</td>
<td>3000</td>
<td>3000</td>
<td>1217.13</td>
<td>9032.94</td>
</tr>
</tbody>
</table>

* (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 $y_1$'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 set: Ethanol-Water-Benzene (VLE, 760 mmHg)

<table>
<thead>
<tr>
<th>Case</th>
<th>Mean β (Max)</th>
<th>T and Y's</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>#</td>
<td>dev** in deg C</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Y1</td>
</tr>
<tr>
<td>03A*</td>
<td>0.28</td>
<td>2.101</td>
</tr>
<tr>
<td></td>
<td>(0.91)</td>
<td>(7.140)</td>
</tr>
<tr>
<td>03B#</td>
<td>0.29</td>
<td>1.953</td>
</tr>
<tr>
<td></td>
<td>(0.83)</td>
<td>(6.790)</td>
</tr>
<tr>
<td>03C+</td>
<td>0.33</td>
<td>1.242</td>
</tr>
<tr>
<td></td>
<td>(0.83)</td>
<td>(3.601)</td>
</tr>
<tr>
<td>03X+</td>
<td>4.65</td>
<td>7.007</td>
</tr>
<tr>
<td></td>
<td>(11.58)</td>
<td>(14.127)</td>
</tr>
</tbody>
</table>

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}) \times 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)

<table>
<thead>
<tr>
<th>Case</th>
<th>Mean &amp; (Max) Abs</th>
<th>Mean Abs. diff. in mole %</th>
<th>Data Sets used in the Regression</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(Te-Tc) deg C</td>
<td>Y₁</td>
<td>Y₂</td>
</tr>
<tr>
<td></td>
<td></td>
<td>System (a)</td>
<td>System (b)</td>
</tr>
<tr>
<td>70A</td>
<td>0.14</td>
<td>0.45</td>
<td>0.55</td>
</tr>
<tr>
<td>71A</td>
<td>-</td>
<td>0.48</td>
<td>0.33</td>
</tr>
<tr>
<td>72A</td>
<td>-</td>
<td>0.12</td>
<td>0.49</td>
</tr>
<tr>
<td>73A</td>
<td>0.14</td>
<td>0.12</td>
<td>0.62</td>
</tr>
<tr>
<td>74A</td>
<td>0.14</td>
<td>0.12</td>
<td>0.14</td>
</tr>
</tbody>
</table>

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)

<table>
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<tr>
<th>Case</th>
<th>Diff. of compositions in mole %, Mean</th>
<th>Mean diff of</th>
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<td>#</td>
<td>Phase Rich in (3)</td>
<td>Phase Rich in (2)</td>
</tr>
<tr>
<td></td>
<td>(1)</td>
<td>(2)</td>
</tr>
<tr>
<td>21B</td>
<td>0.693</td>
<td>0.634</td>
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<td>21C</td>
<td>1.755</td>
<td>3.605</td>
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<table>
<thead>
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<th>Case</th>
<th>Initial Binary Interaction Parameters in deg K</th>
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</tr>
<tr>
<td>21A*</td>
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</tr>
<tr>
<td>21B</td>
<td>1.0</td>
</tr>
<tr>
<td>21C</td>
<td>-19.16</td>
</tr>
</tbody>
</table>

* unconverged case

+ Difference = (X_{i exp} - X_{ical}) / X_{i exp} * 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**

<table>
<thead>
<tr>
<th>Case</th>
<th># of series</th>
<th>Data sets used</th>
<th># of tie cases</th>
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<th>LLEFN</th>
<th>Variable</th>
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<td></td>
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<td>Group I</td>
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<td>40</td>
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<td>21</td>
<td>8</td>
<td>W</td>
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<tr>
<td>41</td>
<td>5</td>
<td>a + b + g</td>
<td><strong>All</strong></td>
<td>21</td>
<td>8</td>
<td>W</td>
</tr>
<tr>
<td>42</td>
<td>3</td>
<td>a + b + g</td>
<td>1</td>
<td>21</td>
<td>11</td>
<td>W</td>
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<tr>
<td>43</td>
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<td>21</td>
<td>11</td>
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<tr>
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<td>46</td>
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<td>8</td>
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<td>9</td>
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<tr>
<td>49</td>
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<td>9</td>
<td>11</td>
<td>W</td>
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<td>W</td>
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<td>51</td>
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<tr>
<td>53</td>
<td>4</td>
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<td><strong>All</strong></td>
<td>10</td>
<td>11</td>
<td>W</td>
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</table>

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<table>
<thead>
<tr>
<th>Case</th>
<th># of Data sets used</th>
<th># of tie series cases</th>
<th>Regression lines</th>
<th>VLEFN</th>
<th>LLEFN</th>
<th>Variables</th>
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<td>60</td>
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<td>W</td>
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<td>21</td>
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<td>W</td>
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<td>All</td>
<td>21</td>
<td>11</td>
<td>W</td>
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<tr>
<td>66</td>
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<td>f + g</td>
<td>All</td>
<td>21</td>
<td>11</td>
<td>W</td>
</tr>
</tbody>
</table>

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 °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 °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 be-
cause 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

<table>
<thead>
<tr>
<th>Stream</th>
<th>Rate lbmole/hr</th>
<th>Composition in mole %</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Ethanol</td>
<td>Water</td>
<td>Benzene</td>
</tr>
<tr>
<td>Entrainer(E)</td>
<td>279.5856</td>
<td>28.104</td>
<td>11.771</td>
<td>60.125</td>
</tr>
<tr>
<td>Feed (F)</td>
<td>115.1506</td>
<td>82.820</td>
<td>17.180</td>
<td>0.0</td>
</tr>
</tbody>
</table>

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

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Table 4.15 (Contd)

**Performance of Azeotropic Column with Various Sets of Modified UNIQUAC Parameters**

**Major fixed conditions**

<table>
<thead>
<tr>
<th>Stream</th>
<th>Rate</th>
<th>Composition in mole %</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>lb mole/hr</td>
<td>Ethanol</td>
</tr>
<tr>
<td>Entrainer (E)</td>
<td>279.5856</td>
<td>28.104</td>
</tr>
<tr>
<td>Feed (F)</td>
<td>115.1506</td>
<td>82.820</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Case</th>
<th>Dist</th>
<th>% Diff</th>
<th>Distillate Comp.</th>
<th>Bottoms Composition</th>
</tr>
</thead>
<tbody>
<tr>
<td># (D) Rate of</td>
<td></td>
<td></td>
<td>EtOH</td>
<td>Wtr</td>
</tr>
</tbody>
</table>

| 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 °C with Various Sets of Modified UNIQUAC Parameters - I

Major fixed conditions

<table>
<thead>
<tr>
<th>Feed Composition in mole %</th>
<th>Temperature</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ethanol</td>
<td>Water</td>
</tr>
<tr>
<td>29.00</td>
<td>17.00</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Case</th>
<th>Frac1 % Diff</th>
<th>Benzene Phase</th>
<th>Water Phase</th>
</tr>
</thead>
<tbody>
<tr>
<td>#</td>
<td>in</td>
<td>EtOH</td>
<td>Wtr</td>
</tr>
<tr>
<td>(λ)</td>
<td>λ *</td>
<td></td>
<td></td>
</tr>
<tr>
<td>NRTL</td>
<td>0.8811</td>
<td>28.104</td>
<td>11.771</td>
</tr>
<tr>
<td>03X</td>
<td>0.8396</td>
<td>4.71</td>
<td>28.666</td>
</tr>
<tr>
<td>21C</td>
<td>0.8456</td>
<td>4.03</td>
<td>28.451</td>
</tr>
<tr>
<td>21X</td>
<td>0.7519</td>
<td>14.66</td>
<td>24.076</td>
</tr>
<tr>
<td>40A</td>
<td>0.8252</td>
<td>6.34</td>
<td>27.904</td>
</tr>
<tr>
<td>40B</td>
<td>0.8155</td>
<td>7.44</td>
<td>27.346</td>
</tr>
<tr>
<td>41A</td>
<td>0.8124</td>
<td>7.80</td>
<td>27.634</td>
</tr>
<tr>
<td>42A</td>
<td>0.8305</td>
<td>5.74</td>
<td>27.925</td>
</tr>
<tr>
<td>42D</td>
<td>0.8257</td>
<td>6.29</td>
<td>27.879</td>
</tr>
<tr>
<td>43B</td>
<td>0.8199</td>
<td>7.85</td>
<td>27.810</td>
</tr>
<tr>
<td>43C</td>
<td>0.7947</td>
<td>9.81</td>
<td>26.817</td>
</tr>
<tr>
<td>43D</td>
<td>0.8410</td>
<td>4.55</td>
<td>28.465</td>
</tr>
</tbody>
</table>
Table 4.16 (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

<table>
<thead>
<tr>
<th>Case</th>
<th>Frac % Diff in (λ)</th>
<th>Benzene Phase</th>
<th>Water Phase</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>EthOH</td>
<td>Wtr</td>
</tr>
<tr>
<td>43E</td>
<td>0.8147</td>
<td>7.54</td>
<td>27.912</td>
</tr>
<tr>
<td>43F</td>
<td>0.8166</td>
<td>7.32</td>
<td>27.806</td>
</tr>
<tr>
<td>47A</td>
<td>0.8050</td>
<td>8.64</td>
<td>27.297</td>
</tr>
<tr>
<td>49A</td>
<td>0.8200</td>
<td>6.93</td>
<td>27.600</td>
</tr>
<tr>
<td>50C</td>
<td>0.8126</td>
<td>7.77</td>
<td>27.175</td>
</tr>
<tr>
<td>53A</td>
<td>0.8244</td>
<td>6.44</td>
<td>27.989</td>
</tr>
<tr>
<td>53B</td>
<td>0.8175</td>
<td>7.26</td>
<td>28.094</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Parameters from case</th>
<th>Absolute difference in λ</th>
<th>Overall mean diff. in phase comp. in mole %</th>
</tr>
</thead>
<tbody>
<tr>
<td>03X</td>
<td>0.0415</td>
<td>5.4772</td>
</tr>
<tr>
<td>21C</td>
<td>0.0354</td>
<td>4.7427</td>
</tr>
<tr>
<td>21X</td>
<td>0.1292</td>
<td>6.1423</td>
</tr>
<tr>
<td>40A</td>
<td>0.0559</td>
<td>3.8038</td>
</tr>
<tr>
<td>40B</td>
<td>0.0665</td>
<td>3.1213</td>
</tr>
<tr>
<td>41A</td>
<td>0.0687</td>
<td>3.9567</td>
</tr>
<tr>
<td>41D</td>
<td>0.3287</td>
<td>20.6315</td>
</tr>
<tr>
<td>42A</td>
<td>0.0505</td>
<td>3.4835</td>
</tr>
<tr>
<td>42D</td>
<td>0.0554</td>
<td>3.6117</td>
</tr>
<tr>
<td>43B</td>
<td>0.0692</td>
<td>4.3940</td>
</tr>
<tr>
<td>43C</td>
<td>0.0863</td>
<td>3.9458</td>
</tr>
<tr>
<td>43D</td>
<td>0.0401</td>
<td>4.7218</td>
</tr>
<tr>
<td>43E</td>
<td>0.0664</td>
<td>4.4683</td>
</tr>
<tr>
<td>43F</td>
<td>0.0644</td>
<td>4.1710</td>
</tr>
<tr>
<td>47A</td>
<td>0.0761</td>
<td>3.3712</td>
</tr>
</tbody>
</table>
Table 4.17 (Contd)

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

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

<table>
<thead>
<tr>
<th>Parameters from case #</th>
<th>Absolute difference in ( \lambda )</th>
<th>Overall mean difference in phase comp. in mole %</th>
</tr>
</thead>
<tbody>
<tr>
<td>49A</td>
<td>0.0611</td>
<td>3.6703</td>
</tr>
<tr>
<td>50C</td>
<td>0.0685</td>
<td>3.8027</td>
</tr>
<tr>
<td>53A</td>
<td>0.0567</td>
<td>4.5048</td>
</tr>
<tr>
<td>53B</td>
<td>0.0640</td>
<td>4.8157</td>
</tr>
</tbody>
</table>

Where \( \lambda \) = 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

<table>
<thead>
<tr>
<th>Case Series</th>
<th>Acceptable Cases for Column</th>
<th>Decanter</th>
<th>Column &amp; Decanter</th>
</tr>
</thead>
<tbody>
<tr>
<td>#</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>03</td>
<td>03X</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>21</td>
<td>21C, 21X</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>40</td>
<td>40A, 40B</td>
<td>40A, 40B</td>
<td>40A, 40B</td>
</tr>
<tr>
<td>41</td>
<td>41A, 41D</td>
<td>41A</td>
<td>41A</td>
</tr>
<tr>
<td>42</td>
<td>42A, 42D</td>
<td>42A, 42D</td>
<td>42A, 42D</td>
</tr>
<tr>
<td>43</td>
<td>43B, 43C, 43D</td>
<td>43C</td>
<td>43C</td>
</tr>
<tr>
<td></td>
<td>43E, 43F</td>
<td></td>
<td></td>
</tr>
<tr>
<td>46</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>47</td>
<td>47A</td>
<td>47A</td>
<td>47A</td>
</tr>
<tr>
<td>48</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>49</td>
<td>49A</td>
<td>49A</td>
<td>49A</td>
</tr>
<tr>
<td>50</td>
<td>50C</td>
<td>50C</td>
<td>50C</td>
</tr>
<tr>
<td>51</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>52</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>53</td>
<td>53A, 53B</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>
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:

\[ A_{12} = -46.98 \quad A_{21} = 336.04 \quad A_{13} = -133.65 \quad A_{31} = 890.55 \]

\[ A_{23} = 187.00 \quad A_{32} = 1249.35 \]
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\degree 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**

<table>
<thead>
<tr>
<th>Stream</th>
<th>Rate</th>
<th>Composition in mole %</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>lb mole/hr</td>
<td>Ethanol</td>
</tr>
<tr>
<td>Entrainer(E)</td>
<td>698.9380</td>
<td>28.104</td>
</tr>
<tr>
<td>Feed(F)</td>
<td>115.1506</td>
<td>85.0</td>
</tr>
</tbody>
</table>

Entrainer/Feed Rate Ratio = 698.938/115.1506 = 6.0698

<table>
<thead>
<tr>
<th>Cas Dist #</th>
<th>D Rate</th>
<th>Distillate Comp.</th>
<th>Bottoms Composition</th>
</tr>
</thead>
<tbody>
<tr>
<td>E+F Ratio</td>
<td>EtOH Wtr Bz</td>
<td>EtOH Wtr Bz</td>
<td></td>
</tr>
<tr>
<td>(1) 2C1</td>
<td>760.0</td>
<td>0.9336 35.196 13.494 51.309 66.178 33.822 0.0</td>
<td></td>
</tr>
<tr>
<td>2C2</td>
<td>684.0</td>
<td>0.8402 28.230 17.668 54.102 84.710 0.259E-5 15.290</td>
<td></td>
</tr>
<tr>
<td>2C3</td>
<td>694.3</td>
<td>0.8528 28.504 17.407 54.089 87.958 0.167E-5 12.042</td>
<td></td>
</tr>
<tr>
<td>2C4</td>
<td>704.7</td>
<td>0.8656 28.786 17.150 54.064 91.799 0.114E-5 8.201</td>
<td></td>
</tr>
<tr>
<td>2C5</td>
<td>708.2</td>
<td>0.8699 28.873 17.065 54.063 93.315 0.104E-5 6.685</td>
<td></td>
</tr>
<tr>
<td>2C6</td>
<td>711.7</td>
<td>0.8743 28.958 16.980 54.062 94.949 0.976E-6 5.051</td>
<td></td>
</tr>
<tr>
<td>2C7</td>
<td>715.3</td>
<td>0.8786 29.038 16.895 54.067 96.748 0.978E-6 3.252</td>
<td></td>
</tr>
<tr>
<td>2C8</td>
<td>718.9</td>
<td>0.8830 29.125 16.811 54.064 98.635 0.113E-5 1.365</td>
<td></td>
</tr>
</tbody>
</table>

**Note:** All the rates and compositions are in lb moles/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 lbmole/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**

<table>
<thead>
<tr>
<th>Stream</th>
<th>Rate (lb mole/hr)</th>
<th>Composition in mole %</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Ethanol</td>
</tr>
<tr>
<td>Entrainer (E)</td>
<td></td>
<td>28.104</td>
</tr>
<tr>
<td>Feed (F)</td>
<td>115.1506</td>
<td>80.0</td>
</tr>
</tbody>
</table>

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

**Note:** All the rates and compositions are in lb moles/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*

<table>
<thead>
<tr>
<th>Stream</th>
<th>Rate (lb mole/hr)</th>
<th>Composition in mole %</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Ethanol</td>
<td>Water</td>
</tr>
<tr>
<td>Entrainer(E)</td>
<td>28.104</td>
<td>11.771</td>
<td>60.125</td>
</tr>
<tr>
<td>Feed(F)</td>
<td>115.1506</td>
<td>83.0</td>
<td>17.0</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th># Rate F</th>
<th>Btms Rate</th>
<th>1.495</th>
<th>Distillate Comp.</th>
<th>Bottoms Composition</th>
</tr>
</thead>
<tbody>
<tr>
<td>6C1 84.5</td>
<td>2.3750</td>
<td>29.149</td>
<td>16.993 53.858 99.152</td>
<td>0.1022 0.746</td>
</tr>
<tr>
<td>6C2 84.0</td>
<td>2.4359</td>
<td>29.265</td>
<td>16.876 53.859 99.049</td>
<td>0.304E-6 0.951</td>
</tr>
<tr>
<td>6C3 80.0</td>
<td>2.4605</td>
<td>29.311</td>
<td>16.830 53.859 98.839</td>
<td>0.137E-6 1.161</td>
</tr>
</tbody>
</table>

**Note:** All the rates and compositions are in lb moles/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

<table>
<thead>
<tr>
<th>Stream</th>
<th>Rate</th>
<th>Composition in mole %</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>lbmole/hr</td>
<td>Ethanol</td>
</tr>
<tr>
<td>Entrainer(E)</td>
<td>28.104</td>
<td>11.771</td>
</tr>
<tr>
<td>Feed(F)</td>
<td>115.1506</td>
<td>85.0</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>#</th>
<th>Rate</th>
<th>Btms E Rate F</th>
<th>Distillate Comp.</th>
<th>Bottoms Composition</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Etoh Wtr Bz</td>
<td>Etoh Wtr Bz</td>
<td></td>
</tr>
<tr>
<td>4C1</td>
<td>88.5</td>
<td>2.1711 29.696</td>
<td>16.453 53.873 97.157</td>
<td>1.4040 1.439</td>
</tr>
<tr>
<td>4C2</td>
<td>85.0</td>
<td>2.3554 29.798</td>
<td>16.325 53.877 99.174</td>
<td>0.811E-4 0.826</td>
</tr>
<tr>
<td>4C3</td>
<td>80.0</td>
<td>2.7531 30.582</td>
<td>15.501 53.917 99.091</td>
<td>0.540E-7 0.909</td>
</tr>
</tbody>
</table>

Note: All the rates and compositions are in lbmole/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

<table>
<thead>
<tr>
<th>Stream</th>
<th>Rate</th>
<th>Composition in mole %</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>lb mole/hr</td>
<td>Ethanol</td>
</tr>
<tr>
<td>Entrainer(E)</td>
<td>28.104</td>
<td>11.771</td>
</tr>
<tr>
<td>Feed(F)</td>
<td>115.1506</td>
<td>0.0</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>#</th>
<th>Etoh comp in F</th>
<th>Rate F</th>
<th>Etoh Rate</th>
<th>Btms Rate</th>
<th>E &amp; SF Ratio</th>
<th>Distillate Comp.</th>
<th>Bottoms Comp.</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>EtoH</td>
<td>Wtr</td>
<td>Bz</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5C1</td>
<td>70.00</td>
<td>60.0</td>
<td>4.1286</td>
<td>29.084</td>
<td>17.084</td>
<td>53.858</td>
<td>99.846</td>
</tr>
<tr>
<td>5C2</td>
<td>75.00</td>
<td>69.0</td>
<td>3.5000</td>
<td>29.171</td>
<td>16.971</td>
<td>53.859</td>
<td>99.421</td>
</tr>
<tr>
<td>5C3</td>
<td>77.50</td>
<td>74.0</td>
<td>3.1387</td>
<td>29.138</td>
<td>17.004</td>
<td>53.858</td>
<td>99.343</td>
</tr>
<tr>
<td>5C4</td>
<td>80.00</td>
<td>79.0</td>
<td>2.8000</td>
<td>29.135</td>
<td>17.007</td>
<td>53.858</td>
<td>99.070</td>
</tr>
<tr>
<td>5C5</td>
<td>82.50</td>
<td>84.1</td>
<td>2.4316</td>
<td>29.070</td>
<td>17.073</td>
<td>53.857</td>
<td>99.037</td>
</tr>
<tr>
<td>5C6</td>
<td>82.75</td>
<td>84.0</td>
<td>2.4413</td>
<td>29.183</td>
<td>16.958</td>
<td>53.859</td>
<td>99.002</td>
</tr>
<tr>
<td>5C7</td>
<td>82.82</td>
<td>84.0</td>
<td>2.4280</td>
<td>29.184</td>
<td>16.957</td>
<td>53.859</td>
<td>99.116</td>
</tr>
<tr>
<td>5C8</td>
<td>83.00</td>
<td>84.0</td>
<td>2.4359</td>
<td>29.265</td>
<td>16.876</td>
<td>53.859</td>
<td>99.049</td>
</tr>
<tr>
<td>5C9</td>
<td>83.50</td>
<td>84.9</td>
<td>2.3750</td>
<td>29.288</td>
<td>16.853</td>
<td>53.859</td>
<td>99.023</td>
</tr>
<tr>
<td>5CA</td>
<td>85.00</td>
<td>84.8</td>
<td>2.3700</td>
<td>29.831</td>
<td>16.290</td>
<td>53.879</td>
<td>99.162</td>
</tr>
<tr>
<td>5CB</td>
<td>89.40</td>
<td>99.0</td>
<td>1.4963</td>
<td>31.137</td>
<td>14.911</td>
<td>53.952</td>
<td>93.626</td>
</tr>
</tbody>
</table>

Note: All the rates and compositions are in lb moles/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 Azeotrope 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:
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)
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).

![Diagram](image)

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**

<table>
<thead>
<tr>
<th>Ser. #</th>
<th>P (psia)</th>
<th>Vapor Distillate</th>
<th>Bottoms</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>EtOH Wtr Bz</td>
<td>EtOH Wtr Bz</td>
</tr>
<tr>
<td>1</td>
<td>14.696</td>
<td>22.928 21.027 56.045</td>
<td>37.683 60.958 1.358</td>
</tr>
<tr>
<td>2</td>
<td>6.0</td>
<td>21.900 18.441 59.579</td>
<td>37.827 61.348 0.825</td>
</tr>
<tr>
<td>3</td>
<td>1.0</td>
<td>22.720 15.955 61.325</td>
<td>37.715 61.724 0.562</td>
</tr>
<tr>
<td>4</td>
<td>0.5</td>
<td>24.039 15.984 59.977</td>
<td>37.516 61.719 0.765</td>
</tr>
<tr>
<td>5</td>
<td>0.25</td>
<td>25.780 16.426 57.793</td>
<td>37.253 61.652 1.095</td>
</tr>
</tbody>
</table>

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).

Overhead Vapor
6.645 lbmoles/hr
25.296 mole % (E)
14.064 mole % (W)
60.641 mole % (B)

SBOX

Feed
47.145 lbmole/h

'Bummy Distillation Column Block'

37.474 mole % (E)
62.526 mole % (W)
0.0 mole % (B)

Bottoms

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

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

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).

![Diagram showing overhead vapor, SBOX block, feed, and bottoms]

Overhead Vapor

5.127 lbmoles/hr
26.554 mole % (E)
11.474 mole % (W)
61.971 mole % (B)

Feed

37.213 lbmole/h

SBOX

'Dummy Distillation Column Block'

37.220 mole % (E)
62.780 mole % (W)
0.0 mole % (B)

Bottoms

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

<table>
<thead>
<tr>
<th>Ser. P # (psia)</th>
<th>Vapor Distillate</th>
<th>Bottoms</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>EtOH</td>
<td>Wtr</td>
</tr>
<tr>
<td>1 14.696</td>
<td>22.936</td>
<td>21.025</td>
</tr>
<tr>
<td>2 6.0</td>
<td>22.000</td>
<td>18.445</td>
</tr>
<tr>
<td>3 1.0</td>
<td>22.761</td>
<td>15.976</td>
</tr>
<tr>
<td>4 0.5</td>
<td>24.029</td>
<td>15.979</td>
</tr>
<tr>
<td>5 0.35</td>
<td>24.887</td>
<td>16.165</td>
</tr>
<tr>
<td>6 0.25</td>
<td>25.765</td>
<td>16.165</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Distillation column performance with ABDIS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ser.</td>
</tr>
<tr>
<td>#</td>
</tr>
<tr>
<td>-----</td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Ser. P # (psia)</th>
<th>Vapor Distillate</th>
<th>Bottoms</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>EtOH</td>
<td>Wtr</td>
</tr>
<tr>
<td>1 14.696</td>
<td>22.028</td>
<td>21.019</td>
</tr>
<tr>
<td>2 6.0</td>
<td>23.633</td>
<td>18.925</td>
</tr>
<tr>
<td>3 1.0</td>
<td>25.375</td>
<td>17.177</td>
</tr>
</tbody>
</table>

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).

Overhead Vapor 5.447 lbmole/hr
24.799 mole % (E)
16.980 mole % (W)
58.221 mole % (B)

Feed 37.161 lbmole/hr
35.751 mole % (E)
55.716 mole % (W)
8.534 mole % (B)

SBOX BLOCK

'Dummy Distillation Column Block'

Bottoms

37.631 mole % (E)
62.369 mole % (W)
0.0 mole % (B)

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

<table>
<thead>
<tr>
<th>Ser. P</th>
<th>Vapor Distillate</th>
<th>Bottoms</th>
</tr>
</thead>
<tbody>
<tr>
<td># (psia)</td>
<td>EtOH</td>
<td>Wtr</td>
</tr>
<tr>
<td>--------</td>
<td>------</td>
<td>-----</td>
</tr>
<tr>
<td>1</td>
<td>22.930</td>
<td>21.021</td>
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<tr>
<td>2</td>
<td>23.040</td>
<td>18.744</td>
</tr>
<tr>
<td>3</td>
<td>24.858</td>
<td>16.931</td>
</tr>
</tbody>
</table>

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).

![Diagram showing overhead vapor, feed, SBOX block, and bottoms with mole percentages.]

Overhead Vapor 5.438 lbmoles/hr
23.320 mole % (E)  
18.342 mole % (W)  
58.339 mole % (B)

Feed 37.148 lbmole/h

35.751 mole % (E)  
55.716 mole % (W)  
8.533 mole % (B)

'SDummy Distillation Column Block'

37.883 mole % (E)  
62.117 mole % (W)  
0.0 mole % (B)

Bottoms

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

<table>
<thead>
<tr>
<th>Ser. P # (psia)</th>
<th>Vapor Distillate</th>
<th>Bottoms</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>EtOH</td>
<td>Wtr</td>
</tr>
<tr>
<td>1 14.696</td>
<td>22.931</td>
<td>21.019</td>
</tr>
<tr>
<td>2 5.0</td>
<td>23.262</td>
<td>18.444</td>
</tr>
<tr>
<td>3 4.8</td>
<td>23.320</td>
<td>18.387</td>
</tr>
<tr>
<td>4 4.0</td>
<td>23.556</td>
<td>18.145</td>
</tr>
</tbody>
</table>

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.

```
Overhead Vapor  4.913 lbmoles/hr
                  23.330 mole % (E)
                  11.992 mole % (W)
                  64.670 mole % (B)

35.751 mole % (E)
55.713 mole % (W)
8.535 mole % (B)

Feed 37.218
lb mole/h

SBOX
BLOCK

'Dummy Distillation
Column Block'

37.640 mole % (E)
62.360 mole % (W)
0.0 mole % (B)

Bottoms
```

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

<table>
<thead>
<tr>
<th>Ser. P</th>
<th>Vapor Distillate</th>
<th>Bottoms</th>
</tr>
</thead>
<tbody>
<tr>
<td># (psia)</td>
<td>EtOH</td>
<td>Wtr</td>
</tr>
<tr>
<td>1</td>
<td>14.696</td>
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<tr>
<td>2</td>
<td>1.0</td>
<td>22.714</td>
</tr>
<tr>
<td>3</td>
<td>0.5</td>
<td>24.037</td>
</tr>
<tr>
<td>4</td>
<td>0.25</td>
<td>25.767</td>
</tr>
<tr>
<td>5</td>
<td>0.1</td>
<td>28.352</td>
</tr>
</tbody>
</table>

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.

```
35.751 mole % (E)
55.715 mole % (W)
8.534 mole % (B)
```

```
Feed 37.364 lbmole/hr
```

```
'Dummy Distillation Column Block'
```

```
Overhead Vapor 4.951 lbmole/hr
16.180 mole % (E)
19.380 mole % (W)
64.630 mole % (B)
```

```
SBOX BLOCK
```

```
Bottoms
38.727 mole % (E)
61.242 mole % (W)
0.0 mole % (B)
```

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

<table>
<thead>
<tr>
<th>Ser. P # (psia)</th>
<th>Vapor Distillate</th>
<th>Bottoms</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>EtOH</td>
<td>Wtr</td>
</tr>
<tr>
<td>1 14.696</td>
<td>22.925</td>
<td>21.026</td>
</tr>
<tr>
<td>2 10.0</td>
<td>22.420</td>
<td>19.851</td>
</tr>
<tr>
<td>3 8.0</td>
<td>22.218</td>
<td>19.247</td>
</tr>
<tr>
<td>4 6.0</td>
<td>21.975</td>
<td>18.439</td>
</tr>
<tr>
<td>5 1.0</td>
<td>22.723</td>
<td>15.952</td>
</tr>
</tbody>
</table>

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.

![Diagram of SBOX block with distillation results]

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

<table>
<thead>
<tr>
<th>Ser. P</th>
<th>Vapor Distillate</th>
<th>Bottoms</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>EtOH</td>
<td>Wtr</td>
</tr>
<tr>
<td>-------</td>
<td>------</td>
<td>-----</td>
</tr>
<tr>
<td>1</td>
<td>14.696</td>
<td>22.935</td>
</tr>
<tr>
<td>2</td>
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<td>21.975</td>
</tr>
<tr>
<td>3</td>
<td>1.0</td>
<td>22.711</td>
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</tbody>
</table>

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.

![Diagram of benzene stripping section](image)

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

<table>
<thead>
<tr>
<th>Ser. P # (psia)</th>
<th>Vapor Distillate</th>
<th>Bottoms</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>EtOH Wtr Bz</td>
<td>EtOH Wtr Bz</td>
</tr>
<tr>
<td>1 14.696</td>
<td>22.919 21.023</td>
<td>56.054 37.700 60.970 1.329</td>
</tr>
<tr>
<td>2 0.5</td>
<td>24.041 15.982</td>
<td>59.989 37.515 61.743 0.732</td>
</tr>
</tbody>
</table>

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.

```
Overhead Vapor
  4.976 lbmoles/hr
  15.112 mole % (E)
  20.797 mole % (W)
  64.089 mole % (B)

35.750 mole % (E)
55.718 mole % (W)
  8.532 mole % (B)

Feed
  37.352 lbmole/hr

SBOX

'B dummy Distillation Column Block'

38.921 mole % (E)
61.079 mole % (W)
  0.0 mole % (B)

Bottoms
```

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

<table>
<thead>
<tr>
<th>Ser. P # (psia)</th>
<th>Vapor Distillate</th>
<th>Bottoms</th>
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</thead>
<tbody>
<tr>
<td></td>
<td>EtOH</td>
<td>Wtr</td>
</tr>
<tr>
<td>-----------------</td>
<td>-------</td>
<td>-------</td>
</tr>
<tr>
<td>2 6.0</td>
<td>21.976</td>
<td>18.440</td>
</tr>
<tr>
<td>3 1.0</td>
<td>22.713</td>
<td>15.952</td>
</tr>
</tbody>
</table>

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 standpoint 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 °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 for an industrial ethanol azeotropic distillation process using PROSIM as a tool, developed as part of the research. The simulation results are classified as shown below:

```
Simulation Results

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<tr>
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<tr>
<td>Concentrator</td>
<td>Concentrator</td>
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<td>(Case A)</td>
<td>(Case B)</td>
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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

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COMPONENTIAL FLOWRATES, LB-MOLES/UNIT TIME

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COMPONENTIAL FLOWRATES, LB-MOLES/UNIT TIME

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**COMPONENTIAL FLOWRATES, LB-MOLES/UNIT TIME**

| ETOH | 13.19192 | 11.97723 | 78.57763 | 0.00000 |
| WATER | 20.58685 | 19.83669 | 32.94643 | 0.00000 |
| BENZENE | 3.13598 | 0.00002 | 168.11349 | 0.80902 |
| TOTAL | 36.91476 | 31.80794 | 279.63757 | 0.80902 |

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**COMPONENTIAL FLOWRATES, LB-MOLES/UNIT TIME**

| ETOH | 1.35585 | 0.00000 | 83.34263 |
| 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

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COMPONENTIAL FLOWRATES, MOLES/UNIT TIME

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COMPONENTIAL FLOWRATES, MOLES/UNIT TIME

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**COMPONENTIAL FLOWRATES, MOLES/UNIT TIME**

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**COMPONENTIAL FLOWRATES, MOLES/UNIT TIME**

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<td>168.12692</td>
<td>0.79995</td>
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<tr>
<td>TOTAL</td>
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<td>279.76068</td>
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<td>95.0000</td>
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</table>

**COMPONENTIAL FLOWRATES, MOLES/UNIT TIME**

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</tr>
</thead>
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<td>WATER</td>
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</tr>
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<td>BENZENE</td>
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<td>0.79995</td>
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<tr>
<td>TOTAL</td>
<td>6.22930</td>
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<td>84.23215</td>
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</tbody>
</table>

**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 flow-schemes (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 Flowshe
(Case B)
The presence of 8.5 mole % benzene in the water phase from the two liquid phase decanter restricts the operability 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:

  o Process simulator -- expansion of the present version of PROSIM
  o 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.
5. Incorporation of the batch distillation model proposed by Clarke (1985) and Springer (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:


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

$$
\ln \gamma_i = \frac{\sum_{j} \tau_{ji} G_{ji} x_j}{\sum_{k} G_{ki} x_k} + \sum_{j} \frac{x_j G_{ji}}{\sum_{k} G_{kj} x_k} \left( \tau_{ij} - \frac{\sum_{k} \tau_{kj} G_{kj} x_k}{\sum_{k} G_{kj} x_k} \right) \quad (A.1)
$$

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

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

$a_{ij} = a_{ji}$ \quad (A.6)
A.1.2 Modified UNIQUAC Equation

For any component $i$, the activity coefficient is given by

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

(2.1)

where segment fraction $\phi$ and area fractions $\theta$ and $\theta'$ are given by

$$
\phi_i = \frac{r_i x_i}{\sum_j r_j x_j} \quad \theta_i = \frac{q_i x_i}{\sum_j q_j x_j}
$$

(A.7, A.8)

$$
\theta_i' = \frac{q_i' x_i}{\sum_j q_i' x_j} \quad l_j = \frac{Z}{2} (r_j - q_j) - (r_j - 1)
$$

(A.9, A.10)

A.1.3 UNIFAC Equation

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

$$
\ln \gamma_i = \ln \gamma_i^C + \ln \gamma_i^R
$$

(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

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

(2.5)

where

$$
l_i = \frac{Z}{2} (r_i - q_i) - (r_i - 1)
$$

(A.11)
\[
\begin{align*}
  r_i &= \sum v_{ki} R_k & q_i &= \sum v_{ki} Q_k \\
  \phi_i &= r_i x_i / \left( \sum_j r_j x_j \right) & \theta_i &= q_i x_i / \left( \sum_j q_j x_j \right)
\end{align*}
\]

(A.12, A.13)  

(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

\[
\ln \gamma_i^R = \sum_k v_{ki} (\ln \gamma_k - \ln \gamma_{k,i}) \tag{2.6}
\]

where the summation are over all groups, and  
\(\gamma_k\) = activity coefficient for group k in the mixture  
\(\gamma_{k,i}\) = activity coefficient for group k in pure component i

The activity coefficient \(\gamma_k\) is computed as follows

\[
\ln \gamma_k = Q_k \left[ 1 - \ln \left( \sum_m \beta_m \xi_{mk} \right) - \sum_m \left( \sum_n \beta_{mn} \xi_{km} \right) \right] \tag{2.7}
\]

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  
\(\xi_{mn} = \exp (-a_{mn}/T)\)  
\(a_{mn}\) = set of group interaction parameters, \(a_{mn} \neq a_{mn}\)

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

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

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

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

$$X_{mi} = \frac{v_{mi}}{\sum_n v_{ni}}, \text{ mole fraction of group } m \text{ in } i \quad (A.20)$$

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

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

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

then

$$h^E = R \sum_i \left[ \sum_j \frac{g_{ij} x_i}{\Theta_{ji} \gamma_{ji}} \Theta_{ji} \gamma_{ji} (a_{ji} + 2b_{ji}/T) \right] \quad (2.3)$$
### 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).

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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

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

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

Component Material Balance

\[
F_1(n,i) = (1 + \frac{S_n}{L_n}) l_{n,i} + (1 + \frac{S_n}{V_n}) v_{n,i} + v_{n-1,i} - l_{n+1,i} f_{n,i} = 0 \tag{2.26}
\]

Linearization of Equation 2.26 leads to

\[
- \Delta v_{n-1,i} + (1 + \frac{S_n}{L_n}) \Delta l_{n,i} - \frac{S_n}{V_n} l_{n,i} \sum_k \Delta l_{n,k} + (1 + \frac{S_n}{V_n}) \Delta v_{n,i} \\
- \frac{S_n}{V_n} l_{n,i} \sum_k \Delta v_{n,k} - \Delta l_{n+1,i} = -F_1(n,i) \tag{B.3}
\]
Equilibrium Relationship coupled with the Murphree stage efficiency, $\eta$

$$F_2(n,i) = \eta_n \frac{K_{iL_n} V_n}{L_n} l_{n,i} - V_{n,i} + (1 - \eta_n) \frac{V_n}{V_{n-1}} l_{n-1} = 0 \quad (2.27)$$

The above equation can be linearized as follows:

$$\begin{align*}
(1 - \eta_n) \frac{V_n}{V_{n-1}} l_{n-1} & - (1 - \eta_n) \frac{V_n}{V_{n-1}} k \sum_{k} \Delta v_{n-1,k} \\
+ \eta_n K_{n,i} \frac{V_n}{L_n} \Delta i_{n,i} - \eta_n K_{n,i} \frac{V_n}{L_n} \sum_{k} \Delta i_{n,k} \\
+ \eta_n K_{n,i} \frac{V_n}{L_n} \sum_{k} \Delta v_{n,k} + (1 - \eta_n) \frac{V_n}{V_{n-1}} \sum_{k} \Delta v_{n,k} \\
+ \eta_n \frac{V_n}{L_n} \sum_{k} \Delta i_{n,k} + \eta_n \frac{V_n}{L_n} \sum_{k} \Delta i_{n,k} \\
+ \eta_n \frac{V_n}{L_n} \sum_{k} \Delta i_{n,k} \\
+ \eta_n \frac{V_n}{L_n} \sum_{k} \Delta i_{n,k} \Delta T_n - \Delta v_{n,i} &= -F_2(n,i) \quad (B.4)
\end{align*}$$

Energy Balance

$$F_3(n) = (1 + \frac{S_{L_n}}{L_n}) h_n + (1 - \frac{S_{V_n}}{V_n}) h_n - h_{n-1} - h_{n+1} - h_F - Q_n +$$

$$h_{n_{mix}} - h_{n+1_{mix}} = 0 \quad (2.30)$$

Linearized Eq. 2.30 is given below:
\[
- \sum_{k} \frac{H_{n-1}}{V_{n-1,k}} \Delta V_{n-1,k} - \frac{\partial H_{n-1}}{\partial T_{n-1}} \Delta T_{n-1} + (1 + \frac{S_{n}}{L_{n}}) \sum_{k} \frac{\partial h_{n}}{\partial l_{n,k}} \Delta l_{n,k} \\
+ (1 + \frac{S_{n}}{L_{n}}) \frac{\partial h_{n}}{\partial T_{n}} \Delta T_{n} + (1 + \frac{S_{n}}{V_{n}}) \sum_{k} \frac{\partial h_{n}}{\partial v_{n,k}} \Delta v_{n,k} - \frac{S_{n}}{V_{n}} H_{n} \sum_{k} \Delta v_{n,k} \\
+ (1 + \frac{S_{n}}{V_{n}}) \frac{\partial h_{n+1}}{\partial T_{n+1}} \Delta T_{n+1} - \sum_{k} \frac{\partial h_{n+1}}{\partial l_{n+1,k}} \Delta l_{n+1,k} + \frac{\partial h_{n+1}}{\partial l_{n+1,1}} \Delta l_{n+1,1} + \\
\sum_{k} \frac{\partial h_{n+1}^{*}}{\partial l_{n,k}} \Delta l_{n,k} + \sum_{k} \frac{\partial h_{n+1}^{*}}{\partial T_{n}} \Delta T_{n} - \sum_{k} \frac{\partial h_{n+1}^{*}}{\partial l_{n+1,k}} \Delta l_{n+1,k} - \\
\sum_{k} \frac{\partial h_{n+1}^{*}}{\partial t_{n,k}} \Delta t_{n,k} = -F_{3}(n)
\]  

(B.5)

B.1.2 Solution Algorithm

Stagewise arrangement of linearized discrepancy functions result in the formation of tridiagonal matrix (N x N) 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

\[
B_{m-1}^{T} \ast S^{T} = A_{m}^{T}
\]  

(B.6)
Figure B1  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:

$$B_N \cdot S = D_N$$

The result of this operation is the set of flow and temperature corrections for the stage $N$.

- $C_m$ is eliminated in the process of back substitution for $m= N-1, N-2, \text{etc.}$ The process is thus:

  a) Eliminate $C$ by subtracting from $D$ the product of $C_m \cdot D_{m+1}$

  b) Perform Gaussian elimination on $B_m \cdot S=D_m$ 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, Ns, Nr, Ncase, Es, Er, Tt, Tb, Pt, Pb, AT, AF, F, N1, N2, N3, N4, Dv, Dl, R, Dc, IM, VF, IMA, 0.0.

IMA = Maximum value of iterations within ACTL block

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

B.2.2 ADFB - 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 separation 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**

\[ EQPAR(J,NE) = NE, N_S, N_R, Ncase, E_S, E_R, T_t, T_b, P_t, P_b, AT, \]
\[ \Delta F, F, N_1, S_{R1}, S_{R2}, S_{R3}, D_V, D_1, R, D_C, I_M, V_F, 2*0.0, \]

- **S_{R1}** = First reference stream number

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\[ S_{R2} = \text{Second reference stream number} \]
\[ S_{R3} = \text{Third reference stream number} \]

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
\[ V_F = \text{Vapor fraction in distillate} \]
\[ x_{di} = \text{Mole fraction guess of ith component in distillate} \]
\[ x_{bi} = \text{Mole fraction guess of ith component in bottoms} \]

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

\[ \geq 2 \text{ default mole fractions are used} \]

B.2.7 DIST - Rigorous Absorption/Distillation Package

\( EQPAR(J,NE) = NE, N_S, N_R, Ncase, E_S, E_R, T_t, T_b, P_t, P_b, \Delta T, \Delta F, F, N_1, N_2, N_3, N_4, D_v, D_1, R, D_C, I_M, V_F, 2*0.0, \)

\( NE = \text{Equipment block/node number} \)
\( N_S = \text{Number of stages in the stripping section} \)
\( N_R = \text{Number of stages in the rectifying section} \)
\( Ncase = \text{Type of process unit} \)

3 Distillation column (reflux ratio specified)
4 Distillation column (Boilup ratio specified)
5 Self refluxing column (Boilup ratio specified)
6 Self reboiling column (reflux ratio specified)

\( E_S = \text{Murphree stage efficiency stripping section} \)
\( E_R = \text{Murphree stage efficiency rectifying section} \)
\( T_t = \text{Temperature at top of column, } ^\circ F \)
\( T_b = \text{Temperature at bottom of column, } ^\circ F \)
\( P_t = \text{Pressure at top of column, } ^\circ F \)
\( P_b = \text{Pressure at bottom of column, } ^\circ F \)
\( \Delta T = \text{Temp. tolerance for convergence (default = 0.01)} \)
\( \Delta F = \text{Flow tolerance for convergence (default = 0.0005)} \)
\( F = \text{Number of feeds to the column (maximum of four)} \)
\( N_1 .. N_4 = \text{Stage for first to fourth feeds} \)
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, AT,
            AF, 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

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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, °F
P_d = Distillate pressure, psia
V_d = Distillate vapor fraction
T_b = Bottoms temperature, °F
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 stream temperature, °F
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
C.2 Sample Input and Azeotropic Column Results for Ethanol-Water-Cyclohexane System
C.3 Sample Input and Azeotropic Column Results for Ethanol-Water-Pentane System
C.4 Sample Input and Azeotropic Column Results for Ethanol-Water-Cyclopentane System
C.5 Sample Input and Azeotropic Column Results for Ethanol-Water-Methyl Cyclopentane System
C.6 Sample Input and Azeotropic Column Results for Ethanol-Water-Isopentane System
C.7 Sample Input and Azeotropic Column Results for Ethanol-Water-n-Hexane System
C.8 Sample Input and Azeotropic Column Results for Ethanol-Water-2-Methyl Pentane System
C.9 Sample Input and Azeotropic Column Results for Ethanol-Water-1 Hexene System
C.10 Sample Input and Azeotropic Column Results for Ethanol-Water-Diethyl Ether System
C.11 Sample Input and Azeotropic Column Results for Ethanol-Water-2,2-Dimethyl Pentane System
C.12 Sample Input and Azeotropic Column Results for Ethanol-Water-2,2,3-Trimethyl Butane System
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,
7.01, 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-01, -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  Azeotropic Distillation Column Bottoms Results

System: Ethanol - Water - Benzene

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

Variable Process Parameters: Pressure and Boilup ratio

<table>
<thead>
<tr>
<th>Case No.</th>
<th>Top Stage Pressure (psia)</th>
<th>Boilup Ratio</th>
<th>Bottoms Product Composition</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>Ethanol</td>
</tr>
<tr>
<td>4A5</td>
<td>12.0</td>
<td>6.015</td>
<td>98.3647</td>
</tr>
<tr>
<td>4A2 *</td>
<td>14.7</td>
<td>6.015</td>
<td>92.0354</td>
</tr>
<tr>
<td>4A3</td>
<td>30.0</td>
<td>6.015</td>
<td>70.9312</td>
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<tr>
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<td>4A13</td>
<td>12.0</td>
<td>5.113</td>
<td>99.4347</td>
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<tr>
<td>4A9</td>
<td>14.7</td>
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<td>97.9300</td>
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<tr>
<td>4A11</td>
<td>14.7</td>
<td>3.680</td>
<td>99.2402</td>
</tr>
</tbody>
</table>

* 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

<table>
<thead>
<tr>
<th>Stg #</th>
<th>( T(F) )</th>
<th>( (1) )</th>
<th>( (2) )</th>
<th>( (3) )</th>
<th>( T(F) )</th>
<th>( (1) )</th>
<th>( (2) )</th>
<th>( (3) )</th>
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</thead>
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<td>8.86</td>
<td>46.09</td>
<td>150.00</td>
<td>48.14</td>
<td>5.27</td>
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<td>46.97</td>
<td>6.91</td>
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<td>151.69</td>
<td>50.49</td>
<td>2.68</td>
<td>46.83</td>
</tr>
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<td>48.68</td>
<td>5.13</td>
<td>46.18</td>
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<td>51.74</td>
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<td>53.39</td>
<td>0.39E-8</td>
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<td>153.93</td>
<td>55.38</td>
<td>0.42E-8</td>
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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

<table>
<thead>
<tr>
<th></th>
<th>ETOH-WTR-CYHEXAN DEHYD: NCASE=5, UNIFAC &amp; VIRIAL VAPOR(EX #4B)</th>
<th></th>
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</thead>
<tbody>
<tr>
<td>3, 7, 1, 2, 0, 0, 0, 1, 0, 0, 0, 202.1, 351.1, -0.3499, 9.559E-03, -37.86E-06, 54.59E-09, 2.153, 5.513E-02, -2.004E-05, 0.328E-09, 12.0457, -3667.705, -46.976, 3*0.0, WATER</td>
<td>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, CYCLOHEXANE</td>
<td>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<em>0.0, 1.40, 1.55, 0.0, 1.55, 1.70, 0.0, 3</em>0.0, 3 ETHANOL</td>
</tr>
<tr>
<td>1, 1, 1, 2, 1, 15, 1, 17, 6, 2, ETOH-WTR-CYCLOHEXANE AZEO DIST COLUMN SIMULATION: UNIFAC</td>
<td>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,</td>
<td></td>
</tr>
</tbody>
</table>
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

<table>
<thead>
<tr>
<th>Case No.</th>
<th>Pressure Ratio (psia)</th>
<th>Boilup</th>
<th>Bottoms</th>
<th>Product Composition (mole%)</th>
</tr>
</thead>
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<td>Cyclohexane</td>
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* 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

<table>
<thead>
<tr>
<th>Stg #</th>
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<th>T(1)</th>
<th>T(2)</th>
<th>T(3)</th>
<th>T(F)</th>
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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

<table>
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</tr>
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<tr>
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<td>2 PENTANE</td>
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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

<table>
<thead>
<tr>
<th>Case No.</th>
<th>Top Stage Pressure (psia)</th>
<th>Boilup Ratio</th>
<th>Bottoms Product Composition (mole%)</th>
</tr>
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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

<table>
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<tr>
<td>5</td>
<td>212.88</td>
<td>78.714</td>
</tr>
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<td>4</td>
<td>213.07</td>
<td>78.133</td>
</tr>
<tr>
<td>3</td>
<td>213.29</td>
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</tr>
<tr>
<td>2</td>
<td>213.57</td>
<td>75.383</td>
</tr>
<tr>
<td>1</td>
<td>213.99</td>
<td>72.187</td>
</tr>
<tr>
<td>R</td>
<td>214.77</td>
<td>65.956</td>
</tr>
</tbody>
</table>

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, 2.1055, 1.9720, 0.92, 0.0, 0.0, 0.253,
2.25, 1.70, 1.40,
202.1, 351.1,
-0.0499, 9.559E-03, -37.86E-06, 54.59E-09,
2.153, 5.1313E-02, -2.004E-05, 0.3209E-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, 0.92, 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, 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,
9.224, -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, 9.59E-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,
MTCYCLOC5
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

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

<table>
<thead>
<tr>
<th>Stage #</th>
<th>T(F)</th>
<th>Liquid Phase Compositions in Mole %</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>(1)</td>
</tr>
<tr>
<td>40</td>
<td>184.24</td>
<td>30.001</td>
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<tr>
<td>39</td>
<td>184.88</td>
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<td>38</td>
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<td>29.166</td>
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<tr>
<td>37</td>
<td>185.38</td>
<td>44.966</td>
</tr>
<tr>
<td>36</td>
<td>187.30</td>
<td>47.298</td>
</tr>
<tr>
<td>35</td>
<td>188.73</td>
<td>48.706</td>
</tr>
<tr>
<td>34</td>
<td>189.67</td>
<td>49.472</td>
</tr>
<tr>
<td>33</td>
<td>190.24</td>
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<tr>
<td>32</td>
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<td>50.069</td>
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<tr>
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<td>190.86</td>
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<td>191.23</td>
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<td>50.393</td>
</tr>
<tr>
<td>22</td>
<td>192.26</td>
<td>50.410</td>
</tr>
<tr>
<td>21</td>
<td>192.41</td>
<td>50.427</td>
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<tr>
<td>20</td>
<td>192.55</td>
<td>50.444</td>
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<td>18</td>
<td>192.84</td>
<td>50.478</td>
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<td>17</td>
<td>192.98</td>
<td>50.495</td>
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<td>193.13</td>
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<td>50.528</td>
</tr>
<tr>
<td>14</td>
<td>193.41</td>
<td>50.545</td>
</tr>
<tr>
<td>12</td>
<td>193.69</td>
<td>50.578</td>
</tr>
<tr>
<td>11</td>
<td>193.83</td>
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<td>50.611</td>
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<tr>
<td>9</td>
<td>194.12</td>
<td>50.628</td>
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<td>8</td>
<td>194.26</td>
<td>50.644</td>
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<tr>
<td>7</td>
<td>194.40</td>
<td>50.661</td>
</tr>
<tr>
<td>6</td>
<td>194.54</td>
<td>50.681</td>
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<tr>
<td>5</td>
<td>194.68</td>
<td>50.747</td>
</tr>
<tr>
<td>4</td>
<td>194.82</td>
<td>51.364</td>
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<td>3</td>
<td>195.12</td>
<td>56.930</td>
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</tr>
<tr>
<td>1</td>
<td>210.70</td>
<td>92.643</td>
</tr>
<tr>
<td>R</td>
<td>221.09</td>
<td>98.345</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>ETOH-WTR-IPENTANE DEHYD. NCASE=5: UNIFAC &amp; VIRIAL (EX #4F)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3, 7, 1, 2, 0, 0, 0, 1, 0, 0, 0, 0, 0, 2.25, 1.70, 1.40,</td>
</tr>
<tr>
<td>202.1, 351.1, -0.3499, 9.599E-03, -37.86E-06, 54.59E-09,</td>
</tr>
<tr>
<td>2.153, 5.113E-02, -2.004E-05, 0.328E-09, 12.0457, -3667.705, -46.976, 3*0.0,</td>
</tr>
<tr>
<td>WATER</td>
</tr>
<tr>
<td>0.0, 0.0, 0.92, 1.40, 1.00, 0.0, 0.0, 0.238,</td>
</tr>
<tr>
<td>0.615, 1.84, 1.70, 538.7, 373.2, 0.6741, 2.825E-03, -8.371E-06, 8.601E-09,</td>
</tr>
<tr>
<td>7.701, 4.595E-04, 2.521E-06, -0.859E-09, 11.9516, -3984.923, -39.734, 3*0.0,</td>
</tr>
<tr>
<td>IPENTANE</td>
</tr>
<tr>
<td>0.0, 0.0, 3.82, 3.31, 3.31, 3.0, 0.0, 0.0, 0.2716,</td>
</tr>
<tr>
<td>3.313, 0.13, 0.0, 81.77, 301.0, -0.5019, 10.1929E-03, -36.5065E-06, 46.8004E-09,</td>
</tr>
<tr>
<td>-2.275, 1.210E-01, -6.519E-05, 1.367E-08, 9.0005, -2348.67, -40.05, 3*0.0,</td>
</tr>
<tr>
<td>1.40, 1.55, 0.0, 1.55, 0.0, 0.0, 3*0.0,</td>
</tr>
<tr>
<td>3 ETHANOL</td>
</tr>
<tr>
<td>3 ISOPENTANE</td>
</tr>
<tr>
<td>1, 1, 1, 2, 1, 15,</td>
</tr>
<tr>
<td>1, 17,</td>
</tr>
<tr>
<td>3, 1, 1, 2, 1, 3,</td>
</tr>
<tr>
<td>ETOH-WTR-IPENTANE AZEO DIST COLUMN SIMULATION: USING UNIFAC</td>
</tr>
<tr>
<td>5, 0, 40, 2, 0, 0, 30, 1, 0,</td>
</tr>
<tr>
<td>1.0, 0.0, 0.0, 726.9, 0.0, 6.015, 200.0, 230.0, 85.0, 0.10,</td>
</tr>
<tr>
<td>40, 0, 98, 0, 169.2, 22.65, 400.0,</td>
</tr>
<tr>
<td>37, 0, 96, 0, 191.9, 66.6, 0.0,</td>
</tr>
</tbody>
</table>
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 VAPOR (EX #4G)
3, 7, 1, 2, 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,
3.17, 351.1,
-0.3499, 9.559E-03, -37.86E-06, 54.59E-09,
2.15, 5.113E-02, -2.004E-05, 0.328E-09,
12.0457, -3667.705, -46.976, 3*0.0,

WATER
0, 0.0, 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,
11.951E, -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, 0.0, 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,
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

<table>
<thead>
<tr>
<th>Case No.</th>
<th>Top Stage Pressure (psia)</th>
<th>Boilup Ratio</th>
<th>Bottoms Product Composition (mole%)</th>
<th>Ethanol</th>
<th>Water</th>
<th>n-Hexane</th>
</tr>
</thead>
<tbody>
<tr>
<td>4G6</td>
<td>49.0</td>
<td>6.015</td>
<td>99.0563</td>
<td>1.3620E-08</td>
<td>0.9437</td>
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</tr>
<tr>
<td>4G2</td>
<td>50.0</td>
<td>6.015</td>
<td>98.3822</td>
<td>1.3613E-08</td>
<td>1.6178</td>
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</tr>
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<td>98.4755</td>
<td>1.7753E-09</td>
<td>1.5245</td>
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<tr>
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<td>3.8490E-10</td>
<td>0.6197</td>
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<td>4G11</td>
<td>50.0</td>
<td>9.624</td>
<td>99.5394</td>
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<td>0.4606</td>
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</tr>
</tbody>
</table>
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

<table>
<thead>
<tr>
<th>Stage #</th>
<th>T(F)</th>
<th>Liquid Phase Comp. in Mole %</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(1)</td>
<td>(2)</td>
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<tr>
<td>40</td>
<td>195.71</td>
<td>26.162</td>
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<td>38</td>
<td>195.30</td>
<td>23.793</td>
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<td>53.443</td>
</tr>
<tr>
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<td>205.38</td>
<td>53.481</td>
</tr>
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<td>205.61</td>
<td>53.532</td>
</tr>
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<td>205.88</td>
<td>54.905</td>
</tr>
<tr>
<td>2</td>
<td>212.60</td>
<td>83.031</td>
</tr>
<tr>
<td>R</td>
<td>235.45</td>
<td>99.056</td>
</tr>
</tbody>
</table>
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

<table>
<thead>
<tr>
<th>ETOH-WTR-2 METHYL C5 DYZD:NCASE=5, UNIFAC &amp; VIRIAL VAPOR(EX#4H)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3, 7, 1, 2, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0</td>
</tr>
<tr>
<td>ETOH</td>
</tr>
<tr>
<td>0, 46.1, 351.1, 516.2, 63.0, 167.0, 0.248, 58.39, 0.635,</td>
</tr>
<tr>
<td>0.0, 0.0, 2.1055, 1.9720, 0.92, 0.0, 0.0, 0.0, 0.252,</td>
</tr>
<tr>
<td>2.25, 1.70, 1.40,</td>
</tr>
<tr>
<td>202.1, 351.1,</td>
</tr>
<tr>
<td>-0.3499, 9.559E-03, -37.86E-06, 54.59E-09,</td>
</tr>
<tr>
<td>2.153, 5.113E-02, -2.004E-05, 0.328E-09,</td>
</tr>
<tr>
<td>12.0457, -3667.705, -46.976, 3*0.0,</td>
</tr>
<tr>
<td>WATER</td>
</tr>
<tr>
<td>0, 18.0, 373.2, 647.6, 217.3, 56.0, 0.348, 18.05, 0.344,</td>
</tr>
<tr>
<td>0.0, 0.0, 0.92, 1.40, 1.00, 0.0, 0.0, 0.238,</td>
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<tr>
<td>0.615, 1.84, 1.70,</td>
</tr>
<tr>
<td>538.7, 373.2,</td>
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<tr>
<td>0.6741, 2.825E-03, -8.371E-06, 8.601E-09,</td>
</tr>
<tr>
<td>7.701, 4.595E-04, 2.521E-06, -0.859E-09,</td>
</tr>
<tr>
<td>11.9516, -3984.923, -39.734, 3*0.0,</td>
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<tr>
<td>2-MET-C5</td>
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<tr>
<td>0, 86.178, 333.4, 497.5, 29.7, 367.0, 0.267, 131.97, 0.279,</td>
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<td>0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.2660,</td>
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<tr>
<td>3.809, 0.0, 0.0,</td>
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<tr>
<td>7.05, 333.4,</td>
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<tr>
<td>-0.3394, 8.3267E-03, -28.6794E-06, 35.3614E-09,</td>
</tr>
<tr>
<td>-2.524, 1.477E-01, -8.533E-05, 1.931E-08,</td>
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<tr>
<td>9.1143, -2614.38, -46.58, 3*0.0,</td>
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<tr>
<td>1.40, 1.55, 0.0,</td>
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<tr>
<td>1.55, 1.70, 0.0,</td>
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<tr>
<td>3*0.0,</td>
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<td>3 ETHANOL</td>
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<tr>
<td>3 2-METHYL PENTANE</td>
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C.8.1.1  ethanol–water–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, 0.6015, 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

<table>
<thead>
<tr>
<th>Case No.</th>
<th>Top Stage Pressure (psia)</th>
<th>Boilup Ratio</th>
<th>Bottoms Product Composition (mole%)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
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<td></td>
<td>Ethanol</td>
</tr>
<tr>
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<td>98.6416</td>
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<tr>
<td>4H10</td>
<td>130.0</td>
<td>6.015</td>
<td>98.1550</td>
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<tr>
<td>4H8</td>
<td>135.0</td>
<td>6.015</td>
<td>96.9976</td>
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<td>4H11</td>
<td>130.0</td>
<td>6.617</td>
<td>98.0819</td>
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<tr>
<td>4H12</td>
<td>130.0</td>
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<td>98.3805</td>
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<td>99.2261</td>
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<tr>
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<td>99.7446</td>
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<td>125.0</td>
<td>5.414</td>
<td>98.3900</td>
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Table C.8.3: **T and x Profiles in the Azeotrop Column Using UNIFAC Model**

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

<table>
<thead>
<tr>
<th>Stage #</th>
<th>T(F)</th>
<th>Liquid Phase Comp. in Mole %</th>
</tr>
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<tbody>
<tr>
<td></td>
<td>(1)</td>
<td>(2)</td>
</tr>
<tr>
<td>---------</td>
<td>-------</td>
<td>-----------------------------</td>
</tr>
<tr>
<td>40</td>
<td>245.43</td>
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<tr>
<td>32</td>
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<td>30</td>
<td>253.38</td>
<td>51.380</td>
</tr>
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<td>28</td>
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<td>51.420</td>
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<td>26</td>
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<td>99.745</td>
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</table>

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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

<table>
<thead>
<tr>
<th>ETOH</th>
<th>WTR</th>
<th>HEXENE</th>
<th>DYHYD</th>
<th>NCASE</th>
<th>UNIFAC &amp; VIRIAL VAPOR(EX #41)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>7</td>
<td>1</td>
<td>2</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>0</td>
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<td>351.1</td>
<td>516.2</td>
<td>63.0</td>
<td>167.0</td>
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<tr>
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<td>2.055</td>
<td>1.9720</td>
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<td>0.0</td>
<td>0.0</td>
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<td>1.70</td>
<td>1.40</td>
<td>0.3499</td>
<td>9.539E-03</td>
<td>-37.86E-06, 54.59E-09</td>
</tr>
<tr>
<td>2.153</td>
<td></td>
<td>5.713E-02</td>
<td>-2.004E-05</td>
<td>0.328E-09</td>
<td>12.0457, -3667.705, -46.976, 3*0.0,</td>
</tr>
<tr>
<td>WATER</td>
<td>0</td>
<td>18.0</td>
<td>373.2</td>
<td>647.6</td>
<td>217.3</td>
</tr>
<tr>
<td>56.0</td>
<td>0.348</td>
<td>18.05</td>
<td>0.3444</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>0.0</td>
<td>0.92</td>
<td>1.40</td>
<td>1.00</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
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<td>1.84</td>
<td>1.70</td>
<td>538.7</td>
<td>373.2</td>
<td>0.6741, 2.8245E-03, -8.371E-06,</td>
</tr>
<tr>
<td>8.601E-09</td>
<td>7.701</td>
<td>4.595E-04</td>
<td>2.521E-06</td>
<td>-0.859E-09</td>
<td>11.9516, -3984.923, -39.734, 3*0.0,</td>
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<tr>
<td>1-HEXENE</td>
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<td>504.0</td>
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<td>350.0</td>
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<td>3 ETHANOL</td>
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<tr>
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<td>1</td>
<td>1</td>
<td>2</td>
<td>1, 15</td>
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<td>17</td>
<td>3</td>
<td>1</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
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<td>3</td>
<td>ETOH-WTR-1 HEXENE AZEO DIST COLUMN SIMULATION: UNIFAC</td>
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<tr>
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<td>2</td>
<td>0</td>
<td>0, 70</td>
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<tr>
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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

<table>
<thead>
<tr>
<th>Case No.</th>
<th>Top Stage Pressure (psia)</th>
<th>Boilup Ratio</th>
<th>Bottoms Product Composition (mole%)</th>
</tr>
</thead>
<tbody>
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<td>97.3042</td>
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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 #: 413

<table>
<thead>
<tr>
<th>Stage ( \delta )</th>
<th>( T(F) )</th>
<th>Liquid Phase Compositions in Mole %</th>
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<tbody>
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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 & V1R1AL (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, 0.0, 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, 0.68367E-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,
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, 40.00,
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

<table>
<thead>
<tr>
<th>Case No.</th>
<th>Top Stage Pressure (psia)</th>
<th>Boilup Ratio</th>
<th>Bottoms Product Composition (mole%)</th>
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* Base case
Table C.10.3: Comparison of T and x Profiles in the Aseptic 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 : 4JL

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<th>(2)</th>
<th>(3)</th>
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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, 0, 0, 0, 0, 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, 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,
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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, 0.0, 0.0, 0.0,
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-09,
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

<table>
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<th>Case</th>
<th>TopStage No.</th>
<th>Pressure (psia)</th>
<th>Boilup Ratio</th>
<th>Bottoms Product Composition (mole%)</th>
<th>Ethanol</th>
<th>Water</th>
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* 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

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<tr>
<th>Stage #</th>
<th>T(P)</th>
<th>Liquid Phase Compositions in Mole %</th>
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---

**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 : VIRTUAL EOS (B BY HAYDEN & 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, 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, 
1.458389E+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, 1.0E-4, 
0.0118, 0.9882, 1.0E-4, 
0.0137, 0.9863, 1.0E-4, 
0.0144, 0.9856, 1.0E-4, 
0.0176, 0.9824, 1.0E-4, 
0.0222, 0.9778, 1.0E-4, 
0.0246, 0.9754, 1.0E-4, 
0.0302, 0.9698, 1.0E-4, 
0.0331, 0.9669, 1.0E-4, 
0.0519, 0.9481, 1.0E-4, 
0.0530, 0.9470, 1.0E-4, 
0.0625, 0.9375, 1.0E-4, 
0.0673, 0.9327, 1.0E-4, 
0.0715, 0.9285, 1.0E-4, 
0.0871, 0.9129, 1.0E-4, 
0.1260, 0.8740, 1.0E-4, 
0.1430, 0.8570, 1.0E-4, 
0.1720, 0.8280, 1.0E-4, 
0.2060, 0.7940, 1.0E-4, 
0.2100, 0.7900, 1.0E-4, 
0.2550, 0.7450, 1.0E-4, 
0.2840, 0.7160, 1.0E-4, 
0.3210, 0.6790, 1.0E-4, 
0.3240, 0.6760, 1.0E-4, 
0.3450, 0.6550, 1.0E-4, 
0.4050, 0.5950, 1.0E-4, 
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0.5450, 0.4550, 1.0E-4, 
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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,
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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, 4*0,
3, 6, 1, 2, 0, 4*0,
11, 4, 0, 3, 0, 10, 21, 11, 0, 3, 2, 0.0, 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,

ETHOH
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
D.2 Objective Functions for Vapor-Liquid Equilibrium Data Regression

The objective functions for the regression of vapor-liquid equilibria are computed for the jth 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,

\[ z_j = \frac{1}{n} \sum_{i=1}^{n} |\gamma_{ei} - \gamma_{ci}| \]  \hspace{1cm} (D2.1)

Function #2: The relative difference of the infinite dilution activity coefficients,

\[ z_j = \frac{1}{n} \sum_{i=1}^{n} \frac{|\gamma_{ei} - \gamma_{ci}|}{\gamma_{ei}} \]  \hspace{1cm} (D2.2)

Function #3: The relative difference of the logarithm of infinite dilution activity coefficients,

\[ z_j = \frac{1}{n} \sum_{i=1}^{n} |\ln \gamma_{ei} - \ln \gamma_{ci}| \]  \hspace{1cm} (D2.3)

Function #4: The difference of activity coefficients,

\[ z_j = \frac{1}{n} \sum_{i=1}^{n} |\gamma_{ei} - \gamma_{ci}| \]  \hspace{1cm} (D2.4)

Function #5: The relative difference of activity coefficients,

\[ z_j = \frac{1}{n} \sum_{i=1}^{n} \frac{|\gamma_{ei} - \gamma_{ci}|}{\gamma_{ei}} \]  \hspace{1cm} (D2.5)
Function # 6: The difference of the logarithm of activity coefficients,

\[ Z_j = \frac{1}{n} \sum_{i=1}^{p} \left| \ln \gamma_{ei} - \ln \gamma_{ci} \right| \]  
(D2.6)

Function # 7: The difference of y's,

\[ Z_j = \frac{1}{n} \sum_{i=1}^{p} \left| y_{ei} - y_{ci} \right| \]  
(D2.7)

Function # 8: The relative difference of y's,

\[ Z_j = \frac{1}{n} \sum_{i=1}^{p} \left| \frac{y_{ei} - y_{ci}}{y_{ei}} \right| \]  
(D2.8)

Function # 9: The difference of the logarithm of y's,

\[ Z_j = \frac{1}{n} \sum_{i=1}^{p} \left| \ln y_{ei} - \ln y_{ci} \right| \]  
(D2.9)

Function # 10: The difference of y's and the relative difference of total P's,

\[ Z_j = \frac{1}{n} \sum_{i=1}^{p} \left| y_{ei} - y_{ci} \right| + \left| \frac{p_e - p_c}{p_e} \right| \]  
(D2.10)

Function # 11: The relative difference of y's and the relative difference of total P's,

\[ Z_j = \frac{1}{n} \sum_{i=1}^{p} \left| \frac{y_{ei} - y_{ci}}{y_{ei}} \right| + \left| \frac{p_e - p_c}{p_e} \right| \]  
(D2.11)

Function # 12: The difference of the logarithm of y's and the difference of logarithm of total P's,

\[ Z_j = \frac{1}{n} \sum_{i=1}^{p} \left| \ln y_{ei} - \ln y_{ci} \right| + \left| \ln p_e - \ln p_c \right| \]  
(D2.12)
Function # 13: The difference of total P's,

\[ Z_j = |P_e - P| \]  \hspace{1cm} (D2.13)

Function # 14: The ratio of total P's,

\[ Z_j = \frac{|P_e|}{P_c} \]  \hspace{1cm} (D2.14)

Function # 15: The relative difference of total P's,

\[ Z_j = \frac{|P_e - P_c|}{P_e} \]  \hspace{1cm} (D2.15)

Function # 16: The difference of the logarithm of total P's,

\[ Z_j = \left| \ln \left( \frac{P_e}{P_c} \right) \right| \]  \hspace{1cm} (D2.16)

Function # 17: The difference of T's,

\[ Z_j = |T_e - T_c| \]  \hspace{1cm} (D2.17)

Function # 18: The ratio of T's,

\[ Z_j = \left| \frac{T_e}{T_c} \right| \]  \hspace{1cm} (D2.18)

Function # 19: The relative difference of T's,

\[ Z_j = \frac{|T_e - T_c|}{T_e} \]  \hspace{1cm} (D2.19)

Function # 20: The difference of the logarithm of T's,

\[ Z_j = \left| \ln \left( \frac{T_c}{T_e} \right) \right| \]  \hspace{1cm} (D2.20)

Function # 21: The difference of T's and the difference of y's,

\[ Z_j = |T_e - T_c| + \frac{1}{n} \sum_{i=1}^{n} |y_{ei} - y_{ci}| \]  \hspace{1cm} (D2.21)
Function # 22: The relative difference of T's and the difference of y's,

\[ z_j = \frac{|T_e - T_c|}{T_e} + \frac{1}{n} \sum_{i=1}^{n} |y_{ei} - y_{ci}| \quad (D2.22) \]
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 superscript 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,

\[
Z_j = \frac{1}{2n} \left( \sum_{i=1}^{n} \left| a_{ci}^I - a_{ci}^{II} \right| \right) \quad (D3.1)
\]

**Function # 2:** The difference in the logarithm of activities,

\[
Z_j = \frac{1}{2n} \left( \sum_{i=1}^{n} \left| \ln a_{ci}^I - \ln a_{ci}^{II} \right| \right) \quad (D3.2)
\]

**Function # 3:** The relative difference in activities,

\[
Z_j = \frac{1}{2n} \left( \sum_{i=1}^{n} \frac{a_{ci}^I - a_{ci}^{II}}{a_{ci}^I + a_{ci}^{II}} \right) \quad (D3.3)
\]

**Function # 4:** The difference in the logarithm of activities, with emphasis on solutes present in the system

\[
Z_j = \frac{1}{2n} \left( \sum_{i=1}^{n} \left| \ln a_{ci}^I - \ln a_{ci}^{II} \right| \right) + \frac{1}{2(n-2)} \left( \sum_{i \neq e, Ir} \left| \ln a_{ci}^I - \ln a_{ci}^{II} \right| \right) x_{ci}^I x_{ci}^{II} \quad (D3.4)
\]
where \( Ie \) and \( Ir \) denotes the rich component in extract and raffinate phases.

Function # 5: The weighted difference in compositions,

\[
Z_j = \frac{1}{2n} \sum_{i=1}^{n} w_i |x_{ei}^I - x_{ci}^I| + w_i^{II} |x_{ei}^{II} - x_{ci}^{II}| \tag{D3.5}
\]

where the associated weights are computed using \( W \) as a constant in the following equations

\[
w_i^I = |1.0 + W \frac{|x_{ei}^I - x_{ci}^I|}{x_{ei}^I}| \quad \text{and} \quad w_i^{II} = |1.0 + W \frac{|x_{ei}^{II} - x_{ci}^{II}|}{x_{ei}^{II}}| \tag{D3.6, 7}
\]

Function # 6: The weighted difference in the logarithm of compositions,

\[
Z_j = \frac{1}{2n} \sum_{i=1}^{n} w_i^I |\ln x_{ei}^I - \ln x_{ci}^I| + w_i^{II} |\ln x_{ei}^{II} - \ln x_{ci}^{II}| \tag{D3.8}
\]

Function # 7: The weighted relative difference in compositions,

\[
Z_j = \frac{1}{2n} \sum_{i=1}^{n} w_i |\frac{x_{ei}^I - x_{ci}^I}{x_{ei}^I}| + w_i^{II} |\frac{x_{ei}^{II} - x_{ci}^{II}}{x_{ei}^{II}}| \tag{D3.9}
\]

Function # 8: The weighted relative difference in compositions,

\[
Z_j = \frac{1}{2n} \sum_{i=1}^{n} w_i |\frac{x_{ei}^I - x_{ci}^I}{x_{ei}^I + x_{ci}^I}| + w_i^{II} |\frac{x_{ei}^{II} - x_{ci}^{II}}{x_{ei}^{II} + x_{ci}^{II}}| \tag{D3.10}
\]

Function # 9: The relative difference in compositions and in the distribution ratios of the solutes,
\[ Z_j = \frac{1}{2n} \sum_{i=1}^{n} w_i \left| \frac{x_{ei}^I - x_{ci}^I}{x_{ei}^I} \right| + \frac{1}{2(n-2)} \sum_{i \neq e,I}^{n} \left| \frac{K_{ei} - K_{ci}}{K_{ei} + K_{ci}} \right| \]

(D3.11)

Function # 10: The weighted difference in the logarithm of compositions and in the logarithm of distribution ratios of solutes,

\[ Z_j = \frac{1}{2n} \sum_{i=1}^{n} w_i \left| \ln \frac{x_{ei}^I}{x_{ci}^I} - \ln \frac{x_{ci}^I}{x_{ei}^I} \right| + \frac{1}{2(n-2)} \sum_{i \neq e,I}^{n} \left| \ln \frac{K_{ei}}{K_{ci}} - \ln \frac{K_{ci}}{K_{ei}} \right| \]

(D3.12)

Function # 11: The weighted relative difference in the compositions and the relative difference in the distribution ratios of solutes,

\[ Z_j = \frac{1}{2n} \sum_{i=1}^{n} w_i \left| \frac{x_{ei}^I - x_{ci}^I}{x_{ei}^I + x_{ci}^I} \right| + \frac{1}{2(n-2)} \sum_{i \neq e,I}^{n} \left| \frac{K_{ei} - K_{ci}}{K_{ei} + K_{ci}} \right| \]

(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,
\[
Z_j = \frac{1}{2n} \sum_{i=1}^{p} w_i \frac{|x_i^I - x_i^I|}{x_i^I + x_i^I} + w_i \frac{|x_i^II - x_i^II|}{x_i^II + x_i^II} + \frac{1}{2(n-2)} \sum_{i \neq e, I, r}^{p} |\ln K_{ei} - \ln K_{ci}| + W_1 \sum_{j=1}^{R} C_j \\
\text{(D3.14)}
\]

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 Regression 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

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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, \( P = 760 \text{ mm Hg} \)
- **Data reference:** Reider, R.M., et al. (1949)
- **No. of data points = 34**

<table>
<thead>
<tr>
<th>Case VLEPN</th>
<th>Binary Interaction Parameters, (^{\circ}K)</th>
<th>( T_{\text{exp}} - T_{\text{cal}} ) in deg C</th>
<th>( Y_{\text{exp}} - Y_{\text{cal}} ) in mole %</th>
<th>Inf. Dilution Activity Coeff</th>
</tr>
</thead>
<tbody>
<tr>
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<td>-68.88</td>
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(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  
No. of data points = 34

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<thead>
<tr>
<th>Case</th>
<th>VLEPN</th>
<th>Binary Interaction Parameters, 0K</th>
<th>T_{exp} - T_{cal} in deg C</th>
<th>Y_{exp} - Y_{cal} in mole %</th>
<th>Inf. Dilution Activity Coeff</th>
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<td>Max</td>
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<tr>
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<td>Max</td>
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<tr>
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<td>-361.09 9963.07</td>
<td>3.00</td>
<td>7.10</td>
</tr>
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<td>0.55</td>
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Note: '-' shows very high calculated values
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<th>Case VLEFN</th>
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<th>P_{exp} - P_{cal} in mm Hg</th>
<th>Y_{leq} - Y_{1cal} in mole %</th>
<th>Inf. Dilution Activity Coeff</th>
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<td>8088.41</td>
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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

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<th>VLEPN</th>
<th>Binary Interaction Parameters, OK</th>
<th>P_{exp}-P_{cal} in mm Hg</th>
<th>Y_{exp}-Y_{cal} in mole %</th>
<th>Inf. Dilution Activity Coeff</th>
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<td>Mean    Max</td>
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<td>0.564   1.460</td>
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<td>08N*</td>
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<td>100    100</td>
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<td>1.66    8.72</td>
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<td>-19.16 272.72</td>
<td>1.66    8.72</td>
<td>0.564   1.239</td>
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<td>1.66    8.72</td>
<td>0.563   1.239</td>
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<td>-19.15 272.70</td>
<td>1.66    8.72</td>
<td>0.564   1.239</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Case</th>
<th>VLEFn</th>
<th>Binary Interaction Parameters, °K</th>
<th>T_{exp} - T_{cal} in deg C</th>
<th>Y_{exp} - Y_{ical} in mole %</th>
<th>Inf. Dilution Activity Coeff</th>
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<td>Final</td>
<td>Mean</td>
<td>Max</td>
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<td>1</td>
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(Cont'd.) Table E.1.3: Regression Results of Isobaric Ethanol-Benzene (VLE) System

<table>
<thead>
<tr>
<th>System: (1) Ethanol - (2) Benzene</th>
<th>Condition: Isobaric, P = 750 mm Hg</th>
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<tr>
<td>Gamma Model: Modified UNIQUAC</td>
<td>Data reference: Tyrer D., (1912)</td>
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<td>Phi Model: Virial EOS</td>
<td>No. of data points = 9</td>
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<th>Case VLEFN</th>
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<th>$^\text{Y}<em>{\text{exp}}$ - $^\text{Y}</em>{\text{cal}}$ in mole %</th>
<th>Inf. Dilution Activity Coeff</th>
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</thead>
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Note: '-' shows very high calculated values
Table E.1.4: *Regression Results of Isothermal Ethanol-Benzene (VLE) System*

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<th>System:</th>
<th>(1) Ethanol - (2) Benzene</th>
<th>Condition: Isothermal, T = 40 °C</th>
<th>Data reference: Udovenko, V.V., et. al. (1952)</th>
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<td>Phi Model: Virial EOS</td>
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</table>

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<th>$y_{\text{exp}} - y_{\text{cal}}$ in mole %</th>
<th>Inf. Dilution Activity Coeff</th>
</tr>
</thead>
<tbody>
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<td>No.</td>
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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

<table>
<thead>
<tr>
<th>Case Reference</th>
<th>Binary Interaction Parameters, 0K</th>
<th>Phase Rich in (1)</th>
<th>Phase Rich in (2)</th>
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<td>Mean % Rel. x Diff.</td>
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System: (1) Benzene - (2) Water  
Gamma Model: Modified UNIQUAC  
Condition: Isothermal, $T = 25$ C  
Data reference: Polak, J. (1973)  
No. of data points = 1
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

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</tr>
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</tr>
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<td>1000</td>
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</tr>
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<td>22V</td>
<td>5</td>
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<td>2000</td>
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</tr>
</tbody>
</table>

* Relative to 25°C
(Cont'd.) Table E.2.1: Regression Results of Benzene-Water (LLF) System at 25 C

System: (1) Benzene - (2) Water  Condition: Isothermal, T = 25 C
No. of data points = 1

<table>
<thead>
<tr>
<th>Case LLEFN</th>
<th>Binary Interaction Parameters, $^\circ$K</th>
<th>Phase Rich in (1)</th>
<th>Phase Rich in (2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>No.</td>
<td># Initial</td>
<td>Final</td>
<td>Mean % Rel. x Diff.</td>
</tr>
<tr>
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<td>$A_{12}$</td>
<td>$A_{21}$</td>
<td>$A_{12}$</td>
</tr>
<tr>
<td>22W</td>
<td>6 2000</td>
<td>2000</td>
<td>-284.78</td>
</tr>
<tr>
<td>22X</td>
<td>7 2000</td>
<td>2000</td>
<td>1424.75</td>
</tr>
<tr>
<td>22Y</td>
<td>8 2000</td>
<td>2000</td>
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</tr>
<tr>
<td>22Z</td>
<td>11 2000</td>
<td>2000</td>
<td>1408.06</td>
</tr>
<tr>
<td>22AA</td>
<td>5 3000</td>
<td>3000</td>
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</tr>
<tr>
<td>22BB</td>
<td>6 3000</td>
<td>3000</td>
<td>1413.35</td>
</tr>
<tr>
<td>22CC</td>
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<td>3000</td>
<td>1413.93</td>
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<tr>
<td>22DD</td>
<td>6 1500</td>
<td>500</td>
<td>1415.42</td>
</tr>
<tr>
<td>22EE</td>
<td>8 1500</td>
<td>500</td>
<td>1409.36</td>
</tr>
</tbody>
</table>

* $(x_{iexp} - x_{ical}) / x_{iexp} \times 100$
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: Sorensen, et. al. (1979)  
No. of data points = 1

<table>
<thead>
<tr>
<th>Case LLEPN</th>
<th>Binary Interaction Parameters, °K</th>
<th>Phase Rich in (1)</th>
<th>Phase Rich in (2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>No. #</td>
<td>Initial</td>
<td>Final</td>
<td>Mean % Rel. x Diff.</td>
</tr>
<tr>
<td></td>
<td>A12</td>
<td>A21</td>
<td>(1)</td>
</tr>
<tr>
<td></td>
<td>A12</td>
<td>A21</td>
<td>(1)</td>
</tr>
<tr>
<td>23A</td>
<td>8</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>23B</td>
<td>8</td>
<td>100</td>
<td>100</td>
</tr>
<tr>
<td>23C</td>
<td>8</td>
<td>200</td>
<td>200</td>
</tr>
<tr>
<td>23D</td>
<td>8</td>
<td>200</td>
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</tr>
<tr>
<td>23E</td>
<td>8</td>
<td>-200</td>
<td>-200</td>
</tr>
<tr>
<td>23F</td>
<td>8</td>
<td>300</td>
<td>300</td>
</tr>
<tr>
<td>23G</td>
<td>8</td>
<td>500</td>
<td>500</td>
</tr>
<tr>
<td>23H</td>
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<td>23I</td>
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<td>500</td>
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<tr>
<td>23J</td>
<td>8</td>
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<td>1000</td>
</tr>
<tr>
<td>23K</td>
<td>8</td>
<td>1000</td>
<td>200</td>
</tr>
<tr>
<td>23L</td>
<td>8</td>
<td>3000</td>
<td>3000</td>
</tr>
</tbody>
</table>

* (xiexp-xical)/xiexp*100
### Table E.2.3: Regression Results of Benzene-Water (LLE) System at 35°C

**System:** (1) Benzene - (2) Water  
**Gamma Model:** Modified UNQUAC  
**Condition:** Isothermal, $T = 35°C$  
**Data reference:** Sorensen, et. al. (1979)  
**No. of data points = 1**

<table>
<thead>
<tr>
<th>Case LLEFN</th>
<th>Binary Interaction Parameters&lt;sup&gt;OK&lt;/sup&gt;</th>
<th>Phase Rich in (1)</th>
<th>Phase Rich in (2)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>No.</td>
<td>Initial</td>
<td>Final</td>
</tr>
<tr>
<td>-------------</td>
<td>-----</td>
<td>---------</td>
<td>-------</td>
</tr>
<tr>
<td></td>
<td>A&lt;sub&gt;12&lt;/sub&gt;</td>
<td>A&lt;sub&gt;21&lt;/sub&gt;</td>
<td>A&lt;sub&gt;12&lt;/sub&gt;</td>
</tr>
<tr>
<td>25A</td>
<td>8</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>25B</td>
<td>8</td>
<td>100</td>
<td>100</td>
</tr>
<tr>
<td>25C</td>
<td>8</td>
<td>200</td>
<td>200</td>
</tr>
<tr>
<td>25D</td>
<td>8</td>
<td>300</td>
<td>300</td>
</tr>
<tr>
<td>25E</td>
<td>8</td>
<td>400</td>
<td>400</td>
</tr>
<tr>
<td>25F</td>
<td>8</td>
<td>500</td>
<td>500</td>
</tr>
<tr>
<td>25G</td>
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<td>1000</td>
<td>1000</td>
</tr>
<tr>
<td>25H</td>
<td>8</td>
<td>2000</td>
<td>2000</td>
</tr>
</tbody>
</table>

* $(x_{\text{exp}}-x_{\text{cal}})/x_{\text{exp}}*100$
**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

<table>
<thead>
<tr>
<th>Case</th>
<th>LLEFN</th>
<th>Binary Interaction Parameters, OK</th>
<th>Phase Rich in (1)</th>
<th>Phase Rich in (2)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>No.</td>
<td>Initial</td>
<td>Final</td>
<td>Mean % Rel. x Diff.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>A_{12}</td>
<td>A_{21}</td>
<td>A_{12}</td>
</tr>
<tr>
<td>24A</td>
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<td>1</td>
<td>1</td>
<td>1072.25</td>
</tr>
<tr>
<td>24B</td>
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<td>1074.55</td>
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<tr>
<td>24C</td>
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<td>200</td>
<td>1076.58</td>
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<tr>
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<tr>
<td>24H</td>
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<td>2000</td>
<td>2000</td>
<td>1868.37</td>
</tr>
</tbody>
</table>

* $(x_{i exp} - x_{ical}) / x_{i exp} \times 100$
Table E.3.1: Regression Results of Ethanol-Water-Benzene (VLE) System

System: (1) Ethanol - (2) Water - (3) Benzene  Condition: Isochoric, P = 760 mmHg
Gamma Model: Modified UNIQUAC  Data Reference: Hands, C.H.G., et. al. (1945)
Phi Model: Virial EOS  Data set: Ethanol-Water-Benzene (VLE, 760 mmHg)

<table>
<thead>
<tr>
<th>Case VLEFN</th>
<th>Final Binary Interaction Parameters in deg K</th>
<th>Mean &amp; (Max) T and y's</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$A_{12}$ $A_{21}$ $A_{13}$ $A_{31}$ $A_{23}$ $A_{32}$</td>
<td>dev$^5$ in T deg C dev$^5$ in mole%</td>
</tr>
<tr>
<td>03A*</td>
<td>21 -180.69 7787.48 -156.49 8696.35 701.73 -16.91</td>
<td>0.28 (0.91) 2.101 (7.140) 3.324 (6.054)</td>
</tr>
<tr>
<td>03B#</td>
<td>21 -177.19 8470.27 -158.48 8365.53 632.96 4.80</td>
<td>0.29 (0.83) 1.953 (6.790) 3.296 (6.001)</td>
</tr>
<tr>
<td>03C+</td>
<td>21 -131.51 1134.12 -179.08 7385.74 311.18 220.55</td>
<td>0.33 (0.83) 1.242 (3.601) 2.597 (5.234)</td>
</tr>
<tr>
<td>03X+</td>
<td>21 -57.02 351.70 -151.47 961.51 375.24 892.72</td>
<td>4.65 (11.58) 7.007 (14.127) 5.370 (5.234)</td>
</tr>
</tbody>
</table>

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

$\text{dev in } T = (T_{\text{exp}} - T_{\text{cal}})$ and $\text{dev in } y_i = (y_{i\text{exp}} - y_{i\text{cal}}) \times 100$
Table E.3.2A: Regression Results of Combinations of Isobaric Binary and Ternary VLE System

System: (1) Etol - (2) Water - (3) Bz  Condition: Isobaric, P = 760 mm Hg
Gamma Model: Modified UNIQUAC  Data Sets and References:
Phi Model: Virial EOS

<table>
<thead>
<tr>
<th>Case</th>
<th>VLEFN</th>
<th>Final Binary Interaction Parameters in deg K</th>
<th>Data Sets used in the Regression</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
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<td>A_{21}</td>
</tr>
<tr>
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<td>330.98</td>
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<td>71A</td>
<td>21</td>
<td>-123.81</td>
<td>1132.14</td>
</tr>
<tr>
<td>72A</td>
<td>21</td>
<td>-127.85</td>
<td>969.31</td>
</tr>
<tr>
<td>73A</td>
<td>21</td>
<td>-48.89</td>
<td>342.70</td>
</tr>
<tr>
<td>74A</td>
<td>21</td>
<td>-56.14</td>
<td>350.85</td>
</tr>
</tbody>
</table>
Table E.3.2R: 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.C., et. al. (1945)

<table>
<thead>
<tr>
<th>Case</th>
<th>VLEFN</th>
<th>Mean &amp; (Max) Abs (Te-Tc) deg C</th>
<th>Mean &amp; (Max) Absolute diff in mole %</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>(a) System (b)</td>
<td>(c)</td>
</tr>
<tr>
<td>70A</td>
<td>21</td>
<td>0.14 (0.56)</td>
<td>0.45 (1.45)</td>
</tr>
<tr>
<td>71A</td>
<td>21</td>
<td>-</td>
<td>0.48 (1.47)</td>
</tr>
<tr>
<td>72A</td>
<td>21</td>
<td>-</td>
<td>0.12 (0.59)</td>
</tr>
<tr>
<td>73A</td>
<td>21</td>
<td>0.14 (0.51)</td>
<td>0.12 (0.50)</td>
</tr>
<tr>
<td>74A</td>
<td>21</td>
<td>0.14 (0.54)</td>
<td>0.12 (0.41)</td>
</tr>
</tbody>
</table>
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)

<table>
<thead>
<tr>
<th>Case</th>
<th>No. LLEFN</th>
<th>W</th>
<th>Final Binary Interaction Parameters in deg K</th>
</tr>
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<tbody>
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<td>$A_{12}$</td>
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<tr>
<td>-------</td>
<td>-----------</td>
<td>---</td>
<td>-----------</td>
</tr>
<tr>
<td>21B</td>
<td>All</td>
<td>11</td>
<td>0</td>
</tr>
<tr>
<td>21C</td>
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</tr>
<tr>
<td>21X</td>
<td>All</td>
<td>11</td>
<td>0</td>
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</table>

Initial Binary Interaction Parameters in deg K

<table>
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<tr>
<th>Case</th>
<th>No. LLEFN</th>
<th>W</th>
<th>Initial Binary Interaction Parameters in deg K</th>
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<td>$A_{12}$</td>
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<tr>
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<td>-----------</td>
<td>---</td>
<td>-----------</td>
</tr>
<tr>
<td>21A*</td>
<td>All</td>
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<td>0</td>
</tr>
<tr>
<td>21B</td>
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<td>11</td>
<td>0</td>
</tr>
<tr>
<td>21C</td>
<td>All</td>
<td>11</td>
<td>0</td>
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</table>

* unconverged case
(Cont'd.) Table E.4: Regression Results of Ethanol-Water-Benzene (LLE) System

<table>
<thead>
<tr>
<th>Case</th>
<th>No. LLEFN</th>
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<th>Diff. of compositions in mole %, Mean &amp; (Max)</th>
<th>Mean diff of d. ratio</th>
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</thead>
<tbody>
<tr>
<td></td>
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<td>Phase Rich in (3)</td>
<td>Phase Rich in (2)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(1)  (2)  (3)</td>
<td>(1)  (2)  (3)</td>
</tr>
<tr>
<td>21B</td>
<td>All</td>
<td>11</td>
<td>0.6929 0.6338 0.5186</td>
<td>0.7065 0.9825 0.4487</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(1.102) (1.484) (1.081)</td>
<td>(1.011) (1.777) (1.947)</td>
</tr>
<tr>
<td>21C</td>
<td>All</td>
<td>11</td>
<td>1.7550 3.6050 4.7180</td>
<td>1.0470 2.2950 1.2480</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(3.225) (15.530) (18.760)</td>
<td>(2.784) (7.314) (4.530)</td>
</tr>
</tbody>
</table>

$\text{Difference} = \frac{(x_{\text{exp}} - x_{\text{calc}})}{x_{\text{exp}}} \times 100$
Table E.5.1A: Regression Results of Isobaric Binary VLE and Isothermal Ternary LLE System

System: (1) EtOH - (2) Water - (3) Bz  Condition: Isobaric for VLE, P = 760 mm Hg
Gamma Model: Modified UNIQUAC  Isothermal for LLE, T = 35 C
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, Morachevskii, A.G., et.al.(1958)

<table>
<thead>
<tr>
<th>Case</th>
<th>No.</th>
<th>LLEFN</th>
<th>W</th>
<th>Final Binary Interaction Parameters in deg K</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>#</td>
<td>of Tie Lines</td>
<td>#</td>
<td>A₁₂</td>
</tr>
<tr>
<td>------</td>
<td>-----</td>
<td>---------------</td>
<td>---</td>
<td>------</td>
</tr>
<tr>
<td>40A</td>
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<td>10</td>
<td>-50.30</td>
</tr>
<tr>
<td>40B</td>
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<td>8</td>
<td>50</td>
<td>-46.98</td>
</tr>
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<td>All</td>
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<td>0</td>
<td>-51.19</td>
</tr>
<tr>
<td>41B</td>
<td>All</td>
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<td>150</td>
<td>-159.10</td>
</tr>
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<td>41C</td>
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<td>8</td>
<td>200</td>
<td>-164.77</td>
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<td>41D</td>
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<td>250</td>
<td>-212.13</td>
</tr>
<tr>
<td>41E</td>
<td>All</td>
<td>8</td>
<td>300</td>
<td>-259.37</td>
</tr>
<tr>
<td>42A</td>
<td>1</td>
<td>11</td>
<td>0</td>
<td>-50.95</td>
</tr>
<tr>
<td>42C</td>
<td>1</td>
<td>11</td>
<td>100</td>
<td>-45.57</td>
</tr>
</tbody>
</table>

246
(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)

<table>
<thead>
<tr>
<th>Case</th>
<th>No. LLEFN</th>
<th>W</th>
<th>Final Binary Interaction Parameters in deg K</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>of Tie</td>
<td></td>
<td>A_{12}</td>
</tr>
<tr>
<td></td>
<td>Lines</td>
<td></td>
<td></td>
</tr>
<tr>
<td>42D</td>
<td>1</td>
<td>11</td>
<td>150</td>
</tr>
<tr>
<td>43B</td>
<td>All</td>
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Table E.5.1B: Regression Results of Isobaric Binary VLE and Isothermal Ternary LLE System

System: (1) Etoh - (2) Water - (3) Bz  Condition: Isobaric for VLE, P = 760 mm Hg
Gamma Model: Modified UNIQUAC  Isothermal for LLE, T = 35 °C
Phi Model: Virial EOS

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(Cont'd.) Table E.5.1B: Regression Results of Isobaric Binary VLE and Isothermal Ternary LLE System

System: (1) Etho - (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) Etho-Water,  
Reider, R.M., et. al. (1949)  
(b) Etho-Bz,  
Tyrer, D., (1912)  
(c) Etho-Wtr-Bz,  
Morachevskii, A.G., et.al.(1958)

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(Cont’d.) Table E.5.1B: Regression Results of Isobaric Binary VLE and Isothermal Ternary LLE System

System: (1) Etoh - (2) Water - (3) Bz  Condition: Isobaric for VLE, P = 760 mm Hg
Gamma Model: Modified UNIQUAC  Isothermal for LLE, T = 35 C
Phi Model: Virial EOS  Data Sets and References:

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Table E.5.1C: Regression Results of Isobaric Binary VLE and Isothermal Ternary LLE System

System: (1) EtOH - (2) Water - (3) Bz  
Condition: Isobaric for VLE, P = 760 mm Hg  
Isothermal for LLE, T = 35 C  
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, Morachevskii, A.G., et.al.(1958)

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* 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-Wt-Bz, Morachevskii, A.G., et.al.(1958)

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System: (1) EtOH - (2) Water - (3) Bz  Condition: Isobaric for VLE, \( P = 760 \) mm Hg
Gamma Model: Modified UNIQUAC                        Isothermal for LLE, \( T = 35 \) C
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, Morachevskii, A.G., et.al.(1958)

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(Cont'd.) Table E.5.2A: **Regression Results of Isothermal Binary VLE and Isothermal Ternary LLE System**

**System:** (1) Ethoh - (2) Water - (3) Bz  
**Gamma Model:** Modified UNIQUAC  
**Phi Model:** Virial EOS  
**Condition:** Isothermal for VLE, T = 40°C  
**Data Sets and References:**  
(a) Ethoh-Water, Mertl, I., et. al. (1972)  
(b) Ethoh-Bz, Udovenko, V.V., et. al. (1952)  
(c) Ethoh-Wtr-Bz, Morachevskii, A.G., et.al. (1958)

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Table E.5.2B: Regression Results of Isothermal Binary VLE and Isothermal Ternary LLR 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)

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<th>Case</th>
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<th>Mean &amp; (Max) Absolute diff in mole %</th>
<th>System</th>
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<th>y2</th>
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<td>44.20 (51.14)</td>
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<td>20</td>
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<td>45.38 (52.38)</td>
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$\phi$ 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  Condition: Isothermal for VLE, T = 40 C
Gamma Model: Modified UNIQUAC  Isothermal for LLE, T = 35 C
Phi Model: Virial EOS  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)

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<th>Mean &amp; (Max) Absolute diff in mole % y1</th>
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@ 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) Etho - (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) Etho-Water, Mertl, I., et. al. (1972)  
(b) Etho-Bz, Udovenko, V.V., et. al. (1952)  
(c) Etho-Wtr-Bz, Morachevskii, A.G., et.al. (1958)

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$\S$ 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) Ethol - (2) Water - (3) Bz  Condition: Isothermal for VLE, T = 40 C  
Gamma Model: Modified UNIQUAC  Isothermal for LLE, T = 35 C  
Phi Model: Virial EOS  

Data Sets and References:  
(a) Ethol-Water, Mertl, I., et. al. (1972)  
(b) Ethol-Bz, Udovenko, V.V., et. al. (1952)  
(c) Ethol-Wtr-Bz, Morachevskii, A.G., et.al. (1958)

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<th>Mean &amp; (Max) Absolute diff in mole %</th>
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<td>30</td>
<td>46.13 (57.04)</td>
<td>74.80 (90.90)</td>
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<td>12.866 (25.172)</td>
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Ω 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) Etho - (2) Water - (3) Bz  
**Condition:** Isothermal for VLE, T = 40 C  
**Gamma Model:** Modified UNIQUAC  
**Phi Model:** Virial EOS  
**Data Sets and References:**  
(a) Etho-Water, Mertl, I., et. al. (1972)  
(b) Etho-Bz, Udovenko, V.V., et. al. (1952)  
(c) Etho-Wtr-Bz, Morachevskii, A.G., et.al. (1958)

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(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

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<th>Case</th>
<th>No. LLEFN W</th>
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<td>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)</td>
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<tr>
<td>47D</td>
<td>All 8 45</td>
<td></td>
<td>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)</td>
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<td>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)</td>
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<td>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)</td>
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<td>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)</td>
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<td>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)</td>
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(Cont'd.) Table E.5.2C: Regression Results of Isothermal Binary VLE and Isothermal Ternary LLE System

System: (1) Ethoh - (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) Ethoh-Water, Mertl, I., et. al. (1972)
(b) Ethoh-Bz, Udozenko, V.V., et. al. (1952)
(c) Ethoh-Wtr-Bz, Morachevskii, A.G., et.al. (1958)

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Table E.5.3A: Regression Results of Isothermal Binary VLE and Isothermal Ternary LLE System

System: (1) EtOH - (2) Water - (3) Bz  
Condition: Isothermal for VLE, T = 40 C  
Isothermal for LLE, T = 35 C  
Gamma Model: Modified UNIQUAC  
Phi Model: Virial EOS  

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)

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(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  
**Condition:** 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)

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<td>3.155 (6.582) 3.398 (12.427) 6.851 (11.968)</td>
<td>(10.895)</td>
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<td>8.37 (22.15) 17.44 (27.14) 8.70 (14.45)</td>
<td>8.185 (12.466) 6.329 (14.134) 6.178 (13.111)</td>
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<td>1.004 (2.178) 1.377 (2.194) 7.052 (13.144)</td>
<td>(10.407)</td>
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@ 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) Eth - (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) Eth-Water, Mertl, I., et. al. (1972)
(b) Eth-Bz, Udovenko, V.V., et. al. (1952)
(c) Eth-Wtr-Bz, Morachevskii, A.G., et.al. (1958)

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<th>Mean &amp; (Max) Absolute diff in molc % y1</th>
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<td>15</td>
<td>32.04 (37.35) 54.21 (64.73) 3.31 (9.59)</td>
<td>2.831 (5.330) 3.365 (5.748) 8.296 (15.559)</td>
<td>4.266 (8.361)</td>
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<td>16.46 (28.09) 28.92 (36.40) 7.08 (13.35)</td>
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<td>13.27 (27.45) 25.50 (33.33) 5.83 (9.86)</td>
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<td>23.98 (29.64) 42.90 (49.32) 5.85 (12.89)</td>
<td>1.690 (3.166) 1.709 (4.706) 7.431 (13.967)</td>
<td>5.922 (11.425)</td>
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@ 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) Ethanol - (2) Water - (3) Benzene  
Condition: Isothermal for VLE, T = 40 C  
Isothermal for LLE, T = 35 C  
Gamma Model: Modified UNIQUAC  
Phi Model: Virial EOS  

Data Sets and References:  
(a) Ethanol-Water, Mertl, I., et. al. (1972)  
(b) Ethanol-Benzene, Udovenko, V.V., et. al. (1952)  
(c) Ethanol-Water-Benzene, Morachevskii, A.G., et.al. (1958)

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<td>26.72 46.78 4.85</td>
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<td>1.901 3.677 13.698</td>
<td>(30.10) (54.41) (11.48)</td>
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<td>4.680 5.490 14.449</td>
<td>(36.40) (65.72) (8.75)</td>
<td>(c)</td>
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© Predicted ternary VLE results, diff. in T's (deg C) and VLEPN # 21  
* Predicted ternary VLE results, VLEPN # 21
Table E.5.3C: Regression Results of Isothermal Binary VLE and Isothermal Ternary LLE System

System: (1) Etoh - (2) Water - (3) Bz  
Condition: Isothermal for VLE, T = 40 C  
Gamma Model: Modified UNIQUAC  
Phi Model: Virial EOS  
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)

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50B 1 21 8 20 7.8460 4.0190 11.2700 4.0370 2.6560 1.6170 5.2402 0.2962

50C 1 21 8 40 1.6540 2.6090 3.6550 1.4720 2.7260 2.4600 2.4293 0.1210

50D 1 21 8 60 1.2860 2.2630 2.5990 1.1370 3.4340 2.5930 2.2187 0.1038
(3.404) (8.271) (7.576) (2.954) (9.763) (9.230) (9.763) (0.269)

51A  All 21 8 0 0.7183 3.4200 2.9600 0.6465 3.3530 2.9040 2.3336 0.0456
(1.351) (9.232) (8.979) (1.497) (10.090) (9.938) (10.090) (0.126)

51B  All 21 8 5 2.6510 4.3430 6.9940 1.5400 1.3970 1.3370 3.0437 0.1282
(4.328) (15.270) (18.470) (2.836) (2.964) (3.308) (15.270) (0.170)

51C  All 21 8 15 1.3740 1.4400 2.8130 1.1670 1.3790 0.8302 1.5005 0.0866
(2.543) (3.802) (6.345) (2.153) (2.551) (3.124) (6.345) (0.148)
(Cont'd.) Table E5.3C: Regression Results of Isothermal Binary VLE and Isothermal Ternary LLE System

System: (1) Eth - (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) Eth-Water, Reider, R.M., et. al. (1949)
(b) Eth-Bz, Tyrer, D., (1912)
(c) Eth-Wtr-Bz, Morachevskii, A.G., et.al. (1958)

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<td>1.2340 3.8270 2.6100 (2.887)(12.000)(9.110) (12.000) (0.150)</td>
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(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)

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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)

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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)

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<th>Mean &amp; (Max) Abs (T_{exp} - T_{cal}) C</th>
<th>Mean &amp; (Max) Absolute diff in mole %</th>
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<td>(a) System (b) (c) (c) System (c)</td>
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<td>11</td>
<td>0</td>
<td>0.15 (0.45) 0.20 (0.61) 0.54 (2.05)</td>
<td>0.933 (2.497) 0.759 (2.394) 0.939 (4.133) 0.973 (3.895)</td>
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<td>0.81 (1.44) 1.00 (1.30) 1.31 (4.58)</td>
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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)

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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)
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 ... \text{cal per gm}
REFERENCE TEMPERATURE ... \text{Deg K}

(2) SPECIFIC HEAT CONSTANTS
\text{LIQUID}
C1=a, C2=b, \ldots, C4=d
\text{cal per gram vs Deg K}
Cp = a + bT + cT^2 + dT^3

(3) SPECIFIC HEAT CONSTANTS
\text{VAPOR}
C1=a, C2=b, \ldots, C4=d
\text{cal per g-mole vs Deg K}
Cp = a + bT + cT^2 + dT^3

(4) VAPOR PRESSURE CONSTANTS
C1, C2, \ldots, C6
C1=a, C2=b, \ldots, C6=f
Atm versus \text{Deg K}
ln(P) = a + b/(c + T) + d*ln(T) + e*T + f*T^2

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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 0
11 BCTL DS-3 30 -21 0 0 0 0 0 0
12 DIST D-3 21 -22 -31 0 0 0 0 0
15 HTCL H-3 32 -17 0 0 0 0 0 0
16 MIXR M-4 33 22 -34 0 0 0 0 0
17 CNTL CT-2 19 35 -36 -33 0 0 0 0

NETWORK COMPLETE
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6 3
7 24
10 1
11 26
12 25
15 2
16 11
17 3

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CASE # A: SIMULATION OF A ZED DIST PROCESS PLANT; VLE NRTL & LLE NRTL & IDEAL

"PROCESS VECTORS"

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CASE # A: SIMULATION OF A ZED DIST PROCESS PLANT; VLE NRTL & LLE NRTL & IDEAL

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CASE # A: SIMULATION OF AZEO DIST PROCESS PLANT; VLE NRTL & LLE NRTL & IDEAL

"OTHER SYSTEM VARIABLES"

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"INPUT DATA"

**CASE A: SIMULATION OF AZEO DIST PROCESS PLANT: VLE NRTL & LLE NRTL & IDEAL**

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**COMPOSITION, LB-MOLES/UNIT TIME**

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**COMPOSITION, LB-MOLES/UNIT TIME**

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### BEGIN TRIAL AND ERROR RECYCLE CALCULATIONS WITH EQUIPMENT LIST:

4, 15, 8, 11, 12, 17, 16, 7, 10

*** SUBSET LOOP COMPLETE ***
## FINAL RESULTS

**CASE # A: SIMULATION OF AZEO DIST PROCESS PLANT; VLE NRTL & LLE NRTL & IDEAL**

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**COMPOSITION, LB-MCLES/UNIT TIME**

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**COMPOSITION, LB-MCLES/UNIT TIME**

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**COMPOSITION, LB-MOLES/UNIT TIME**

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**COMPOSITION, LB-MOLES/UNIT TIME**

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**TOTAL** 6.25012 0.80902 84.15167

**CASE A: SIMULATION OF AZED 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
CASE B: SIMULATION OF AJOE DIST PROCESS PLANT; VLE NRTL & LLE NRTL & IDEAL

NUMBER OF COMPONENTS = 3

VAPOUR-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 LIG 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

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 M-1 11 -14 0 0 9 0 0
4 MIXR M-2 15 16 -1 2 0 0 0
6 ACTL CT-1 17 14 -18 -19 0 0 0
7 DVGR CV-1 34 -16 -23 0 0 0 0
10 SMIX M-3 18 23 -15 -30 0 0 0
11 DCTL CS-3 30 -21 0 0 0 0 0
12 DIST D-3 21 -22 -31 0 0 0 0
15 HTCL M-3 32 -17 0 0 0 0 0
16 MIXR M-4 33 22 -34 0 0 0 0
17 CNTRL CT-2 19 35 -36 -33 0 0 0

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3 2
4 11
6 3
7 24
10 1
11 26
12 23
15 2
16 11
17 3

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**CALCULATION DATA COMPLETE**
CASE # B: SIMULATION OF AIEO DIST PROCESS PLANT; VLE NRTL & LLE NRTL & IDEAL

"PROCESS VECTORS"

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CASE # B: SIMULATION OF AIEO DIST PROCESS PLANT; VLE NRTL & LLE NRTL & IDEAL

"STREAM CONNECTIONS"

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CASE # 8: SIMULATION OF AIEO DIST PROCESS PLANT; VLE NRTL & LLE NRTL & IDEAL
"OTHER SYSTEM VARIABLES"

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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
### Case B: Simulation of Azeo Dist Process Plant: VLE NRTL & LLE NRTL & Ideal

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#### Composition, lb-moles/unit time

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*** SUBSET LOOP COMPLETE ***
## Final Results

### Case B: Simulation of Azed Dist Process Plant; VLE NRTL & LLE NRTL & Ideal

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<td>0.0000</td>
<td>168.12692</td>
<td>167.32634</td>
</tr>
<tr>
<td><strong>TOTAL</strong></td>
<td>279.73398</td>
<td>0.0000</td>
<td>279.76068</td>
<td>310.67633</td>
</tr>
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</table>

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<table>
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<tr>
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<tbody>
<tr>
<td>EQUIP CONNION</td>
<td>FR 6 TO 17</td>
<td>FR 11 TO 12</td>
<td>FR 12 TO 16</td>
<td>FR 7 TO 10</td>
</tr>
<tr>
<td>VAPOR FRACTION</td>
<td>0.0000</td>
<td>0.0000</td>
<td>1.0000</td>
<td>0.8775</td>
</tr>
<tr>
<td>TEMPERATURE, F</td>
<td>171.6569</td>
<td>95.0000</td>
<td>101.9489</td>
<td>99.6651</td>
</tr>
<tr>
<td>ENTHALPY, K-BTU</td>
<td>-1.5339</td>
<td>-79.2645</td>
<td>73.4274</td>
<td>71.3476</td>
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<tr>
<td>L/H LIQUID FRAC</td>
<td>1.0000</td>
<td>1.0000</td>
<td>1.0000</td>
<td>1.0000</td>
</tr>
</tbody>
</table>

**COMPOSITION, LB-MOLES/UNIT TIME**

| ETHOH | 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 |

<table>
<thead>
<tr>
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<th>31</th>
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<tbody>
<tr>
<td>EQUIP CONNION</td>
<td>FR 10 TO 11</td>
<td>FR 12 TO 1</td>
<td>FR 4 TO 15</td>
<td>FR 17 TO 16</td>
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<tr>
<td>VAPOR FRACTION</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
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<tr>
<td>TEMPERATURE, F</td>
<td>95.0000</td>
<td>129.9099</td>
<td>94.9976</td>
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<td>ENTHALPY, K-BTU</td>
<td>-79.3082</td>
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<td>-669.0167</td>
<td>-2.0798</td>
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<td>L/H LIQUID FRAC</td>
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<td>1.0000</td>
<td>1.0000</td>
<td>1.0000</td>
</tr>
</tbody>
</table>

**COMPOSITION, LB-MOLES/UNIT TIME**

| ETHOH | 13.280933 | 12.02075 | 78.63961 | 0.00000 |
| WATER | 20.70906 | 19.70135 | 32.95416 | 0.00000 |
| BENZENE | 3.17323 | 0.00008 | 168.12692 | 0.79995 |

**TOTAL** | 37.17162 | 31.72217 | 279.76068 | 0.79995 |
<table>
<thead>
<tr>
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<td>FR 0 TO 17</td>
<td>FR 17 TO 0</td>
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<td>VAPOR FRACTION</td>
<td>0.8775</td>
<td>0.0000</td>
<td>0.0000</td>
</tr>
<tr>
<td>TEMPERATURE, F</td>
<td>99.6651</td>
<td>95.0000</td>
<td>171.6569</td>
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<td>PRESSURE, PSIA</td>
<td>48000</td>
<td>146960</td>
<td>146960</td>
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<td>ENTHALPY, K-BTU</td>
<td>713476</td>
<td>-20798</td>
<td>-15339</td>
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<tr>
<td>L/H LIQUID FRAC</td>
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**COMPOSITION, LB-MGLES/UNIT TIME**

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<th>Component</th>
<th>34</th>
<th>35</th>
<th>36</th>
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</thead>
<tbody>
<tr>
<td>ETHOH</td>
<td>1.26078</td>
<td>0.0000</td>
<td>83.43219</td>
</tr>
<tr>
<td>WATER</td>
<td>0.95885</td>
<td>0.0000</td>
<td>0.00000</td>
</tr>
<tr>
<td>BENZENE</td>
<td>3.96967</td>
<td>0.79995</td>
<td>0.79995</td>
</tr>
<tr>
<td>TOTAL</td>
<td>6.22930</td>
<td>0.79995</td>
<td>84.23215</td>
</tr>
</tbody>
</table>

**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, flagged 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

PROSIM (main program)

<table>
<thead>
<tr>
<th>PROSIM1</th>
<th>PROSIM2</th>
<th>PROSIM3</th>
<th>THERMOL</th>
</tr>
</thead>
<tbody>
<tr>
<td>(file)</td>
<td>(file)</td>
<td>(file)</td>
<td>(library)</td>
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</table>

<table>
<thead>
<tr>
<th>Prog.</th>
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<th>Prog.</th>
<th>Library</th>
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<tr>
<td>ABSR</td>
<td>ACTL*</td>
<td>ABSR1</td>
<td>ANYONE</td>
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<tr>
<td>ADBF*</td>
<td>BCTL*</td>
<td>ABSR2</td>
<td>INTLIZ</td>
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<tr>
<td>BZTL*</td>
<td>CLEAN</td>
<td>DIST1</td>
<td>DEWT1</td>
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<tr>
<td>CNTL*</td>
<td>COMP</td>
<td>DIST2</td>
<td>DEWP</td>
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<tr>
<td>CTRL</td>
<td>DCHECK</td>
<td>MATRIX</td>
<td>BUBT1</td>
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<tr>
<td>DCTL*</td>
<td>DENETS</td>
<td>CORECT</td>
<td>BUBT2</td>
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<tr>
<td>DIST</td>
<td>DPRINT</td>
<td>GAUSL</td>
<td>BUBP</td>
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<tr>
<td>DREAD</td>
<td>DSPT*</td>
<td>KCOLMN</td>
<td>TWOLIQ*</td>
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<tr>
<td>DVDR</td>
<td>ECTL*</td>
<td>KFAC</td>
<td>FLSH1*</td>
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<tr>
<td>EPRINT</td>
<td>EQCALL</td>
<td>TESTCL</td>
<td>FLSH2*</td>
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<tr>
<td>EQUIP</td>
<td>GSXP</td>
<td>SUMUP</td>
<td>AFLSH2*</td>
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<td>HTCL</td>
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<td>HYTR</td>
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<td>UNQAC2*</td>
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<td>UNIFAC*</td>
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</table>
G.2 Absorption/Distillation Program and Affiliated Subprograms

ABDIS (main program)

<table>
<thead>
<tr>
<th>ABDIS1 (file)</th>
<th>ABDIS2 (file)</th>
<th>ABDIS3 (file)</th>
<th>THERMOL (library)</th>
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G.3 Three Phase Flash Program and Affiliated Subprograms

FLASH2* (main program)

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<td>DEWP</td>
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<tr>
<td>BUBT1</td>
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</tr>
<tr>
<td>BUBT2</td>
<td></td>
</tr>
<tr>
<td>BUBP</td>
<td></td>
</tr>
<tr>
<td>TWOLIQ*</td>
<td></td>
</tr>
<tr>
<td>FLSH1*</td>
<td></td>
</tr>
<tr>
<td>FLSH2*</td>
<td></td>
</tr>
<tr>
<td>AFLSH2*</td>
<td></td>
</tr>
<tr>
<td>KCALC2*</td>
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</tr>
<tr>
<td>PRINT2*</td>
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<td>PRCKH</td>
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G.4 Non-linear Regression Program and Affiliated Subprograms

MARQDT (main program)

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<tr>
<th>Executive</th>
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<tbody>
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<td>(file)</td>
<td>(library)</td>
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FOFX*
INTLIZ*
BUBP
BUBPTL
TWOLIQ*
FXVLE*
FX2LIQ*
INFY*
KCALC2*
PRINT2*
PRINT3*
TALLY1*
PROGRAM PROSIM

VERSION # MARCH 1985

THE FOLLOWING ARE THE MAIN PROGRAM FILE AND OTHER SUPPLEMENTARY FILES:

(A) PROSIM1.FOR
(B) PROSIM2.FOR
(C) PROSIM3.FOR
(D) THERMO1.FOR
(E) THERMO2.FOR
(F) THERMO3.FOR
(G) DATABANK.UNIT (ONLY WITH UNIFAC ACTIVITY COEFFICIENT MODEL)

MODULES DELCP, GSXP AND COMP USE ONLY R-K EOS.

COMMON /CINIT/ NIN, NOUT, NOCOMP, NE, NEN, KUNIT
COMMON /EQPA/ BC(1252)
COMMON /ECBP/ CFC(150)
COMMON /HTST/ HC(300)
COMMON /STMA/ J(2403)
COMMON /STRMIN/ K(128)
COMMON /STMOUT/ LL(128)
COMMON /SYSAA/ M(70)
COMMON /SYSA/ NC(801)
COMMON /SYSB/ ND(127)
COMMON /SYSC/ PP(5)
COMMON /SYSD/ QFC(154)
COMMON /BLANK/ NCR, NPRT, KEEPIT(22)
COMMON /CMR/ NK, NCM1, NCP1, IDL, IDL, IDH, IDB, ISW,
* NDIM, ZNAME(2, 10), L(10), NDCOMP(10), NLQ, IPSET
COMMON /CLMN/ TIGER(22)
COMMON /ZDATA/ CAT(1107)
COMMON /STRT/ DDG(82)
COMMON /THML/ DUMB(71)
COMMON /ZFEED/ AAAA(15)

WRITE (6, 9999)
9999 FORMAT (" ", 30X, "PROGRAM PROSIM")

SYSTEM LIMITS
10 COMPONENTS
50 STREAMS
100 NODES (PIECES OF EQUIPMENT)

NCR=5
NPRT=6

KODE = 0 REQUIRES AN INITIALIZATION OF ALL VARIABLES
KODE = -1 IMPLIES A VARIATION OF THE PREVIOUS CASE
KODE = 1 PROBLEM DATA HAS ERRORS - TERMINATE PROGRAM

DEC Error-Set Routines Activated
Errset 72 = Floating Point Overflow
Errset 73 = Divide Check
Errset 74 = Floating Point Underflow
Errset 77 = Subscript Out Of Range

CALL ERRSET (72, .TRUE., .TRUE., .FALSE., .FALSE., 999)
CALL ERRSET (73, .TRUE., .TRUE., .FALSE., .FALSE., 999)
THIS BLOCK (ACTL) SIMULATES THE DISTILLATE RATE
OF AN AZEOTROPIC DISTILLATION COLUMN
BASED ON THE COMPUTED BOTTOMS PRODUCT COMPOSITION

* NEW ESTIMATE OF THE DISTILLATE RATE USING SECANT METHOD
  (IN CASE OF WET ALCOHOL PRODUCT)

* NEW ESTIMATE OF THE DISTILLATE RATE BY HEURISTIC METHOD
  (IN CASE OF DRY AND IMPURE ALCOHOL)

COMMON /BLANK/ NCR, NPPT, KEEPIT(22)
COMMON /CMPRO/ NK, NCM1, NCP1, IDLL, IDLV, IDM, LDBG, ISW,
* NDIM, ZNAME(2,10), L(10), NTCOMP(10), ALIQ, IPSET
COMM /CONTL/ NZIN, NGUT, NOCOMP, NE, NEN, KUNITS
COMMON /SYSC/ LA, LB, LC, LOOP, LOOPS
COMMON /SYSD/ KEFLAG(50), KSFLAG(100), KTRACE, DERRGR, NP_FREQ,
* IPUNCH
COMMON /EQPA/ ECPAR(25,50), NMAX, MAXEQP
COMMON /STRMIN/ SINUM(4), SIFLAG(4), SIVPRF(4), SITEMP(4), SIPRES(4),
* SINTH(4), SIVISC(4), SITHK(4), SIZ(4), SISC(4),
* SIFR(4), SIMO(4), SICOMP(10,4), SIKV(10,4)
COMMON /STMUT/ SGNUM(4), SOFLAG(4), SQVPRF(4), SQITEMP(4), SQIPRES(4),
* SGINTH(4), SGOVISC(4), SGITHK(4), SGZ(4), SGISC(4),
* SGIFR(4), SIMO(4), SGICOMP(10,4), SGKV(10,4)
REAL SIUM(4,12), SODUM(4,12), COMIN(10), ZF(10), XF(10)
REAL XBT(3), XBSRV(3)
INTEGER ISAVE(10)
EQUIVALENCE (SIDUM(1,1), SINUM(1)), (SDDLM(1,1), SONUM(1))
REAL XBSET(3)/0.99, 5.0E-3, 0.01/
REAL XBC(3)/0.99, 1.5E-4, 0.01/
REAL XCC(3)/0.28, 0.18, 0.54/

EQPAR(1, NE) = EQUIPMENT NUMBER
EQPAR(2, NE) = NUMBER OF STAGES IN STRIPPING SECTION
EQPAR(3, NE) = NUMBER OF STAGES IN RECTIFYING SECTION
EQPAR(4, NE) = TYPE OF UNIT
EQPAR(5, NE) = STAGE EFFICIENCY STRIPPING SECTION ... FRACTION
EQPAR(6, NE) = STAGE EFFICIENCY RECTIFYING SECTION ... FRACTION
EQPAR(7, NE) = TCP STAGE TEMPERATURE (DEG K)
EQPAR(8, NE) = BCTGM STAGE TEMPERATURE (DEG K)
EQPAR(9, NE) = TCP STAGE PRESSURE (ATM)
EQPAR(10, NE) = DOTTM STAGE PRESSURE (ATM)
EQPAR(11, NE) = TEMPERATURE TOLERANCE (DEFAULT = 0.01)
EQPAR(12, NE) = FLOW TOLLERANCE (DEFAULT = 0.0005)
EQPAR(13, NE) = NUMBER OF FEEDS
EQPAR(14, NE) = STAGE NUMBER FOR THE 1ST FEED
EQPAR(15, NE) = STAGE NUMBER FOR THE 2ND FEED
EQPAR(16, NE) = STAGE NUMBER FOR THE 3RD FEED
EQPAR(17, NE) = STAGE NUMBER FOR THE 4TH FEED
EQPAR(18, NE) = SPECIFIED DISTILLATE VAPCR RATE, DESTV
EQPAR(19, NE) = SPECIFIED DISTILLATE LIQUID RATE, DESTL
EQPAR(20, NE) = REFLEX RATIO OR BOILUP RATIO
EQPAR(21, NE) = DISTILLATE CCDE (ICODE)
   -1 : SUBCOOLED LIQUID
   0 : VAPO/LIQUID DISTILLATE
   +1 : LIQUID AT BUBBLE POINT
EQPAR(22, NE) = ITMAX (MAXIMUM VALUE FOR ITERATIONS)
EQPAR(23, NE) = DISTILLATE VAPOR/(V+L) FRACTION
EQPAR(24, NE) = MAX ITERATION FOR ACTL BLOCK
INPUT VALUES  NCASE  DESCRIPTION
3     3  DISTILLATION COLUMN (RR SPECIFIED)
4     4  DISTILLATION COLUMN (BOILUP SPECIFIED)
5     5  SELF REFLUXING COLUMN (BOILUP SPECIFIED)
6     6  SELF REBOILING COLUMN (RR SPECIFIED)

IOK=0 SUCCESSFUL CALCULATIONS
IOK=1 EXCESS BENZENE IN THE BTMS (ACTION INC DIST RATE)
IOK=1 EXCESS WATER IN THE BTMS (ACTION DEC DIST RATE)

DO LOOP ON SODUM=SIDUM

IF (LDBG * GE. 1) WRITE (6,9999)
9999 FORMAT ("","30X,"SUBROUTINE ACTL")

IF (LDBG * GE. 1) THEN
WRITE (NPRT,4)
4   FORMAT (/" PARAMETERS IN SUB. ACTL ARE:"/)
WRITE (NPRT,*) (C(J),J=1,12)
WRITE (NPRT,*) (ALPHA(J),J=1,6)
END IF

IOK=0
KNT=0
D RATE=0
ISW=0
SUM1=0.0
SUM2=0.0

DO 30 I=1,NCCOMP
      XF(I)=0.0
      ZF(I)=0.0
30   COMIN(I)=0.0
   DO 50 I=1,NCCOMP
   DO 50 J=1,NIN
   COMIN(I)=COMIN(I)+SICOMP(I,J)
50  SICOMP(I,J)=SICOMP(I,J)

   DO 60 J=3,12
   DO 60 I=1,NIN
   SODUM(I,J)=SIDUM(I,J)
60   D RATE=0.0
   FRATE=0.0
   DO 100 J=1,NIN
   SMOLE(J)=SIMOLE(J)
100  FRATE=FRATE+SMOLE(J)

   DO 150 I=1,NOCOMP
150  XF(I)=COMIN(I)/FRATE

LOOP FOR NEW ESTIMATION OF DISTILLATE RATE BY CHANGING
XD(2) BECAUSE X6(2)=0.0, OTHERWISE SET NEW VALUES OF
OTHER X6"S AND XD"S
EQPAR(18,NE)/EQPAR(19,NE) INITIALLY CARRIES FIRST GUESS

KUNITS=EQPAR(25,NE)+0.1
IF (KUNITS .EQ. 0) THEN
   D RATE=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
FXTSV = 0.95 * XB(2) - XBSET(2)

155 CONTINUE
SUM1 = 0.0
SUM2 = 0.0
SUM3 = 0.0
DO 160 I = 1, NCOMP
SUM1 = SUM1 + XF(I)
SUM2 = SUM2 + XD(I)
SUM3 = SUM3 + XB(I)
160 CONTINUE
DO 170 I = 1, NCOMP
XF(I) = XF(I) / SUM1
XD(I) = XD(I) / SUM2
XB(I) = XB(I) / SUM3
170 CONTINUE

C IF (LDBG .GE. 1) THEN
WRITE (NPRT, 240)
240 FORMAT (" SUB ACTL: FEED, DIST AND BTMS COMPOSITIONS /")
WRITE (NPRT, *) (XF(J), J = 1, NCOMP), (XD(J), J = 1, NCOMP),
* (XB(J), J = 1, NCOMP)
WRITE (NPRT, *)
WRITE (NPRT, 250) DRATE, FRATE
250 FORMAT (" CHECK IN ACTL: DRATE & FRATE ", 2E20.8)
END IF
C 290 IF (FRATE - DRATE) .LT. 300, 300, 350
300 DRATE = 0.9 * FRATE
GO TO 290
C WRITE (NPRT, 310)
C 310 FORMAT (" PROGRAM 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)) .GE. 400, 420, 400
400 EQPAR(18, NE) = 0.0
EQPAR(19, NE) = DRATE
GO TO 560
420 EQPAR(18, NE) = DRATE - EQPAR(23, NE)
EQPAR(19, NE) = DRATE + (1.0 - EQPAR(23, NE))
500 IF (LDBG .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 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 IDIST
WRITE (NPRT, 578)
578 FORMAT (" SUB ACTL STMT#578: RETURNED FROM DIST")
C
C CHECK WHETHER THE BTMS COMPOSITION IS CORRECT
C SDCOMP(I,2)
DO 600 I=1,NOCOMP
600 XBT(I)=SDCOMP(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 ETCH & 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 C LESS ETCH & MORE WATER IN BTMS
IF (XBT(1) .LT. XBSET(1) .AND.
 % XBT(2) .GT. XBSET(2)) IOK=2
C C LESS ETCH, 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 D RATE
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*(D RATE-DRSV)/(FXN-FXNSV)
END IF
IF (IOK .EQ. 1) DELTA=0.0005*DRAT E
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
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

THIS MODULE HAS BEEN EXPANDED TO TAKE CARE OF 13 DIFFERENT CASES BY CALLING SUBPROGRAM ANYONE, A GENERALIZED FLASH ALGORITHM

COMMON /BLANK/ NCR, NPRT, KEEPIT(22)
COMMON /CONTL/ NIN, NOUT, NOCOMP, NE, NEN, KUNITS
COMMON /CMRDO/ NK, NCM1, NCPI, IDLL, IDLV, IDM, LDEBUG, ISW,
* NDIM, NAME(2,10), L(10), NTCOMP(10), NLIQ, IPSET
COMMON /SYSB/ KRET(66), KCNT, KDUM(4), IRGMAN(56)
COMMON /SYSC/ KERFLAG(50), KSFLAG(100), KTRACE, ERRDR, NPFR, NPFR, *
* IPUNCH
COMMON /ECPA/ ECPAR(25,50), NEMAX, MAXEQP
COMMON /STRMIN/ SINUM(4), SIFLAG(4), SIVPFRC(4), SITEMP(4), SIPRES(4), *
* SIENTH(4), SIVISC(4), SITHK(4), SIZ(4), SIS(4), *
* SIFRAL(4), SIMOLE(4), SIMO(10,4), SIKV(10,4)
COMMON /STHOUT/ DONUM(4), SOFLAG(4), SOVPFRC(4), SORTMP(4), SOPRES(4), *
* SDENTH(4), SDOVISC(4), SOTHK(4), SIZ(4), SSO(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), VPC(10), FUG(10), GAMC(10), SVAP, *
* HOFZ, HVAP, HLTIQ, DHV, XSH, NOBUB, NODEW
COMMON /TWCLQ/ XI(10), X2(10), DUMB1(40), DHL(2), HIDLL(2), *
* HRELL(2), FRAO, DUMB2(4)
COMMON /ZFEEDZ/ PF, TF, FEED(10), AAA(3)

EQPAR(1,NE) = EQUIPMENT NUMBER
EQPAR(2,NE) = MODE OF FLASH CALCULATION

WRITE (6,9999)
9999 FORMAT(’”.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

NOUT=1 FOR MODE # 5 AND PRESET IN THE CALLING PROGRAM
NOUT=2 FOR MODE # 1, 3, 6, 11, 13
NOUT=3 FOR MODE # 2, 4, 7, 8, 9, 10, 12

OPTIONS AVAILABLE FOR TOTAL # OF OUTPUT STREAMS FROM THE EQUIPMENT MODULE "ADB" ARE: 1, 2 OR 3.

MODE=NTYPE

<table>
<thead>
<tr>
<th>NTYPE</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>DEW POINT TEMPERATURE</td>
</tr>
<tr>
<td>2</td>
<td>BUBBLE POINT TEMPERATURE (1/2 LIQ)</td>
</tr>
<tr>
<td>3</td>
<td>ALL VAPOR ENTHALPY WITH PRIOR DEW POINT</td>
</tr>
<tr>
<td>4</td>
<td>ALL LIQUID ENTHALPY WITH PRIOR BUBBLE POINT (1/2 LIQ)</td>
</tr>
<tr>
<td>5</td>
<td>ALL VAPOR ENTHALPY</td>
</tr>
<tr>
<td>6</td>
<td>ALL LIQUID ENTHALPY (1/2 LIQ)</td>
</tr>
<tr>
<td>7</td>
<td>ISOTHERMAL FLASH (1/2 LIQ)</td>
</tr>
<tr>
<td>8</td>
<td>ISOTHERMAL FLASH ... NO DEW/BUBBLE POINT (1/2 LIQ)</td>
</tr>
<tr>
<td>9</td>
<td>ADIABATIC FLASH (1/2 LIQ)</td>
</tr>
<tr>
<td>10</td>
<td>ADIABATIC FLASH ... NO DEW/BUBBLE POINT (1/2 LIQ)</td>
</tr>
<tr>
<td>11</td>
<td>DEW POINT PRESSURE</td>
</tr>
</tbody>
</table>
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GO TO 200
END IF

C NOUT=2 & MCCE<>13: OUTPUT STREAM (1) VAPOR & (2) 1/2 LIQUID
C NOUT=2 & MODE=13 : OUTPUT STREAMS ARE ONLY LIQUID
   (1) LIGHT PHASE
   (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
  SITEMP(1)=T
  SITEMP(2)=T
  SDTEMP(1)=T
  SDTEMP(2)=T
  GO TO 36
  SOPRES(1)=P
  SOPRES(2)=P
  CONTINUE
C
C IF (MODE .EQ. 13) THEN
  SGVPFR(1)=0.0
  SGVPFR(2)=0.0
  SORFAL(1)=1.0
  SORFAL(2)=1.0
  SMLOLE(1)=SIMOLE(1)*FRACL
  SMLOLE(2)=SIMOLE(1)*(1.0-FRACL)
  SENTH(1)=HREAL(1)*SMLOLE(1)
  SENTH(2)=HREAL(2)*SMLOLE(2)
  DO 38 I=1,NOCOMP
       SCOMP(I,1)=X1(I)*SMLOLE(1)
  38 SCOMP(I,2)=X2(I)*SMLOLE(2)
  GO TO 200
ELSE
  SGVPFR(1)=1.0
  SGVPFR(2)=0.0
  SORFAL(1)=0.0
  SORFAL(2)=FRACL
  SMLOLE(1)=SIMOLE(1)*FRACV
  SMLOLE(2)=SIMOLE(1)*(1.0-FRACV)
  SENTH(1)=HVAP*SMLOLE(1)
  SENTH(2)=(HREAL(1)*FRACL+HREAL(2)*(1.0-FRACL))*SMLOLE(2)
  SGZ(I)=IVAP
  DO 40 I=1,NOCOMP
       SCOMP(I,1)=Y(I)*SMLOLE(1)
  40 SCOMP(I,2)=(X1(I)*FRACL+X2(I)*(1.0-FRACL))*SMLOLE(2)
  GO TO 200
END IF
END IF

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 SDTEMP(I)=T
  GO TO 56
  SOPRES(I)=P
  CONTINUE
CONTINUE
SOPVFRC(1)=1.0
SOPFRA(1)=0.0
DO 60 I=2,3
SOPFRA(I)=1.0
60    SOPVFRC(I)=0.0

SOMOLEC1=SOMOLEC1*FRACV
SOMOLEC2=SOMOLEC1*(1.0-FRACV)*FRACL
SOMOLEC3=SOMOLEC1*(1.0-FRACV)*(1.0-FRACL)
SOENTH(1)=MVAP*SCMOLE(1)
SOENTH(2)=MREALL(1)*SOMOLE(2)
SOENTH(3)=MREALL(2)*SOMOLE(3)
SOZ(1)=ZVAP
DO 70 I=1,NCOMP
SOCOMP(I,1)=YC(I)*SOMOLEC1
SOCOMP(I,2)=XC(I)*SOMOLEC2
70    SOCOMP(I,3)=XZ(I)*SOMOLEC3
GO TO 200
END IF

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

RETURN
END SUBROUTINE ECTL

BCTL BLOCK TAPS THE VALUES FROM THE REFERENCE STREAMS
C + VE FOR INCOMING C - VE FOR OUTGOING STREAMS] AND
MAKE NEW ESTIMATE OF DISTILLATE OF THE TARGET DIST
BLOCK. AT PRESENT BLOCK IS DESIGNED FOR THE BENZENE
STRIPPING COLUMN

COMMON /BLANK/ NCR, NPRT, KEEPIT(22)
COMMON /COMPO/ NK, NCM1, NCP1, IDLL, IDLV, IDH, LDBG, ISW,
     NDIM, ZNAMEC(2,10), L(10), NTCOMP(10), NLIQ, IPSET
COMMON /CON TL/ NIN,NOUT,NCOMP,NE,NEK,NUMITS
COMMON /SYSC/ LA,LB,LC,LOOP,LOGPS
COMMON /SYSD/ KEFLAG(50),KSFLAG(100),KTRACE,ERROR,NPFRQ,
     IPCUNCH
COMMON /EQPA/ EQPARD(25,50),NMAX,MAXEQP
COMMON /STMA/ SEXTSV(13,100),SINTSV(11,100),NSMAX,MAXSEX,MAXSM
COMMON /STRMIN/ SINUM(4),SFILAG(4),SIVPFRC(4),SITEMP(4),SIPRES(4),
     SIVTH(4),SIVISC(4),SITHK(4),SIZ(4),SIS(4),
     SIFRAC(4),SIMOLE(4),SCOMP(10,4),SIK(10,4)
COMMON /STOUT/ SONUM(4),SOFLAG(4),SOVPFRC(4),SOTEMP(4),SOPRES(4),
     SCENTH(4),SOVIS(4),SOTHK(4),SOZ(4),SOS(4),
     SOFRA(4),SOMOLE(4),SOCOMP(10,4),SOV(10,4)
REAL SNUMC(4,12),SDUMC(4,12),CNUMC(10),DR(10),XFC(10)
INTEGER ISAVE(10), ISTRM(4), IOCMP(3)
EQUIVALENCE (CSDUM(1,1),CINUM1), (CSUMC(1,1),CSUMK(1))
DATA K, MAXEQP /0, 10/
REAL X(3)/0.995, 1.0E-5, 0.005/
REAL X(3)/0.31642, 0.14041, 0.54317/
C EQPAR(1,NE) = BLOCK/NODE #
C EQPAR(2,NE) = DISTILLATION COLUMN BLOCK/NODE #
C EQPAR(3,NE) = CODE FOR DIST STREAM TYPE
    (-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 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 EQPAR(13,NE) TO EQPAR(25,NE) = 0.0
C
C LOAD THE OUTPUT STREAM WITH THE INPUT STREAM
C DO LOOP ON SODUM=SIDUM
C
DO 30 I=1,NCCOMP
   XFI(I)=0.0
   DRI(I)=0.0
30   COMIN(I)=0.0
   ITAG1=0
   IF (EQPAR(9,NE) LT 0.0) ITAG1=1
   DO 50 I=1,NCCOMP
   DO 50 J=1,NIN
      COMIN(I)=COMIN(I)+SICOMP(I,J)
      SICOMP(I,J)=SICOMP(I,J)
50
   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(14,NE) NE 0.0) THEN
      ISTRM(I)=SIGN(ABS(EQPAR(14,NE))+0.1,EQPAR(14,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(I)
   J2=ICOMP(2)
   IF (ISTRM(I) GT 0.0) THEN
      IF (SEXPSV(J1+3,ISTRM(I)) GT 0.0 AND.
         SEXPSV(J2+3,ISTRM(I)) GT 0.0 ) THEN
         B1=B1+SEXPSV(J1+3,ISTRM(I))
         B2=B2+SEXPSV(J2+3,ISTRM(I))
      END IF
   ELSE IF (ISTRM(I) LT 0.0) THEN
      INITM=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

85 CONTINUE

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 (NPR,T,90) B1, B2
90 FORMAT (' SUB BCTL: ESTIMATED B1 AND B2 FOR BZ
  % STRIPPING COLUMN ARE '/2E25.8)

C THIS IS FOR THE 1ST ENTRY IN BCTL BECAUSE
C SEXTSV ARRAY IS CLEAN IF THE REFERENCE STREAMS ARE
C NOT YET PROCESSED FOR A SINGLE TIME.
C
C IF (DRATE .EQ. 0.0) DRATE=2*COMIN(3)
C
C IF (ITAG1 .EQ. 1) GO TO 350
FRATE=0.0
DO 100 J=1,NIN
  SGMLE(J)=SIMCLE(J)
100 FRATE=FRATE+SGMLE(J)

C IF (LDBG .GE. 1) THEN
WRITE (NPR,T,240)
240 FORMAT (' SUB BCTL: FEED, DIST AND BTMS COMPOSITIONS '/)
WRITE (NPR,T,250) (XF(J),J=1,NOCOMP),(XF(J),J=1,NOCOMP),
  (XF(J),J=1,NOCOMP)
WRITE (NPR,T,250) DRATE, FRATE, B1, B2
250 FORMAT (' CHECK IN BCTL: DRATE / FRATE / B1 / B2'/4E16.5)
END IF
C
C IF (FRATE=CRATE) 300,300,350
300 WRITE (NPR,T,310)
310 FORMAT (' PROGRAM STOPPED ... DISTILLATE RATE TOO HIGH. READ
  * PROPER VALUES OF XC & XB ARRAYS IN BCTL 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 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 (LDBG = NE. 1) THEN  
WRITE (NPRINT, 550) EQPAR(18, II), EQPAR(19, II)  
WRITE (NPRINT, *)  
END IF  
550 FORMAT (/" SUB DSPT: DESTV = "+E13.5," & DESTL = "+E13.5)  
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 = E13.5) GC 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  
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, IDM, LDBG, ISW,  
* NCIM, ZNAME(2, 10), L(10), NTCOMP(10), KLIG, IPSET  
COMMON / CONTL / NIN, NOT, NOCOMP, NE, NEN, KUNITS  
COMMON / Sysc / LA, LB, LC, LOOP, LOOP  
COMMON / SYSO / KEFLAG(50), KSFLAG(100), KTRACE, CERROR, NPFREK,  
* IPLNCH  
CCOMMON / EPQA / EQPAR(25, 50), NMAX, MAXEQP  
COMMON / STMHA / SEX, TS(13, 100), SINTV(11, 100), NSMAX, MAXSEX, MAXSIN  
COMMON / STRMIN / SINUM(4), Sigflag(4), SIVPFR(4), SITEMP(4), SIPRES(4),  
* SENTH(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), SOVPF(4), SGTEMP(4), SOPRES(4),  
* SGENTH(4), SIVISC(4), SOTHK(4), SIZ(4), SOS(4),  
* SGFRL(4), SISMOLE(4), SICOMP(10, 4), SOKV(10, 4)  
REAL SIDUM(4, 12), SODUM(4, 12), COMIN(10), DRC(10), XK(10)  
INTEGER ISAVE(10), ISTRM(4)  
EQUIVALENCE (SIDUM(1, 1), SINUM(1)), (SDDUM(1, 1), SODUM(1))  
DATA K, ISV, ERROR /0, 0, 0.01/
DATA BTM1, BTM2 / 10.995, 17.2726/
INTEGER ICOMP(3)/ 1, 2, 0/

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) = TCP STAGE TEMPERATURE (DEG K)
C EQPAR(8,NE) = BOTTOM STAGE TEMPERATURE (DEG K)
C EQPAR(9,NE) = TCP STAGE PRESSURE (ATM)
C EQPAR(10,NE) = BOTTOM STAGE PRESSURE (ATM)
C EQPAR(11,NE) = TEMPERATURE TOLERANCE (DEFAULT = 0.01)
C EQPAR(12,NE) = FLOW TOLERANCE (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)
   -1 : SUBCOOLED LIQUID
   0 : VAPOR/LIQUID DISTILLATE
   +1 : LIQUID AT BUBBLE POINT
C EQPAR(22,NE) = ITRMAX (MAXIMUM VALUE FOR ITERATIONS)
C EQPAR(23,NE) = DISTILLATE VAPOR/(V+L) FRACTION

C INPUT VALUES NGASE DESCRIPTION
C 3 3 DISTILLATION COLUMN (RR SPECIFIED)
C 4 4 DISTILLATION COLUMN (BGILUP SPECIFIED)
C 5 5 SELF REFLUXING COLUMN (BOILUP SPECIFIED)
C 6 6 SELF REBOILING COLUMN (RR SPECIFIED)

C
C IGK=0 SUCCESSFUL CALCULATIONS
C IGK=1 EXCESS BENZENE IN THE BTMS (ACTION INC DIST RATE)
C IGK=1 EXCESS WATER IN THE BTMS (ACTION DEC DIST RATE)

C
C IF (LDBGUG .GE. 1) WRITE (6,9999)
9999 FORMAT("",30X,"SUBROUTINE BITL")
ISV=0
C
C IF (LDBGUG .GE. 1) THEN
C WRITE (NPRP,4)
C 4 FORMAT (/" PARAMETERS IN SUB. ACTL ARE:"/)
C WRITE (NPRP,*),(C(J),J=1,12)
C WRITE (NPRP,*),(ALPHA(J),J=1,6)
C END IF
DO 30 I=1,NCCOMP
30 COMINC(I)=0.0
DO 50 I=1,NCCOMP
DO 50 J=1,NIN
50 COMINC(I)=COMINC(I)+SICOMP(I,J)
C 50 SICOMP(I,J)=SICOMP(I,J)
C DO 60 J=3,12

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DO 60 I=1,HIN
60 SUMD(I,J)=SIDUM(I,J)

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

CASE THE BLOCK IS USED STAND ALONE
KOUNT=0
DO 75 I=1,3
75 IF (ISTRM(I) .EQ. 0) KOUNT=KOUNT+1

ALL STREAM NUMBERS ARE 0
IF (KOUNT .EQ. 3) THEN
  B1=BTM1*453.59
  B2=BTM2*453.59
  GO TO 85
END IF

DO 80 I=1,3
80 ICOMP(I)=ECPAR(I,B,NE)+0.1

COMPUTE BTMS RATE OF 1 AND 2 BY ESTABLISHING MASS
BALANCE BASED UPON THE REFERENCE STREAMS

B1=0
B2=0
DO 85 I=1,4
J1=ICOMP(I)
J2=ICOMP(2)
IF (ISTRM(I) .GT. 0) THEN
  IF (SEXSV(J1+3,ISTRM(I)) .GT. 0.0 .AND.
    (SEXSV(J2+3,ISTRM(I)) .GT. 0.0) ) THEN
    B1=B1+SEXSV(J1+3,ISTRM(I))
    B2=B2+SEXSV(J2+3,ISTRM(I))
  END IF
ELSE IF (ISTRM(I) .LT. 0) THEN
  ICMPM=ABS(ISTRM(I))
  IF (SEXSV(J1+3,ICMPM) .GT. 0.0 .AND.
    (SEXSV(J2+3,ICMPM) .GT. 0.0) ) THEN
    B1=B1-SEXSV(J1+3,ICMPM)
    B2=B2-SEXSV(J2+3,ICMPM)
  END IF
END IF
85 CONTINUE

COMPUTATION OF COMPONENT DISTILLATE RATE

IF (B1 .LT. 0.0) B1=0.0
IF (B2 .LT. 0.0) B2=0.0
D1=COMIN(I)-B1
D2=COMIN(2)-B2
D3=COMIN(3)
D RATE=D1+D2+D3
D RMIN=COMIN(3)
WRITE (NPRT,90) B1, B2
90 FORMAT (*) SUB BITL: ESTIMATED B1 ANO B2 FOR B2
  STRIPPING COLUMN ARE */2E25.6)
THIS IS FOR THE 1ST ENTRY IN BCTL BECAUSE
SEXTSV ARRAY IS CLEAN IF THE REFERENCE STREAMS ARE
NOT YET PROCESSED FOR A SINGLE TIME.

IF (D RATE .EQ. 0.0) D RATE = 2 * COMIN(3)

FRATE = 0.0
DO 100 J = 1, NMIN
   SDMCL(J) = SMQLE(J)
100   FRATE = FRATE + SIMOLE(J)

IF (LDBG .GE. 1) THEN
   WRITE (NPRT, 240)
240 FORMAT (' SUB BZTL: 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) D RATE, FRATE, B1, B2, (COMIN(I), I = 1, NOCOMP)
250 FORMAT (' CHECK IN BZTL: D RATE / FRATE / B1 / B2 / COMIN/
   4E16.5 / 5E16.5 )
END IF

SETTING MAX AND MIN DIST RATES W.R.T. BENZENE SPECS IN THE
DISTILLATE/BOTTOMS
MAX RATE: 0.98 * FRATE (ARBITRARY) OR COMPUTE BASED UPON
BZ SPECS
MIN RATE: DIST RATE (WITH BZ IN DIST = 0.995 TO 0.997
OF ENTERING BZ)
IF MIN RATE DOES NOT SATISFY THE ETHANOL SPECS IN BOTTOMS,
SEARCH FOR DIST RATE BETWEEN MIN AND MAX RATES FIXED.
IF EACH SPECS ARE NOT MET, SELECT MIN DIST RATE FOR
SEPERATION.
LOOP STARTS HERE
KNT = 0
DRSV = 0.9 * D RATE
275 IF (FRATE - D RATE) 300, 300, 350
300 D RATE = 0.9 * FRATE
   GO TO 275
WRITE (NPRT, 310)
310 FORMAT (' PROGRAM STOPPED ... DISTILLATE RATE TOO HIGH. READ
   # PROPER VALUES OF XC & XB ARRAYS IN DCTL BLOCK ')
   CALL EXIT
   RETURN

   350 IF (EQPAR(21, NE)) 400, 420, 400
400 EQPAR(18, NE) = 0.0
   EQPAR(19, NE) = D RATE
   GO TO 500
420 EQPAR(18, NE) = D RATE * EQPAR(23, NE)
   EQPAR(19, NE) = D RATE * (1.0 - EQPAR(23, NE))
500 IF (LDBG .GE. 1) THEN
      WRITE (NPRT, 550) EQPAR(18, NE), EQPAR(19, NE)
      WRITE (NPRT, *)
END IF

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*(SOCCOMP(1, ICOMP(1), 2) - B1)
C IF (KNT .GT. 0) CALL ZDIST
WRITE (NPRT, 578)
578 FORMAT (" SUB BZTL STMT 578: RETURNED FROM DIST")
C CHECK WHETHER THE BTMS COMPOSITION IS CORRECT
C
SOCCOMP(I, 2)
IF (LDBG .GE. 1) THEN
WRITE (NPRT, 550) EQPAR(18, NE), EQPAR(19, NE)
WRITE (NPRT, *)
END IF
IOK = 0
XD3 = ABS(CMIN(3) - SOCCOMP(3, 1)) / CMIN(3)
C IF (XD3 .GE. 0.995 AND XD3 .LE. 0.997) DRMIN = DRATE
C IF (SOCCOMP(3, 2) .GT. ERROR) IOK = 3
C IF (IOK .NE. 0) GO TO 600
C IF (KNT .LE. 10) THEN
FX = SOCCOMP(1, 2) - B1
C ELSE
FX = SOCCOMP(3, 2)
C END IF
C FX = SOCCOMP(1, 2) - B1
IF (FX - ERRCR) 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. (IICK .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. IICK .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, " ICK = " , 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) GC TO 275
WRITE (NPRT, 690)
690 FORMAT (" BZTL STOPPED: ITERATION LIMIT EXCEEDED")
CALL EXIT
C
700 WRITE (NPRT, 710)
710 FORMAT ('BITL SUCCESSFULLY COMPLETED')

RETURN
END

SUBROUTINE CNTL

OPTIONS IN CNTL

1. MANIPULATION OF THE COMPONENTIAL FLOW OF THE TARGET STREAM
   BASED UPON DIFFERENCE IN TWO RATES

2. MANIPULATION OF THE COMPONENTIAL FLOW OF THE TARGET STREAM
   BASED UPON RATIOS OF TWO STREAM RATES

THIS BLOCK USES SECOND STREAM AS THE TARGET STREAM, THE
COMP. FLOW IS CHANGED WITH REFERENCE TO THE FIRST INCOMING
STREAM.

COMMON /BLANK/ NCR, NPRT, KEEPIT(22)
COMMON /CMPRO/ NK, NCMI, NPCI, IDIL, IDLV, IDH, LDBG, ISW,
* NDIM, ZNAMEC(2,10), LC(10), NTCOMP(10), ALIQ, IPSET
COMMON /CONTL/ NIN,NOUT, NOCOMP, NE, NEN, KUNIT5
COMMON /SYSC/ LA, LB, LC, LOOP, LOOPS
COMMON /SYSD/ KEFLAG(50), KSFLAG(100), KTRACE, DERROR, NPFREQ,
* IPUNCH
COMMON /EGPA/ ECPAR(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 /STMON/ SDNUM(4), SDFLAG(4), SODPFR(4), SOTEMP(4), SDPRES(4),
* SODENTH(4), SODVISC(4), SOTHK(4), SGZ(4), SOS(4),
* SDRALF(4), SSMOLE(4), SSOCOMP(10,4), SSOV(10,4)
REAL SICUM(4,12), SODUM(4,12), SICK(12), SICO(12)
INTEGER ISAVE(10)
EQUIVALENCE (SINUM(1,1), SINUM(1,1)), (SDODM(4,1,1), SDUM(1,1))
DATA K, MIG, 250 /0, 10/
DATA RMIN, RMAX /1.05, 2.12/

EQPAR(1,NE) = BLOCK/NODE #
EQPAR(2,NE) = OPTION #
EQPAR(3,NE) = COMPONENT # TO BE CONTROLLED
EQPAR(4,NE) = MIN RAT. FOR OPTION 2
EQPAR(5,NE) = MAX RAT. FOR OPTION 2
EQPAR(6,NE) = MAX FLOW OF COMPONENT # IN EQPAR(3,NE)
EQPAR(7,NE) THRU EQPAR(25,NE) = 0.0

LOAD THE OUTPUT STREAM WITH THE INPUT STREAM

DO LOOP ON SDUM=SICUM
KUNIT5=EQQPAR(25,NE)+0.1
IF (KUNIT5 .LT. 0) GO TO 10
EQPAR(6,NE)=EQPAR(6,NE)+453.59
EQPAR(25,NE)=0.0
CONTINUE

IF (EQPAR(2,NE) = 2.0) GO TO 250

OPTION 1
ICOMP=EQQPAR(3,NE)+0.1
IF (SICOMP(1,ICOMP)+EQ. 0.0) GO TC 350
DIFF=SICOMP(1,ICOMP)-SICOMP(1,ICOMP)
SOCOMP(ICOMP,2)=SICOMP(ICOMP,2)+DIFF
IF (SGCOMP(ICOMP,2) GT E QPAR(6,NE)) SOCOMP(ICOMP,2)=E QPAR(6,NE)
SUM=0.0
DO 150 J=1,NOCOMP
  SICOMP(J,2)=SOCOMP(J,2)
150 SUM=SUM+SGCOMP(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=SOMCLE(1)/SOMOLE(2)
    IF (RATIO LT RMIN) THEN
      SUM=0.0
      DO 280 I=1,NOCOMP
        SCOMP(I,2)=0.99*SCOMP(I,2)
      280 SUM=SUM+SCOMP(I,2)
      SOMOLE(2)=SUM
      GO TO 275
    ELSE
      IF (RATIO GE RMAX) THEN
        SUM=0.0
        DO 300 I=1,NOCOMP
          SCOMP(I,2)=1.01*SCOMP(I,2)
        300 SUM=SUM+SCOMP(I,2)
        SOMOLE(2)=SUM
        GO TO 275
      END IF
    END IF
END IF

C 350 CONTINUE C

ESTABLISHING STREAM # 2 VIA ISOTHERMAL FLASH

ESAVE=EQPAR(2,NE)
NSE=NUM
DO 360 I=3,12
  SID(I)=SIDUM(1,I)
360 SICUM(I,1)=SIDUM(2,I)
DO 370 I=1,NOCOMP
  SIC(I)=SICOMP(I,1)
370 SICOMP(I,1)=SICCMP(I,2)

C E QPAR(2,NE)=8.0
NCUT=1
CALL ADIF
C RESTORE THE STREAM VARIABLES E QPAR(2,NE)=ESAVE
NSE=NSE
DO 372 I=3,12
  SIDUM(2,I)=SIDUM(1,I)
372 SICUM(I,1)=SID(I)
DO 374 I=1,NOCOMP
  SICOMP(I,2)=SICOMP(I,1)
374 SICOMP(I,1)=SIC(I)

C DO 380 J=3,12
DO 380 I=1,12
380

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380 SODUM(I,J)=SIDUM(I,J)
390 DO 390 I=1,NIN
       DO 390 J=1,NOCOMP
390 SGCMP(J,I)=SGICMP(J,I)
       IF (LDBUG .GE. 1) WRITE (6,400) ICOMP, SICMP(ICOMP,2),
          * SGCMP(ICOMP,2)
400 FORMAT (/" IN SUB CNTL: ICOMP, SICMP & SGCMP OF (ICOMP,2)
          * ARE "/,I5,2E15.5)
900 RETURN
END

SUBROUTINE DCTL

DCTL DYNAMICALLY SIMULATES THE FEED-FORWARD CONTPLIC
OF THE SPLIT IN AN AIEOTROPIC DISTILLATION COLUMN
BASED UPON THE COMPSITE FEED COMPOSITION AND RATE
AND THE ASSUMED DISTILATE AND BOTTOMS COMPOSITION.
THIS BLOCK CAN BE EASILY EXTENDED TO ANY DISTILLATION
COLUMN.

COMMON /BLANK/ NCRT, NPRET, KEEPIT(22)
COMMON /CMRO/ NK, NC1, NCP1, IDL1, IDL2, IDH, LDBG, ISW,
               NDIM, NZNAMEC(2,10), L(10), NTCOMP(10), NLIQ, IPSET
COMMON /CROUTE/ NIN, NOUT, NOCOMP, NE, NEN, KUNITS
COMMON /SYS/ LA, LB, LC, LOOP, LOOPC
COMMON /SYSD/ KEFLAG(503), KSFLAG(100), KTRACE, QERROR, NPFRQ,
               * IPUNCH
COMMON /ECPAR/ ECPAR(25,50), NEMAX, MAXEOP
COMMON /STRMIN/ SINUM(4), SIFLAG(4), SIVPFR(4), SITEMP(4), SIPRES(4),
                * SIENTH(4), SIVISC(4), SITHK(4), SIZ4, SIS(4),
                * SIFRAC(4), SIMOLE(4), SICOMP(10), SIKV(10),
COMMON /STMOUT/ SONUM(4), SGFLAG(4), SOVPF(4), SQTEMP(4), SQPRES(4),
                * SCENTH(4), SOVISC(4), SOTHK(4), SIZ(4), SIS(4),
                * SCIFRAC(4), SMCLE(4), SICOMP(10), SCKV(10),
REAL SUDUM(4,12), SDUM(4,12), COMINC(10), ORC(10), XCF(10)
REAL XD(3), X(3)
INTEGER ISAVE(10)
EQUIVALENCE (SIDUM(1,1), SINUM(1,1), (SODUM(1,1), SDUM(1,1))
DATA K, MAXGSP /0, 10/
REAL XE(3)/0.995, 1.0-5, 0.005/
REAL XD(3)/-31642, 0.14041, 0.54317/

EQPAR(1,NE) = BLOCK/NO
EQPAR(2,NE) = DISTILLATION COLUMN BLOCK/NO
EQPAR(3,NE) = CODE FOR DIST STREAM TYPE
   (-1:SUBCCCLED LIQUID, 0:VAPOR/LIQUID, +1:LC AT BUS T)
EQPAR(4,NE) = DISTILLATE VAPOR/(V+L) FRACTION
EQPAR(5,NE) THRU EQPAR(NOCOMP+4,NE) = XD (I), I=1,NOCOMP
EQPAR(NOCOMP+5,NE) THRU EQPAR(2*NOCOMP+4,NE) = XB (I), I=1,NOCOMP
   XD AND XB ARE GUESSED VALUES OF DISTILLATE
   AND BOTTOMS COMPONENT MOLE FRACTIONS
IF EQPAR(5,NE) .GE. 2.0 THEN DEFAULT VALUES ARE USED
IF EQPAR(5,NE) < 0 NO CHANGE IS MADE IN DIST RATE,
ITAG1 IS USED WITH REFERENCE TO IT.
LOAD THE OUTPUT STREAM WITH THE INPUT STREAM
DG LOOP ON SODUM=SIDUM
IF (EQPAR(5,NE) .GE. 2.0) GO TO 20
DO 20 I=1,NCCOMP
  XDC(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
  SGMLE(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+XDC(I)
  SUM3=SUM3+XB(I)
160 CONTINUE
DO 170 I=1,NOCOMP
  XF(I)=XF(I)/SUM1
  XDC(I)=XDC(I)/SUM2
  XB(I)=XB(I)/SUM3
170 CONTINUE

C
C
DO 180 I=1,NOCOMP
180 DR(I)=(XF(I)-XB(I))/(XDC(I)-XB(I))=CCMIN(I)
C
DO 190 I=1,NOCOMP
190 DRATE=DRATE+DR(I)

C
C
DO 180 I=1,NOCOMP
180 DR(I)=(XF(I)-XB(I))/(XDC(I)-XB(I))=FRATE
C
DO 190 I=1,NOCOMP
190 DRATE=DRATE+DR(I)

C
C
CALCULATION OF CRATE USING ASSUMED VALUES OF DIST AND BTMS
C COMPOSITIONS THRU EQPAR MATRIX

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DRATE=(X8(2)*COMIN(1)-X8(1)*COMIN(2))/
%  (X8(2)*XD(1)-X8(1)*XD(2))

C
IF (LDBG .GE. 1) THEN
  WRITE (NPRT,240)
240  FORMAT (" SUB DCTL: FEED, DIST AND BTMS COMPOSITIONS ")
  WRITE (NPRT,*) (X(J),J=1,NOCOMP),(XD(J),J=1,NOCOMP),
  * (X8(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 ",2E20.6)
END IF

C
IF (FRATE-DRATE) 300,300,350
300  WRITE (NPRT,310)
310  FORMAT ("PROGRAM STOPPED ... DISTILLATE RATE TOO HIGH. READ
* PROPER VALUES OF XD & XB ARRAYS IN DCTL BLOCK ")
  CALL EXIT
  RETURN

C
DIST RATE ASSIGNED TO EQPAR OF THE PROPER DISTILLATION BLOCK
UNITS OF EQPAR AND DRATE ARE DIFFERENT

C
ISAVE ARRAY STORES THE DIST COLUMN BLOCK # WHICH HAS BEEN
PROCESSED ONCE. SECOND TIME, FOR THE SAME BLOCK #, UNITS
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
402  EQPAR(19,II)=DRATE
    GO TO 500
420  EQPAR(18,II)=DRATE*EQPAR(4,NE)
422  EQPAR(19,II)=DRATE*(1.0-EQPAR(4,NE))
500  IF (LDBG .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
DSFMAX IS THE MAX # OF DSPT MODULES IN A FLGWSHEME

C
560  K=K+1
  IF (K .GE. MAXDSP) GO TO 700
DG 570  I=K,MAXDSP
570  ISAVE(I)=0
  ITAG=0

C
  GO 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

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C 700 RETURN
END

SUBROUTINE DSPT

DSPT SIMULATES THE FEED-FORWARD CONTROL OF THE SPLIT IN A
DISTILLATION COLUMN. THE SPLIT (ASSUMING NO SIDE STREAMS)
IS COMPUTED BASED ON THE MULTIPLIERS CORRESPONDING TO EACH
OF THE COMPONENTS AND COMPONENTIAL FEED RATES.

COMMON /BLANK/ NCR, NPRT, KEEPIT(22)
COMMON /CMPOS/ NK, NC+1, NCP1, IDL, IDLV, ICH, LDBG, ISW,
* NDIM, ZNAME(2,10), LC(10), NTCOMP(10), NLIG, IPSET
COMMON /CONLT/ NIN,NCHT,NOCOMP,NE,NEI,KUNITS
COMMON /SYSC/ LA,LB,LC,LOOP,LOOPS
COMMON /SYSO/ KEFLAG(50),KSFLAG(100),KTRACE,CEHR,NPREG,
* IPUNCH
COMMON /ECOP/ EGPACT(25,50),NMAX,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),SMODEL(4),SMCOMP(10,4),SIK(10,4)
COMMON /STMDT/ SONUM(4),SDFLAG(4),SDVPR(4),SDTEMP(4),SDPRES(4),
* SCENTH(4),SOVISC(4),SOTHK(4),SZ(4),SOS(4),
* SDFRAL(4),SMODEL(4),SOMCOMP(10,4),SOK(10,4)
REAL SIDUM(4,12),SDUM(4,12)
INTEGER ISAVE(10)
EQUIVALENCE (SIDUM(1,1),SINUM(1)),(SDUM(1,1),SONUM(1))

DATA K, MAXDSP /0, 10/

EQPAR(1,NE) = BLOCK/NODE *
EQPAR(2,NE) = DISTILLATION COLUMN BLOCK/NODE *
EQPAR(3,NE) = CODE FOR DIST STREAM TYPE
  (-1:SUBCOLED LIQUID, 0:VAPO/LIQUID, +1:LIQ AT BUB TL)
EQPAR(4,NE) = DISTILLATE VAPO/(V+L) FRACTION

EQPAR(5,NE) = FEED MULTIPLIER COMPONENT 1
EQPAR(6,NE) = FEED MULTIPLIER COMPONENT 2
EQPAR(7,NE) = FEED MULTIPLIER COMPONENT 3
EQPAR(8,NE) = FEED MULTIPLIER COMPONENT 4
**
EQPAR(14,NE) = FEED MULTIPLIER COMPONENT 10
EQPAR(15,NE) = THRU EQPAR(25,NE) = 0.0

IF EQPAR(5,NE) < 0 NO CHANGE IS MADE IN DIST RATE,
ITAG1 IS USED WITH REFERENCE TO IT.

LOAD THE OUTPUT STREAM WITH THE INPUT STREAM

DO LOOP ON SDUM=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+=SICOMP(I,J)
  50      SDUM(I,J)=SICOMP(I,J)

  DO 60 J=3,12
  DC 60 I=1,NIN
  60      SDUM(I,J)=SIDUM(I,J)

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C
IF (ITAG1 .EQ. 1) GO TO 175
DRATE=0.0
FRATE=0.0
DO 100 J=1,NIN
SIMOLE(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 (LDBG .GE. 1) THEN
WRITE (NPR2,*)
WRITE (NPR2,120) 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 (NPR2,160)
160 FORMAT (' PROGRAM STOPPED ... DISTILLATE RATE TOO HIGH. READ
* PROPER VALUES OF MULTIPLIERS FOR DSPT PROCESS')
CALL EXIT
RETURN
C
DIST RATE ASSIGNED TO EQPAR OF THE PROPER DISTILLATION BLOCK
UNITS OF EQPAR AND DRATE ARE DIFFERENT
C
ISAVE ARRAY STORES THE DIST COLUMN BLOCK # WHICH HAS BEEN
PROCESSED ONCE. SECOND TIME, FOR THE SAME BLOCK #, UNITS
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 (LDBG .GE. 1) THEN
WRITE (NPR2,550) EQPAR(18,II),EQPAR(19,II)
WRITE (NPR2,*)
END IF
550 FORMAT (' SUB DSPT: DESTV = ',E13.5,' & DESTL = ',E13.5)
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

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IF (ITAG1 .EQ. 1) GC TO 700
EQPAR(18,II)=ECPAR(18,II)/453.59
EQPAR(19,II)=ECPAR(19,II)/453.59

700 RETURN
END

SUBROUTINE ECTL

THIS BLOCK IS DEDICATED (AT PRESENT) FOR AZEOTROPIC
DISTILLATION COLUMN (ETCH-WATER-BENZENE).

ECTL DYNAMICALLY SIMULATES THE FEED-FORWARD CONTROL
OF THE SPLIT IN A AZEOTROPIC DISTILLATION COLUMN
BASED UPON THE COMPOSITE FEED COMPOSITION AND RATE
AND THE ASSUMED ENTRAINER RATE.

1. DETERMINATION OF ENTRAINER RATE (TOP FEED, WITH FIXED
COMPOSITION) WITH FIXED, ETHANOL*WATER FEED
COMPOSITION, BOTTOMS SPECS AND THEIR RATES.
2. IF SATISFACTORY SOLUTION IS NOT OBTAINED FROM DIST,
DIST CALCULATIONS ARE REPEATED WITH NEW ESTIMATE OF THE
ENTRAINER RATE.
3. CALL EXIT IF CONVERGENCE IS IN UNSATISFACTORY.

COMMON /BLANK/ NCR, NPRT, KEEPIT(22)
COMMON /CMPOD/ NK, NCM1, NCP1, IDLL, IDLV, IDH, LDBG, ISW,
              NCIM, ZNAME(2,10), LC(10), NTCOMP(10), NLIQ, IPSET
COMMON /CONLT/ NIN, NGUT, NCOMP, NE, NEN, KUNITS
COMMON /SYSC/  LA, LB, LC, LOOP, LOOPS
COMMON /SYSO/  KEFLAG(50), KSFLAG(100), KTRACE, CERROR, NPRES,
              IPUNCH
COMMON /ECPO/  EQPAR(25,50), NMAX, MAXEQP
COMMON /STRMIN/ SINUM(4), SIFLAG(4), SIVPFR(4), SITEMP(4), SIPRES(4),
                SIENTHC(4), SIVISC(4), SITHKC(4), SIZC(4), SISC(4),
                SIFRAC(4), SIMOLE(4), SICOMP(10,4), SIKV(10,4)
COMMON /STMOV/  SQNUM(4), SQFLAG(4), SQVPFR(4), SQTEMP(4), SQPRES(4),
                SCOENTHC(4), SQVISC(4), SOTHC(4), SQSC(4), SOSC(4),
                SQFRA(4), SQMOLE(4), SQCOMP(10,4), SQKV(10,4)
REAL           SIUUM(4,12), SODUM(4,12), COMP(10), IF(10), XF(10)
REAL           SDC(12), SOC(12)
REAL           XBT(3), XE(3), XBS(3)
INTEGER        ISAVE(10)
EQUIVALENCE   (SIDIUM(1,1),SINUM(1)),(SODUM(1,1),SQNUM(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 /

EQPAR(1,NE) = EQUIPMENT NUMBER
EQPAR(2,NE) = NUMBER OF STAGES IN STRIPPING SECTION
EQPAR(3,NE) = NUMBER OF STAGES IN RECTIFYING SECTION
EQPAR(4,NE) = TYPE OF UNIT
EQPAR(5,NE) = STAGE EFFICIENCY STRIPPING SECTION ... FRACTION
EQPAR(6,NE) = STAGE EFFICIENCY RECTIFYING SECTION ... FRACTION
EQPAR(7,NE) = TDP STAGE TEMPERATURE (DEG K)
EQPAR(8,NE) = BOTTOM STAGE TEMPERATURE (DEG K)
EQPAR(9,NE) = TDP STAGE PRESSURE (ATM)
EQPAR(10,NE) = BOTTOM STAGE PRESSURE (ATM)
EQPAR(11,NE) = TEMPERATURE TOLLERANCE (DEFAULT = 0.01)
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 VAPCR 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)
  -1 : SUBCOOLED LIQUID
  0 : VAPOR/LIQUID DISTILLATE
  +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
  (DEFAULT: SUM OF ALL THE INCOMING STREAMS
  EXCEPT THE FIRST ONE)
C
C
INPUT VALUES
C
CASE NCASE DESCRIPTION
  3 3 DISTILLATION COLUMN (RR SPECIFIED)
  4 4 DISTILLATION COLUMN (BCILUP SPECIFIED)
  5 5 SELF REFLUXING COLUMN (BCILUP SPECIFIED)
  6 6 SELF REBOILING COLUMN (RR SPECIFIED)
C
ICK=0 SUCCESSFUL CALCULATIONS
ICK=1 EXCESS BENZENE IN THE BTMS (ACTION INC DIST RATE)
ICK=1 EXCESS WATER IN THE BTMS (ACTION DEC DIST RATE)
C
DO LOOP ON SODUM=SICUM
C
IF (LDEBUG .GE. 1) WRITE (6,9999)

9999 FORMAT("
",30X,"SUBROUTINE ECTL")
C
C
IF (LDEBUG .GE. 1) THEN
  WRITE (NPRT,4)
  4 FORMAT ("/ PARAMETERS IN SUB. ECTL ARE:\n")
  WRITE (NPRT,4) (CC(J),J=1,12)
  WRITE (NPRT,4) (ALPHA(J),J=1,6)
C
END IF
ICK=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(1)
ELSE
  KUHITS=EQPAR(25,NE)+0.1
  IF (KUHITS .EQ. 0.0) GO TO 17
  EQPAR(24,NE)=EQPAR(24,NE)*45.59
  17 BRATE=EQPAR(24,NE)
END IF
C
DJ 20 I=1,NCCOMP
20 XE(I)=0.0
DJ 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 CGMIN(I)=0.0
   DO 50 I=1,NOCOMP
      SICOMP(I,1)=XE(I)#SIMOLE(1)
   DO 50 J=1,HIN
50 CGMIN(I)=CGMIN(I)+SICOMP(I,J)
C   UPDATING ENTHALPY OF INCOMING ENTRAINER STREAM VIA ADBF
   NSAVE=NSUT
   ESAVE=EQPAR(2,NE)
   NOUT=1
C   SAVE OUTPUT STREAM # 1
   DO 100 I=3,12
100 SOC(I)=SODUM(1,I)
   DO 110 I=1,NOCOMP
110 SOC(I)=SODUM(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
120 SODUM(1,I)=SODUM(1,I)
   DO 130 I=1,NOCOMP
130 SICOMP(I,1)=SOC(I)
   FRATE=0.0
   DO 140 J=1,HIN
140 FRATE=FRATE+SIMOLE(J)
C
   DO 150 I=1,NOCOMP
150 XF(I)=CCMIN(I)/FRATE
   ORATE=FRATE-BRATE
C
155 CONTINUE
   SUM1=0.0
   SUM2=0.0
   SUM3=0.0
   DO 160 I=1,NOCOMP
160 SUM1=SUM1+XF(I)
   SUM2=SUM2+XD(I)
   SUM3=SUM3+XB(I)
160 CONTINUE
   DO 170 I=1,NOCOMP
170 XF(I)=XF(I)/SUM1
   XD(I)=XD(I)/SUM2
   XB(I)=XB(I)/SUM3
170 CONTINUE
C
C   IF (LDBG .GE. 1) THEN
      WRITE (NPRT,240)
      240 FORMAT (* SUB ECTF:FEED, DIST AND BTMS COMPOSITIONS * )
WRITE (NPRT,*) (XF(J),J=1,NOCOMP),(XD(J),J=1,NOCOMP),
* (XBJ(J),J=1,NOCOMP)
WRITE (NPRT,*)
WRITE (NPRT,250) FRATE, ERATE, DRATE, BRATE
250 FORMAT (* CHECK IN ECTL: FRATE / ERATE / DRATE / B RATE /*
* 4E16.5)
END IF
C
290 IF (FRATE=DRATE) 300,300,350
300 WRITE (NPRT,310)
310 FORMAT (* PROGRAM 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 (LOBUG .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 .GE. 0) CALL ZDIST
WRITE (NPRT,578)
578 FORMAT (* SUB ECTL STMT#578: RETURNED FROM DIST*)
C
CHECK WHETHER THE BTMS COMPOSITION IS CORRECT C
SCOMP(I,Z)
DG 600 I=1,NOCOMP
600 XBTE(I)=SOCCOMP(I,Z)/SOCDLE(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)) ICK=2
% XBT(3) .LT. XBSET(3)) ICK=3

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IF (ICK .EQ. 0) GO TO 700

SECANT METHOD FOR NEW VALUE OF D RATE

CONTINUE

SUMA=0.0
DO 610 I=1,NDCOMP
610 SUMA=SUMA+XBT(I)
DO 612 I=1,NDCOMP
612 XBT(I)=XBT(I)/SUMA

FXN=XBT(2)-XBTSET(2)
IF (ICK .EQ. 2 .OR. IOK .EQ. 3) THEN
    DELTA=-FXN*(ERATE-ERSV)/(FXN-FXNSV)
END IF

IF (ICK .EQ. 1) DELTA=0.010*ERATE
IF (ICK .EQ. 10) DELTA=0.02*ERATE
IF (ICK .EQ. 11) DELTA=0.075*ERATE
IF (ICK .EQ. 12) DELTA=0.20*ERATE
FXNSV=FXN
ERSV=ERATE
ELIMIT=0.25*ERATE
DELTA=SIGN(AMIN(FABS(Delta),ELIMIT),DELTA)
ERATE=ERATE-DELTA
KNT=KNT+1
WRITE (NPRT,625) LOOP, KNT, IOK, ERATE, DELTA

FORMAT (" IN ECTL: LOOP ="I3," IOK ="I3," ERATE ="F15.5," DELTA ="F15.5)
CALL EXIT

700 WRITE (NPRT,710)

RETURN

SUBROUTINE RCTL

RCTL BLOCK TAPS THE VALUES FROM THE REFERENCE STREAMS
[+ VE FOR INCOMING & -VE FOR OUTGOING STREAMS] AND
MAKE NEW ESTIMATE OF CCMONENTIAL RATES OF THE OUTPUT
STREAM.

ONLY 1 INPUT AND 1 OUTPUT STREAM ALLOWED

COMMON /BLANK/ NCR, NPRT, KEEPIT(22)
COMMON /CMRGC/ NK, NCM1, NCP1, IDLL, IDLV, IDH, LDBG, ISW,
*          NDIM, ZNAMEC(2,10), L(10), NTCOMP(10), NLIQ, IPSET
COMMON /CNGT/ NIN, NOUT, NDCOMP, NE, NEN, KUNITS
COMMON /SYS/ LA, LB, LC, LOOP, LOOPS
COMMON /SYS/ KEFLAG(50), KSFLAG(100), KTRACE, DERRCR, NPFREQ,
*            IPUNCH
COMMON /EGPA/ ECAPAR(25,50), NMAX, MAXEQP
COMMON /STM/ SEXTSV(13,100), SINTSV(11,100), NSMAX, MAXSXY, MASIN
COMMON /STMIN/ SINUM(4), SIFLAG(4), SIFRAC(4), SIMP(10,4), SITEMP(4), SIPRES(4),
*            SINTH(4), SIVISC(4), SITHK(4), SIZ(4), SIS(4),
*            SIFRLAC(4), SIMDL(4), SICOMP(10,4), SIKV(10,4)
COMMON /STMOUT/ SDNUM(4), SDFLAG(4), SDVPFR(4), SCITEMP(4), SDPRES(4),
*            SCENTH(4), SDVISC(4), STHK(4), SIC(4), SICOMP(4),
*            SDFRLAC(4), SDML(4), SDCOMP(10,4), SCKV(10,4)

REAL SIGUM(4,12), SoDUM(4,12), COMIN(10), CR(10), XF(10)
INTEGER ISA(10), ISRM(4), ICMP(4)
EQUIVALENCE (SIDUM(1,1), SINUM(1)), (SODUM(1,1), SDNUM(1))
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 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 EQPAR(13,NE) TO EQPAR(25,NE) = 0.0
C LOAD THE OUTPUT STREAM WITH THE INPUT STREAM
C DO LDGP ON SODUM=SIGUM
C DO 30 I=1,NOCOMP
   XF(I)=0.0
   DRI(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
       CMIN(I)=CMIN(I)+SICOMP(I,J)
50 SICOMP(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
C DO 80 I=1,4
80 ICOMP(I)=EQPAR(I+8,NE)+0.1
C COMPUTE BKMS 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

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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

WRITE (NPRT,90) B1, B2
90 FORMAT ('SUB RCTL: B1 AND B2 = ',2E20.8)
ADD1 = 61
ADD2 = 2.0

IF (B1 .LE. 0.0) ADD1 = 0.0
IF (B2 .LE. 0.0) ADD2 = 0.0

ITAR = EQPAR(2,NE)+0.1
IF (J1 .NE. 0) SOCCMP(J1,1) = ADD1 + COMIN(1)
IF (J2 .NE. 0) SOCCMP(J2,1) = ADD2 + COMIN(2)
IF (SOCCMP(1,1) .LT. 0.0) SOCCMP(1,1) = 0.0
IF (SOCCMP(2,1) .LT. 0.0) SOCCMP(2,1) = 0.0

C
C THIS IS FOR THE 1ST 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 + SOCCMP(I,1)
100   SICOMP(I,1) = SOCCMP(I,1)
   SGMOLE(I) = SUM
120   SIMCLE(I) = SGMOLE(I)

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

700 RETURN

ENC

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 I + 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, IDL, IDLV, IDH, LDBUG, ISW,
  * NDIM, ZNAME2(10), L(10), KTCOMP(10), NLIQ, IPSET
COMMON /CONTL/ NIN, NOUT, NOCOMP, NE, NEN, KUNITS
COMMON /SYSCL/ LA, LB, LC, LGOP, LOOPS
COMMON /SYSD/ KEFLAG(50), KSFLAG(100), KTRACE, CERRDR, NPFREG,
* 
COMMON /EQPA/    EQPAR(25,50), NEMAX, MAXEOP 
COMMON /STMA/    SEXTSV(13,100), SINTSV(11,100), NMAX, MAXSEX, MAXSIN 
COMMON /STRMIN/  SINU(4), SIFLAG(4), SIVPFR(4), SIEMPC(4), SIREPS(4), 
*               SIENTH(4), SIVISC(4), SITHK(4), SIZ(4), SIZ(4), 
*               SIRAL(4), SIMCLE(4), SICOMP(10,4), SIKV(10,4) 
COMMON /STMOUT/  SONUM(4), SOFLAG(4), SOVPPR(4), SGTEMP(4), SOSPRES(4), 
*               SOENTH(4), SOVIS(4), SOTHK(4), SOZ(4), SOS(4), 
*               SORAL(4), SSMCLE(4), SSCOMP(10,4), SSKV(10,4) 
REAL             SIDUM(4,12), SIDUM(4,12), CCWIN(10), DR(10), XF(10) 
REAL             SIC(12), SIC(12), SOC1(12), SOC1(12) 
INTEGER          ISAVE(10), ISTRM(4), ICOMP(4) 
EQUIVALENCE      (SIDUM(1,1), SINUM(1)), (SIDUM(1,1), SONUM(1)) 
C 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 SGMICLE(*) 
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 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 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 C EQPAR(18,NE) TO EQPAR(25,NE) = 0.0 
C C LOAD THE OUTPUT STREAM WITH THE INPUT STREAM 
C DO LOOP ON SODUM=SIDUM 
C KUNITS=EQPAR(25,NE)+0.1 
C IF (KUNITS .EQ. 0) GO TO 10 
C EQPAR(13,NE)=(EQPAR(13,NE)-32.0)/1.8+273.16 
C EQPAR(14,NE)=EQPAR(14,NE)/14.696 
C EQPAR(16,NE)=(EQPAR(16,NE)-32.0)/1.8+273.16 
C EQPAR(17,NE)=EQPAR(17,NE)/14.696 
C EQPAR(25,NE)=0.0 
10 CONTINUE 
C DO 30 I=1,NCOMP 
30 COMINC(I)=0.0 
C ITAG1=0 
C IF (EQPAR(9,NE) .LT. 0.0) ITAG1=1 
C DO 50 I=1,NCOMP 
C DO 50 J=1,NIN 
50 COMINC(I)=COMINC(I)+SICOMP(I,J) 
C C DO 70 I=1,4 
C IF (EQPAR(I+4,NE) .LE. 0.0) THEN 
C ISTRM(I)=SIGN(ABS(EQPAR(I+4,NE)))+0.1,EQPAR(I+4,NE))
END IF
70 CONTINUE
DO 80 I=1,4
80 ICMP(I)=ECPAR(I+8,NE)+0.1
C C
C COMPUTE BMRS 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
DC 85 I=1,4
J1=ICMP(I)
J2=ICMP(I)
IF (ISTRM(I) .GT. 0) THEN
IF (SEXTS(V(J1+3,ISTRM(I)) .GT. 0.0) AND.
% (SEXTS(V(J2+3,ISTRM(I)) .GT. 0.0)) THEN
B1=B1+SEXTS(V(J1+3,ISTRM(I))
B2=B2+SEXTS(V(J2+3,ISTRM(I))
END IF
ELSE IF (ISTRM(I) .LT. 0) THEN
ITEMP=ABS(ISTRM(I))
IF (SEXTS(V(J1+3,ITEMP) .GT. 0.0) AND.
% (SEXTS(V(J2+3,ITEMP) .GT. 0.0)) THEN
B1=B1-SEXTS(V(J1+3,ITEMP))
B2=B2-SEXTS(V(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=ECPAR(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 SOCMP(I,J)=0.0
IF (J1 .NE. 0) SOCMP(J1,ITAR)=ADD1
IF (J2 .NE. 0) SOCMP(J2,ITAR)=ADD2
DO 98 I=1,NOCOMP
IF (I .EQ. J1 OR. I .EQ. J2) GO TO 98
SOCMP(I,1)=COMINI(I)
98 CONTINUE
C SUM=0.0
SUM1=0.0
DO 100 I=1,NOCOMP
SUM=SUM+SOCMP(I,1)
SUM1=SUM1+SOCMP(I,ITAR)
SOCMP(I,1)=COMINI(I)-SOCMP(I,ITAR)
IF (SOCMP(I,1) .LT. 0.0) SOCMP(I,1)=0.0
100 SUM=SUM+SOCMP(I,1)
SOMOLE(ITAR)=SUM1
SGM0LE(1)=SUM
C IF (LDBUG .GE. 0) THEN
   WRITE (NPRT,105) (SGM0LE(J), (SGCOMP(I,J),I=1,N0COMP),*
   * J=1,N0IN)
105 FORMAT (* SUB SBQX STMT#105: SGM0LE / SGCOMP ARE */
   * 10((4G18.5)/))
C END IF
DO 130 I=1,N0IN
IF (SGM0LE(I) .LT. 0.0) THEN
   WRITE (NPRT,110) I, SGM0LE(I)
110 FORMAT (* SUB SBQX: NEGATIVE FLOWS, I / SGM0LE ARE *,
   * 13.2X,9G13.5)
   CALL EXIT
END IF
130 CONTINUE
C THE OUT GOING STREAMS ARE ESTABLISHED BY
C COMPUTING BUBBLE/DW POINT TEMPERATURE
C ENTHALPIES
C 1 - DISTILLATE (VAPCR)
C 2 - BOTTOMS
C
NSAVE=NOUT
NSAVE1=N0IN
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
   SIC(I)=SIDUM(1,I)
150 SIDUM(1,I)=SODUM(1,I)
DO 155 I=1,N0COMP
   SIC(I)=SICOMP(I,1)
155 SICOMP(I,1)=SCOMP(I,1)
   SITEMP(I)=EQPAR(13,NE)
   SIPRES(I)=EQPAR(14,NE)
   SIVPFR(I)=EQPAR(15,NE)
C DW POINT AND ENTHALPY CALCULATION
   EQPAR(2,NE)=1.0
   CALL ADF
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)
   SODUM(1,I)=SOD1(I)
DO 165 I=1,N0COMP
165 SOD1(I)=SCOMP(I,1)
C SECOND STREAM
DO 170 I=3,12
170 SIDUM(1,I)=SIDUM(2,I)
   SIDUM(2,I)=SIDUM(1,I)
DO 175 I=1,N0COMP
175 SICOMP(I,1)=SCOMP(I,2)
   SITEMP(I)=EQPAR(16,NE)
   SIPRES(I)=EQPAR(17,NE)
   SIVPFR(I)=0.0
C BUBBLE POINT AND ENTHALPY
   EQPAR(2,NE)=2.0
   CALL ADF
C RESTORE THE SAVED VALUES

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EQPAR(2,NE)=ESAVE
NOUT=NSAVE
NIN=NSAVE1
C RESTORE INPUT STREAM #1
DO 180 I=3,12
180 SIDUM(1,I)=SIDO(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
SGCOMP(I,2)=SGCOMP(I,1)
SUM=SUM+SGCOMP(I,2)
195 SGCMP(I,1)=SGC1(I)
SGMOL(I,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 1ST 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 (LDBGU *GE.* 0) THEN
DO 230 I=1,NIN
230 WRITE (NPR,240) I, SGMOLE(I)
240 FORMAT (" SUB SBOX STMT#240: SGMOLE(I) =",G15.5)
WRITE (NPR,*)
WRITE (NPR,245) EQPAR(3,NE)*3.96887E-6, SUM
245 FORMAT (" HEAT BALANCE IN (K BTU) =",G15.5/
" HEAT BALANCE IN (CAL) =",G15.5)
WRITE (NPR,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, NPR, KEEPIT(22)
COMMON /CONTL// NIN,NOUT,NOCOMP,NE,NEN,KUNITS
COMMON /CMRMP// NK, NC11, NCPI, IDLL, IDLV, IDHI, LDBG, ISW,*
NDIM, INAMEC2,10, L(10), NTCOMP(10), NLIG, IPSET
COMMON /SYSB// KRET(66), KCNT,KDM(4), IRGMA(96)
COMMON /SYSC// LA, LB, LC, LOOP, LOOPSPA
COMMON /SYSD// KEFLAG(50), KSFLAG(100), KTRAC, DERROR, NPFRG, *
IPUNCH
COMMON /ECPS// ECPAR(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),

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* COMMON /STOUT/ SIFRAL(4), SIMOLE(4), SICOMP(10,4), SIKV(10,4)
* COMMON /STRA/ SDNUM(4), SOFLAG(4), SOVPFR(4), SOTEMP(4), SOPRES(4),
* COMMON /STHM/ S0NTH(4), S0VIS(4), S0THK(4), SCG(4), S0S(4),
* COMMON /STRF/ S0FRAL(4), S0MOL(4), S0COMP(10,4), S0KV(10,4)
* COMMON /STM/ T, P, Z(10), Y(10), X(10), FRACV, ZVAP,
* COMMON /TVCL/ X1(10), X2(10), DUMB1(40), DHL(2), MIDL(2),
* COMMON /ZZE/ PF, TF, FEED(10), AAAA(3)

REAL SICUM(4,12), SICUM(4,12), SIC(12), SID(12)

EQUIVALENCE (SINUM, SIDUM), (SONUM, SODUM)

EQPAR(1,NE) = EQUIPMENT NUMBER
EQPAR(2,NE) = TEMPERATURE (F) OF ALL OUTPUT STRMS
EQPAR(3,NE) = PRESSURE (PSIA) OF ALL OUTPUT STRMS
EQPAR(4,NE) = HEAT REMOVED/ADDED IN THE OPERATION
EQPAR(5,NE) = MODE OF FLASH CALCULATION
EQPAR(6,NE) TO EQPAR(25,NE) = 0.0

MODE=NTYPE

<table>
<thead>
<tr>
<th>NTYPE</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>DEW POINT TEMPERATURE</td>
</tr>
<tr>
<td>2</td>
<td>BUBBLE POINT TEMPERATURE (1/2 LIQ)</td>
</tr>
<tr>
<td>3</td>
<td>ALL VAPOR ENTHALPY WITH PRIOR DEW POINT</td>
</tr>
<tr>
<td>4</td>
<td>ALL LIQUID ENTHALPY WITH PRIOR BUBBLE POINT (1/2 LIQ)</td>
</tr>
<tr>
<td>5</td>
<td>ALL VAPOR ENTHALPY</td>
</tr>
<tr>
<td>6</td>
<td>ALL LIQUID ENTHALPY (1/2 LIQ)</td>
</tr>
<tr>
<td>7</td>
<td>ISOTHERMAL FLASH (1/2 LIQ)</td>
</tr>
<tr>
<td>8</td>
<td>ISOTHERMAL FLASH ... NO DEW/BUBBLE POINT (1/2 LIQ)</td>
</tr>
<tr>
<td>9</td>
<td>ADIABATIC FLASH (1/2 LIQ)</td>
</tr>
<tr>
<td>10</td>
<td>ADIABATIC FLASH ... NO DEW/BUBBLE POINT (1/2 LIQ)</td>
</tr>
<tr>
<td>11</td>
<td>DEW POINT PRESSURE</td>
</tr>
<tr>
<td>12</td>
<td>BUBBLE POINT PRESSURE (1/2 LIQ)</td>
</tr>
<tr>
<td>13</td>
<td>LIQ - LIQ SEPERATION BELOW BUBBLE POINT (2 LIQ)</td>
</tr>
</tbody>
</table>

WRITE (6,9999)
9999 FORMAT("",30X,"SUBROUTINE SMIX")

KUNITS=EQPAR(25,NE)+0.1
IF (KUNITS .EQ. 0) GO TO 11
EQPAR(2,NE)=CEQPAR(2,NE)-32.0)/1.8+273.16
EQPAR(3,NE)=EQPAR(3,NE)*14.696
EQPAR(25,NE)=0.0

11 CONTINUE

T=EQPAR(2,NE)
P=EQPAR(3,NE)
MODE=EQPAR(5,NE)+0.1
IF (MODE .EQ. 0) MODE=13

DO 1 I=1,NIN
IF (SIMCLE(I) .GT. 0.) GO TO 2
1 CONTINUE
RETURN
SML=SIRES(I)
J=I+1
IF (J.GT.NIN) GO TO 4
DO 3 J=1,NIN
3  IF (SIRES(I).LT.SMALL.AND.SMOLE(I).GT.0.) SMALL=SIRES(I)
4  SOMPRES(I)=SMALL
5  SMOLE(I)=SOMPRES(I)
DO 5 J=1,NCOMP
6  SOMPRES(J,1)=SOMPRES(J,1)+SICOMP(J,1)
IF (SORTMP(1).EQ.0.) SORTMP(1)=273.16
DO 12 I=3,12
12  SICOMP(I,1)=SICOMP(I,1)
DO 13 I=1,NCOMP
13  SICOMP(I,1)=SICOMP(I,1)
C
SVNOUT=NOUT
DO 17 I=1,NOUT
SOMPRES(I)=P
17  SORTMP(I)=T
C
HOFZ=SIENTH(I)/SICOMP(I)
FRAC=SVPFRC(I)
FRACL=SAFRAL(I)
DO 19 I=1,NCOMP
19  FEED(I)=SICOMP(I,1)
C
IF (LDBGU.EQ.0) THEN
  WRITE (NPRT,21)
  WRITE (NPRT,*) FRACV,FRACL,T,P,HOFZ,(FEED(J),J=1,NCOMP)
21  FORMAT (" SUB SMIX AT FTN#21: FRACV/ FRACL / T / P /
* HOFZ / FEED /"
END IF
C
CALL ANYONE (MODE)
C
IF (LDBGU.EQ.0) THEN
  WRITE (NPRT,25)
  WRITE (NPRT,*) FRACV,FRACL,T,P,HOFZ,(FEED(J),J=1,NCOMP)
25  FORMAT (" SUB SMIX AT FTN#25: FRACV/ FRACL / T / P /
* HOFZ / FEED /"
END IF
C
NOUT=2 & MODE<>13: OUTPUT STREAMS (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
    SVPFRC(1)=0.0
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SQVPFR(2)=0.0
SCFRAL(1)=1.0
SCFRAL(2)=1.0
SDMCL(1)=SIMC(1)*FRACL
SDMCL(2)=SIMC(1)*(1.0-FRACL)
SGENTH(1)=MREAL(1)*SDMCL(1)
SGENTH(2)=MREAL(2)*SDMCL(2)
DO 38 I=1,NOCOMP
  38 SCOMP(I,1)=X1(I)*SDMCL(1)
  SCOMP(I,2)=X2(I)*SDMCL(2)
GO TO 200
ELSE
  SQVPFR(1)=1.0
  SQVPFR(2)=0.0
  SCFRAL(1)=0.0
  SCFRAL(2)=FRACL
  SDMCL(1)=SIMC(1)*FRACY
  SDMCL(2)=SIMC(1)*(1.0-FRACY)
  SGENTH(1)=MYP*SDMCL(1)
  SGENTH(2)=CHREAL(1)*FRACL+MREAL(2)*(1.0-FRACL)*SDMCL(2)
  SQZ(I)=IVAP
  DO 40 I=1,NOCOMP
  40 SCOMP(I,1)=Y(I)*SDMCL(1)
  SCOMP(I,2)=(X1(I)*FRACL+X2(I)*(1.0-FRACL))*SDMCL(2)
GO TO 200
END IF
END IF

200 CONTINUE
DO 202 I=3,12
  202 SIDUM(I,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+SGENTH(I)
  DO 208 I=1,NOUT
  208 SUM2=SUM2+SGENTH(I)
  EQPAR(N,NE)=SUM1-SUM2
C
  NOUT=SVOUT
  IF (LDBUG .GE. 0) THEN
    WRITE (NPRT,209)
    WRITE (NPRT,*), (SDMCL(I), (SCCOMP(J,I), J=1,NOCOMP), I=1,NOUT)
    209 FORMAT (/" SUB SMIX AT FTM#209: SDMCL / SCOMP / */
     & 4E15.5/4E15.5)
  END IF
  IF (KTRACE .LT. 2) GO TO 250
  WRITE (NPRT,210)
  210 FORMAT ("O SUB SMIX AT STM#210 : NTYPE / NOUT / FRACY / FRACL /")
  WRITE (NPRT,*), MODE, NOUT, FRACY, FRACL
C
  250 RETURN
END
PROGRAM FLASH2

GENERALIZED VAPOR- LIQUID- LIQUID FLASH PROGRAM FOR
THE NON-Ideal NON-ELECTROLYTIC SYSTEMS

VERSION #2 AUGUST 1984.
VERSION #3 FEBRUARY 1995. INCLUSION OF SUBROUTINE SWITCH
FOR THE OPTION OF TWO DIFFERENT SETS OF PARAMETERS
FOR GAMMA MODEL

COMMON /BLANK/ NCR, NPRT, NSTART, KUNITS, TITLE(20)
COMMON /CMPS0/ NC, NCM1, NCP1, ICLL, IDLV, IDHM, LDBUG, ISW,
# NDIM, INAME(2,10), L(10), NTCOMP(10), NLIQ, IPSET
* COMMON /ZDATA/ CPL(10,4), CPV(10,4), ENP(10,10), ANT(6,10),
* WC(10), AX, BX, OMEG(A10), 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), RC(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,
* HOFI, HVAP, HLIQ, DNV, XSH, NOBUB, NODEW
COMMON /CONTRL/ ITF, IPF, N, NTYP, JCDE
COMMON /WORK/ X1(10), X2(10), GAM1(10), GAM2(10), EK1(10),
* EK2(10), OML(2), HIDLL(2), MREALL(2), FRACL,
* IE, IR, XMAX, XMIN
COMMON /IFEEED/ PF, TF, FEED(10), FMOL, TREF, MI
COMMON /DUMMY/ XX(10,2), SX(10,2), XC(10,2), YY(10), SY(10),
* YC(10), RMAX, RMIN
DIMENSION DEW(10), BUBC(10), IJK(7), HLIQ(2)
REAL FDC(11), BUBVAP(10), DEWLIQ(10)
EQUIVALENCE (FEED(1),FDC(1))

DATA IJK '/"T","P","F","G","M","N"'/
DATA DOLLAR '/$$$/'

CALL ERRSET (73.,TRUE.,TRUE.,TRUE.,FALSE.,FALSE.,999)
CALL ERRSET (74.,TRUE.,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

READ IN THE MAIN TITLE

READ (NCR,16,END=1500,ERR=7) TITLE
WRITE (NPRT,17) TITLE
CALL START (IDATA, MFEEDS, MCASES, &1500)

The following codes and values are read in addition to those read in START.

PARAMETERS READ CARDS

<table>
<thead>
<tr>
<th>JCODE</th>
<th>CASE CALCULATION CODE</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>USE THE USER INTERACTIVE MODE</td>
</tr>
<tr>
<td>1</td>
<td>BYPASS THE USER INTERACTIVE MODE</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>IE</th>
<th>COMPONENT #: E-PHASE RICH IN THAT COMPONENT</th>
</tr>
</thead>
<tbody>
<tr>
<td>IR</td>
<td>COMPONENT #: R-PHASE RICH IN THAT COMPONENT</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>XMAY</th>
<th>X TO INITIALIZE X(E) &amp; XR(IR) IN INTLIZ</th>
</tr>
</thead>
<tbody>
<tr>
<td>XMN</td>
<td>X TO INITIALIZE X(IR) &amp; XR(E) IN INTLIZ</td>
</tr>
</tbody>
</table>

READ (NCR,=) JCODE, IE, IR, XMAY, XMN
WRITE (NPRT, 8) JCODE, IE, IR, XMAY, XMN
8 FORMAT ('DEFINED 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//

IF (NLIQ .EQ. 0) NLIQ=1
NLIQSY=NLIQ
IF (IDATA .NE. 0) GO TO 11
CALL CDATA
WRITE (NPRT, 9)
9 FORMAT ('GENERALIZED NONIDEAL FLASH (1/2 LIQ) PROGRAM')
GO TO 665

WRITE (NPRT, 8)
CALL ZPVY
CALL ZNRPL
WRITE (NPRT, 13)
13 FORMAT ('OCOMPONENTS 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)

*** *** *** RETURN POINT FOR MULTIPLE CASES *** *** ***

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

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WRITE (NPRT,20) PF,TF,FRACV,MRUN,NTYPE
20 FORMAT ("0 PARAMETERS FOR EQUILIBRIUM CALCULATION:",/  
  5X,"P, PSIA =", F14.3/  
  5X,"T, DEG F =", F13.2/  
  5X,"FRACV =", F16.5/  
  5X,"M, K-BTU =", 1PE13.5/  
  5X,"NTYPE =", I16)

CONVERT PSIA, F, BTU TO ATM, K, CAL (INTERNAL UNITS)

PF=PF/14.696  
P=PF  
TF=(TF-32.0)/1.8+273.16  
TSAVE=TF  
MRUN=MRUN+252.16+1.0E3  
MDFZ=MRUN

INITIAL SETTING OF GAMMA, FUGACITY AND DISTRIBUTION COEFF. BASED  
UPON THE TYPE OF COMPONENT

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

READ IN LB-MOLES OF COMPONENT FLOWRATES IN THE FEED

READ (NCR,*) (FD(J),J=1,NC)  
FMOL=0.0  
DO 35 J=1,NC  
35 FMCL=FMOL+FD(J)  
DO 40 I=1,NC  
40 Z(I)=FD(I)/FMCL

WRITE (NPRT,80)
80 FORMAT ("OUTPUT SUMMARY:",/  
  13," NAME",15X,"MCLS",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 (13,2X,2A4,F17.4,F15.6)  
WRITE (NPRT,110) FMCL  
110 FORMAT (" TCAL",F24.4)

CONVERT MCLAR UNITS FROM LB-MOLE TO GM-MOLE

FMCL=FMCL*453.59  
FD(NC+1)=FMCL  
MRUN=MRUN/FMCL  
TERM=FMCL/252.16+1.0E3

FRACV USED AS SWITCH
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**DEW POINT TEMPERATURE DETERMINATION**

**DEW POINT TEMPERATURE DETERMINATION**

```c
146 GO TO (150, 220, 150, 220, 350, 410, 150, 440, 150, 440, 1000,
   1000, 612), NTYPE

*** DEW POINT TEMPERATURE DETERMINATION ***
NTYPE=1, 3, 7 & 9

WRITE (NPRT, 151)
IF (NODW.EQ.0) GO TO 170
WRITE (NPRT, 160)
WRITE (NPRT, 185) T, TF, TSAVE
FORMAT (*.1RESULTS OF DEW POINT CALCULATION")
IF (NODEW.EQ.0) GO TO 170
WRITE (NPRT, 160)
FORMAT (*.1NO DEW POINT SINCE NONVOLATILE COMPONENTS ARE PRESENT")
TDew=1.0E6
DO 165 I=1, NC

165 DEW(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

WRITE (NPRT, 180) I=1, NC
Y(I)=Z(I)
FORMAT (*.1T, TF & TSAVE IN FLASH2 AT STEM& 185 ARE *.3F12.4)
NHold=NLIQ
NLIQ=1
CALL DEW(T)
TDew=T
TDew=(TDew-273.16)*1.8+32.0
DO 190 I=1, NC

DEW(I)=X(I)
WRITE (NPRT, 200) PRES, TDew
WRITE (NPRT, 205) (INAME(J), J=1, 2), I=1, NC
FORMAT (*.1DEW POINT OF FEED AT", F7.2, " PSIA IS", F7.2, " DEG F")
WRITE (NPRT, 210) (DEW(I), I=1, NC)
FORMAT (*.1DEW PT LIQ MCLF FRAC", 2X, 10F10.5)
CALL PRINT2
NLIQ=NHold
WRITE (NPRT, 320) I=1, NC
IF (NTYPE.EQ.3) GO TO 320
IF (NTYPE.EQ.7) GO TO 220
IF (NTYPE.EQ.9) GO TO 220
GO TO 665

*** BUBBLE POINT TEMPERATURE DETERMINATION ***

NTYPE=2, 4, 6, 7 & 9

WRITE (NPRT, 221)
WRITE (NPRT, 240)
WRITE (NPRT, 230)
FORMAT (*.1"RESULTS OF BUBBLE POINT CALCULATION")
IF (NODW.EQ.0) GO TO 240
WRITE (NPRT, 230)
WRITE (NPRT, 230)
FORMAT (*.1ONC BUBBLE POINT SINCE NONCONDENSIBLE COMPONENTS ARE PRESE")
NT"

TBUB=-459.0
DO 235 I=1, NC

235 BUB(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 (NLIG.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('"FEED 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('"BUBBLE POINT OF FEED AT","T"," PSIA IS","T"," DEG F"
DO 265 I=1,NC
265 BUIC(I)=Y(I)
WRITE (NPRT,205) ((ZNAME(J,I),J=1,2),I=1,NC)
WRITE (NPRT,270) (BUIC(I),I=1,NC)
270 FORMAT('" BUB PT VAP MOL 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
ISO FLASH TEMP TF MAY NOT BE SUITABLE AS INITIAL GUESS FOR BUBT2

C
IF (NTYPE.EQ.7) T=0.96*TF
FRACL=0.50
CALL INTLIZ
CALL BUBT2
IF (NLIG.EQ.1) GO TO 245
WRITE (NPRT,285) FRACL
285 FORMAT('"TWO LIQ PHASE REGION, LIQUID PHASE MOLE RATIO", F12.6)
GO TO 245

C
### ALL VAPOR ENTHALPY WITH PRIOR DEW POINT ###

C
NTYPE=3 & 5

C
320 IF (TF LT TDEW) GO TO 665
330 WRITE (NPRT,340)
340 FORMAT('"FEED AT CR 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
MIDLV=M-DHV
WRITE (NPRT,370) PRES,TDEG,H,MIDLV,DHV
370 FORMAT('"VAPOR PHASE ENTHALPY SUMMARY:"')

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* 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-STU =",F13.5)
GO TO 605

*** ALL LIQUID ENTHALPY WITH PRIOR BUBBLE POINT ***

NTYPE= 4 & 6

380 IF (T > TUB) GO TO 665
390 WRITE (NPR,400)
400 FORMAT ("0FEED AT CR BELOW BUBBLE POINT")
410 T=TF
NLIQ=NLIQSV
GO TO (415,420), NLIQ

415 DO 416 I=1,NC
416 X1(I)=Z(I)
DO 418 I=1,NC
418 X(I)=X1(I)
CALL LIQH
MREALL(I)=MLIQ
M=MREALL(I)
MIDLL(I)=MLIQ-XSH
DHL(I)=XSH
GO TO 429

420 CONTINUE
CALL INITL
CALL TWDLIQ
WRITE (NPR,285) FPACL
421 DO 423 I=1,NC
423 X(I)=X1(I)
CALL LIQH
MREALL(I)=MLIQ
MIDLL(I)=MLIQ-XSH
DHL(I)=XSH
DO 424 I=1,NC
424 X(I)=X2(I)
CALL LIQH
MREALL(2)=MLIQ
MIDLL(2)=MLIQ-XSH
DHL(2)=XSH
M=MREALL(1)*FRACL+MREALL(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
M=M*TERM
DO 430 N =1,NLIQ
MREALL(N)=MREALL(N)*TERM
MIDLL(N)=MIDLL(N)*TERM
DHL(N)=DHL(N)*TERM
430 CONTINUE

CALL PRINT2
WRITE (NPR,435) PRES,TDEG,M
435 FORMAT ("OLIQUID PHASE ENTHALPY SUMMARY:")
* 5X, "P, PSIA =", F21.3/
* 5X, "T, DEG F =", F20.2/
* 5X, "MLIQ (REAL), K-BTU =", F13.5)
C
DG 439 N=1, NLIQ
WRITE (NPRT, 437) N
437 FORMAT ("ENTHALPY SUMMARY OF LIQUID PHASE # ", I1)
WRITE (NPRT, 438) HREAL(N), HIDL(N), DML(N)
438 FORMAT (" MLIQ (REAL), K-BTU =", F13.5/
* 5X, "MLIQ (IDEAL), K-BTU =", F13.5/
* 5X, "DELTA MLIQ , K-BTU =", F13.5)
439 CONTINUE
GO TO 665
C
C
INITIALIZE VAPOR & LIQUID PHASES FOR ISO & ADIABATIC FLASH
C
440 CONTINUE
IF (NDUBU.EQ.0) GO TO 480
IF (NDDEW.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)
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

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
*** ADIABATIC FLASH ***

NTYPE=9 & 10

IF (HRUN .EQ. 0.0) GO TO 1000
WRITE (NPRT, 581)

561 FORMAT ("RESULTS OF ADIABATIC FLASH CALCULATION")
T=TF
HI=HRUN
CALL AFLSH2
GO TO 600

*** ISOTHERMAL FLASH ***

NTYPE=7 & 8

585 CONTINUE
IF (TF .GT. TDEW) GO TO 330
IF (TF .LT. T8UB) GO TO 390

590 T=TF
WRITE (NPRT, 591)

591 FORMAT ("RESULTS OF ISOTHERMAL FLASH CALCULATION")
IF (LDBG .GE. 2) WRITE (NPRT, 594) (X1(I), I=1, NC), (X2(I), I=1, NC)

594 FORMAT ("IN 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

600 TDEG=(T-273.16)*1.8+32.0
WRITE (NPRT, 610) TDEG, PRES, FRACV

610 FORMAT ("SYSTEM IS IN THE V/L PHASE REGION AT \$F7.2, \" DEG F AND \$","
* F7.2, \" PSI:\$/"
VAPOR/FEED MCLE RATIO\$", 2X, F9.6)
IF (NLIQ .EQ. 2) WRITE(NPRT, 285) FRACL

CALL PRINT2
GO TO 620

*** LIQ - LIQ SEPERATION AT T BELOW BUBBLE POINT ***

NTYPE=13

612 T=TF
FRACL=0.5
CALL TWQLIQ
WRITE (NPRT, 614)

614 FORMAT ("LIQUID - LIQUID SEPERATION BELOW BUBBLE POINT")
TDEG=(T-273.16)*1.8+32.0
WRITE (NPRT, 616) NLIQ, TDEG

616 FORMAT ("SYSTEM IS IN THE \$", I1, \" LIQUID PHASE REGION AT \$",
* F7.2, \" DEG F\")
IF (NLIQ .EQ. 2) WRITE(NPRT, 285) FRACL
GO TO 421

CALL CALCULATION OF VAP/LIQ ENTHALPIES AFTER ISO/ADIAB FLASH

620 DO 622 I=1, NC
622 X(I)=X1(I)
CALL LIQH
MREAL(1)=HLIQ
HIDL(1)=HLIQ-XSH
DLH(1)=XSH
IF (NLIQ .NE. 2) GO TO 625
DO 624 I=1,NC
624 X(I)=X2(I)
CALL LIQH
MREAL(2)=HLIQ
HIDL(2)=HLIQ-XSH
DLH(2)=XSH
625 CALL VAPH

C
TDEG=(T-273.16)*1.8+32.0
HVAPOR=HVAP*TERM
DVH=DVH*TERM
HIDLV=HVAPOR-DHV
WRITE (NPRT,370) PRES,TDEG,TVAPOR,HIDLV,DHV
GO TO (631,632),NLIQ
631 HLIQCD(1)=MREAL(1)
HLIQCD(2)=0.0
GO TO 633
632 HLIQCD(1)=MREAL(1)
HLIQCD(2)=MREAL(2)
C
DO 635 N=1,NLIQ
HIDL(N)=HIDL(N)*TERM
HLIQCD(N)=HLIQCD(N)*TERM
DLH(N)=(HLIQCD(N)-HIDL(N))
WRITE (NPRT,437) N
WRITE (NPRT,438)HLIQCD(N),HIDL(N),DLH(N)
635 CONTINUE
H=HVAPOR*FRACV+HLIQCD(1)*(1.0-FRACV)*FRACL
IF (NLIQ .EQ. 2) H=H+HLIQCD(2)*(1.0-FRACV)*(1.0-FRACL)
C
WRITE (NPRT,440) PRES,TDEG,H
640 FORMAT ("TOTAL ENTHALPY SUMMARY:"/
* 5X,"P, PSIA =", F21.3/
* 5X,"T, DEG F =", F20.2/
* 5X,"H (REAL), K-BTU =", F13.5)
C
HI IS THE ENTHALPY ASSOCIATED WITH THE ADIABATIC
FLASH FEED STREAM.
C
ISOTHERMAL FLASH CAN BE PERFORMED BEFORE THE ADIABATIC
FLASH TO ESTABLISH FEED, IN THE MULTIPLE CASE PROBLEM.
C
IF (NTYPE .EQ. 7 OR NTYPE .EQ. 8) THEN
H=HVAPOR*FRACV+MREAL(1)*(1.0-FRACV)*FRACL+
MREAL(2)*(1.0-FRACV)*(1.0-FRACL)
END IF
C
665 IF (JCODE .NE. 0) GO TO 15
C
CODE FOR INTERACTIVE MODE HAS TO BE MODIFIED.
C
INDEX=3
670 WRITE (6,680)
680 FORMAT (" ENTER CHANGES/"
WRITE (6,690)
690 FORMAT ("/"

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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
    CALL M19P (IPF,P)
    GO TO 700
760 IF (INDX .GT. 3) INDX=3
    TF=S
    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 INPUT *T DATA CARDS")
C
930 GO TO (15,150,320), INDX
C
940 NTYPE=1
    MI=MI+S
    WRITE (6,850) S
950 FORMAT(" ONNISO THERMAL MODE ENTERED.  Q ="/"	BTU/LAMOL"/
    "")
    GO TO 700
960 NTYPE=S
    GO TO 700
C
1000 WRITE (NPRT,1100)
1100 FORMAT(" EXITING FLASH2 WITH INCOMPLETE CALCULATIONS")
1500 CALL EXIT
STOP
END
SUBROUTINE TWOLIQ

TWO PHASE MATERIAL BALANCE USED FOR
  * BUBBLE POINT
  * SUBCOOLED LIQUID

OPTION OF DIFFERENT PARAMETER SETS FOR VLE AND LLE INCLUDED
  THROUGH IPSET.

COMMON /BLANK/ NCR, NPRT, NSSTART, KUNIT5, 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), ANTC(6,10),
  * W(10), AX, BX, OMEGA(10), AVAL(10), BVAL(10),
  * AK(10,10), RC(10), QC(10), QC(10), XL(10),
  * VQL(10), CC(160), ALPH(45), VC(10), TC(10),
  * PC(10), ZC(10), THBP(10), GA(10), DB(10),
  * A(10,10), G(10,10), ZRA(10), RD(10), DMU(10),
  * ETA(10)
COMMON /STRM/ T, P, I(10), Y(10), X(10), FRACV, ZVAP,
  * ER(10), VP(10), FUG(10), GAM(10), SVAP,
  * HG1, HVAP, HLIQ, DHV, XSM, NDBUG, NODEW
COMMON /CCNTRL/ ITF, IPE, N, NTYPE, JCODE
COMMON /TWOLIQ/ X(10), X2(10), GAM1(10), GAM2(10), EK1(10),
  * EK2(10), DHL(2), HIDLL(2), HREAL(2), FRACL,
  * IE, IR, XMAX, XMIN
COMMON /ZFEEDZ/ PF, TF, FEED, FMOL, TREF, HI
COMMON /DUMMY/ XX(10,2), SX(10,2), X(10,2), Y(10), SY(10), YC(10),
  * RMAX, RMIN
DIMENSION RG(10), XTEMP(10,2)

DATA CONV/1.0E-5/, CONV1/1.E-5/, CONV2/1.E-3/,
  * NDBJ /3/, GUESS /0.50/, KMAX/100/

ENTRY TO SUBROUTINE SWITCH IS MADE TO LOAD LLE PARAMETERS IF
SEPERATE SETS OF PARAMETERS ARE USED

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 =I,NC
  GAM1(I)=1.0
  GAM2(I)=1.0
5 CONTINUE
FRACL=0.5
IF (LDBG .GE. 2) THEN
  WRITE (NPRT,6)
  FORMAT (/"CHECK ON PARAMETER VALUES IN TWOLIQ SMT # 6")
  CALL PRCHK
END IF
IF (LDBG .GE. 2) WRITE (NPRT,7) IDLL
7 FORMAT ("IDLL AT THE BEGINING OF TWOLIQ IS ",I4)
  CALL ACTVY(T,P,X1,GAM1)

KNTX=0
IZERO$=0
DO 8 I=1,NC
IF (X2(I) .GT. 0.0) GO TO 8
KNTX=KNTX+1
8 CONTINUE
IF (KNTX .GE. NC) THEN
  DO 9 I=1,NC
  GM2(I)=1.0
  IZERO$=1
  GO TO 11
ELSE
  CALL ACTVY(T,P,X2,GAM2)
END IF
C
11 ISW=1
IF (LDBG. 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 (IZERO$ .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 (LDBG. 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
  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 (LC(I),EQ.0.OR.Z(I),LT.1.0E-12) GO TO 60
B=Z(I)*(1.0-RG(I))
WW=FRACL+B/RG(I)
DWW=1.0-RG(I)
F2=F2+B/WW
DF2=DF2-B/WW**2*DWW
DDF2=DDF2+2.0*B/WW**3*DWW**2
60 CONTINUE
C
C
C
C
C
C
C
60 DO 70 F=0.0,F2+DDF2
70 CONTINUE
C
C
C
C
C
C
C
C
C
C
C
C
IF (LDBG. GE. 1) WRITE(NPRT,62) KNT,T,F2,FRACL,DEL
62 FORMAT(' KNT-T-F2-FRACL-DEL', I3,F12.4,3E14.5)

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C
IF (K.LT. 20) GO TO 70
63 WRITE(NPRT, 64)
64 FORMAT ("0WOLI Q. CALCLUATION TERMINATED"/
+ "CALCULATION CONTINUING")
   DO 66 I = 1, NC
   Ww = FRACL + (1.0 - FRACL) * RG(I)
   XI(I) = Z(I) / WW
   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
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 .LE. 0.5
GO TO 75
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
   MOLD = X1(I)
   X1(I) = X2(I)
   X2(I) = MOLD
   MOLD = XX(I, 1)
   XX(I, 1) = XX(I, 2)
   XX(I, 2) = MOLD
   MOLD = SX(I, 1)
   SX(I, 1) = SX(I, 2)
   SX(I, 2) = MOLD
   MOLD = GAM1(I)
   GAM1(I) = GAM2(I)
81 GAM2(I) = MOLD
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
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GG 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
C IF (DBUG.GE.1) THEN
   WRITE(NPRT,102) (XX(I,1),I=1,NC)
   WRITE(NPRT,103) (XX(I,2),I=1,NC)

102 FORMAT ("XX1-CALC ",10E13.5)
103 FORMAT ("XX2-CALC ",10E13.5)
END IF
C
C INNER LOOP: SOLVING FOR FRACL FOR A SET OF COMPOSITIONS
C
KNT=KNT+1
C 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)
   SUM2=SUM2+X2(I)
   DO 130 I=1,NC
   X1(I)=X1(I)/SUM1
   130 X2(I)=X2(I)/SUM2
   GO TO 20
C
C 150 CONTINUE
C
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
C
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 (LC(I).EQ.0 .GR. LZ(I).LT.1.0E-12) GO TO 164
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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 NOBJ=3 : TEST ON SUMMATION OF ACTIVITIES
159 SUM=SUM+ABS(X1(I)*GAM1(I)-X2(I)*GAM2(I))
   GO TO 164
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 ENTRY TO SUBROUTINE SWITCH IS MADE TO LOAD BACK VLE PARAMETERS
C IF SEPERATE SETS OF PARAMETERS ARE USED
C IF (IPSET .EQ. 0) GC 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("OTWO LIQUID CALCULATIONS SUCCESSFULLY COMPLETED")
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) GC TO 185
   IPSET=1

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CALL SWITCH

185 RETURN

C

190 CONTINUE
C WEG BYPASSED
C IF (KNT .GE. 0) GO TO 240
IF (LDBG .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 220 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 (LDBG .GE. 1) WRITE (NPRT, 195) XTEMP(I, N), XX(I, N), SX(I, N),
* XC(I, N)
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 (LDBG .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
IF (N .EQ. 2) X2(I) = XTEMP(I, N) / SUM2
210 CONTINUE
IF (LDBG .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
X1(I) = X(1, I)
X2(I) = X(1, I)
X1(I) = (X(I, 1) + X1(I)) / 2.0
X2(I) = (X(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

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GO TO 20
END
SUBROUTINE FLUSH

ISOTHERMAL FLASH *** ONE LIQUID

COMMON /BLANK/ NCR, NPRT, NSTART, KUNITS, TITLE(20)
COMMON /CMPO/ NC, NCM1, NCP1, IDLL, IDLV, IDM, LDBG, ISW,
* NDIM, ZNAME(2,10), LC(10), NTCOMP(10), NLIOQ, IPSET
* COMMON /ZDATA/ CPL(10,4), CPV(10,4), ENP(10,10), ANTE(10),
* WC(10), AX, BX, DMEQAC(10), AVAL(10), BVAL(10),
* AK(10,10), R(10), Q(10), QPC(10), XLC(10),
* VCL(10), C(180), ALPHA(45), VC(10), TC(10),
* PC(10), ZC(10), TNBP(10), GA(10), ORC(10),
* AIC(10,10), G(10,10), ZRA(10), ROC(10), DUC(10),
* ETA(10),
COMMON /STRM/ T, P, Z(10), Y(10), X(10), FRACV, ZVAP,
* EK(10), VP(10), FUG(10), GAM(10), SVAP,
* HDFZ, HVAP, HLIOQ, DWH, XSH, NOBU6, NODEW
COMMON /CONTU/ ITF, IFH, N, NTYP, JCODE
COMMON /T.mul/ XIC(10), XIC(10), GAMIC(10), GAMIC(10), EKIC(10),
* EK2(10), DHIIL(2), HREAL(2), KREAL, FRACL,
* IE, IR, XMAX, XMIN
COMMON /Z.FEED/ PF, TF, FEED(10), FMO, TREF, HI
COMMON /DUMMY/ XIC(20), XIC(20), XIC(20), YX(10), SYC(10), YC(10),
* RMAX, RMN

EQUIVALENCE (RVF,FRACV)

DATA CONV/1.0E-4/, CONV1/1.E-5/

RVF IS VAPOR FRACTION
CALLING PROGRAM MUST SUPPLY INITIAL VALUE FOR RVF, X, Y

KNT=0
IDO=1
ISH=0
CALL KCALC2
ISH=1
IF (NK.GT.1) GO TO 21

Y(1)=1.0
X(1)=1.0
RETURN

20 CALL KCALC2

21 IF (LDBG.GE.1) WRITE(NPRT,25) KNT,T,RFV

25 FORMAT ("NKNT = ",I3, " FLUSH#1 T&RFV", F12.4,E14.5)
IF (LDBG.GE.2) WRITE(NPRT,26) (YI(I),I=1,N,C), (XI(I),I=1,N,C)

26 FORMAT ("Y-ASS ",3E13.5/ X-ASS ",3E13.5)

29 K=0
30 AMAX=RMAX
AMIN=RMN
F=0.0
DF=0.0
DD 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
90 K=K+1
C
IF (LDBG .GE. 2) WRITE(NPRT,90) K,F,DF,RFV
90 FORMAT (5X,"K = ",I2," F=DF-RVF",E14.5)
C
IF (K.LT.20) GO TO 99
91 WRITE (NPRT,92)
92 FORMAT ("OPRINT#1 CALCULATION TERMINATED"
+" CALCULATION CONTINUING")
GO TO 320
99 IF (ABS(F) .LT. CONV1) GO TO 190
C
99 IF (F) 100,190,110
100 AMIN=RFV
C
GO TO 120
110 AMAX=RFV
C
120 IF ((AMAX-AMIN).LT.CONV1)GO TO 170
C
DF=-F/DF
C
130 F=RFV+DF
C
140 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
170 IF (ABS(RVF-AMIN).LT.CONV1 .OR. ABS(RVF-AMAX).LT.CONV1) GO TO 190
C
DR=-F/DF
130 RNEXT=RFV+DR
C
IF (RNEXT .GE. AMIN) GO TO 150
140 DR=DR*.50
GO TO 130
C
150 IF (RNEXT .GT. AMAX) GO TO 140
C
RNEXT=RNEXT
C
IF (ABS(DF)-CONV1)190,30,30
IF (ABS(DR) .GT. CONV1) GO TO 30
C
170 CONTINUE
C
SUM=0.0
C
180 X1(I)=(X1(I)+SX(I))/2.0
C
190 SUM=SUM+X1(I)
C
DD 185 I=1,NC
C
200 XX(I)=X1(I)/SUM
C
GO TO 20
C
190 IF (LDBG .GE. 2) WRITE (NPRT,200) RVF
200 FORMAT (5X,"RVF",E14.5)
DD 240 I=1,NC
IF (L(I)) 210,220,230
210 XX(I)=I(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 (CLC(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 (CLC(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 350 I=1,NC
X1(I)=X1(I)/UX
350 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)
XX(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)
Y(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 (CLC(I).EQ.0) .OR. (Z(I).LT.1.0E-12) GO TO 430
CALL WEG (X1(I),XX(I),SX(I),XX(I))
SUM=SUM+X1(I)
430 CONTINUE
DO 440 I=1,NC
440 X(I)=X(I)/SUM

C

450 IF (IDLV.EQ.0) GO TO 500
SUM=0.0
DO 470 I=1,NC
IF ((LC(I) .LT. 0) .OR. (I(I) .LT. 1.0E-12)) GO TO 470
CALL WEGC(Y(I),YY(I),SY(I),Y(I))
SUM=SUM+Y(I)
470 CONTINUE
DO480 I=1,NC
480 Y(I)=Y(I)/SUM
500 FRACV=(CRM+RMIN)*0.5
GO TO 20
C
END
SUBROUTINE FLUSH2

C

ISOTHERMAL FLASH *** TWO LIQUIDS

C

COMMON /BLANK/NCR, NPRT, NSTART, KUNITS, TITLE(20)
COMMON /CMPRO/NC, NCM1, NCPI, IDLL, IDLV, IDH, LDBG, ISW,
*NDIM, ZNAME(2,10), L(10), NTCOMP(10), NLIQ, IPSET
COMMON /ZDATA/CPL(10,*), CPY(10,4), ENP(10,10), ANTC(6,10),
*W(10), AX, BX, OMEG(10), AVAL(10), EVAL(10),
*AK(10,10), RC(10), QP(10), XL(10),
*VDC(10), C(180), ALPHA(45), VC(10), TC(10),
*PC(10), ZC(10), TNBP(10), CA(10), DB(10),
*AK(10,10), G(10,10), ZR(10), RC(10), DMU(10),
*ETF(10)
COMMON /STRM/T, P, Z(10), Y(10), X(10), FRACV, ZVAP,
*EK(10), V(PC(10), FUG(10), GAM(10), SVAP,
*HGFX, HVAP, MLQ, DMV, XSH, NDBB, NODEW
COMMON /CONT/ITF, ICP, N, NTYPE, JCODE
COMMON /TWCLG/X(10), ZX(10), GAM(10), GAM2(10), EK(10),
*EKZ(10), DHL(2), MIDLL(2), REALL(2), FRACL,
*IE, IR, XMAX, XMIN
COMMON /ZFEED/PF, TF, FEEDC(10), FMCL, TREF, HI
COMMON /DUMMY/XE(10), SX(10,2), XC(10,2), YC(10,2), SYC(10), YC(10),
*RMX, RMIN
C

DIMENSION RKS(10), ZJ(2,2), RMS(2), XTEMP(10,2)
EQUIVALENCE (U,FRACV), (V,FRACL)
C
DATA CONV/1.0E-4/, CONV1/1.0E-5/, CONV2/1.0E-5/
C
KNT=0
ICX=1
ISW=0
FRACV=0.5
FRACL=0.5
IF (LDBG .GE. 2) WRITE (NPRT,5) (?I),I=1,NC)
5 FORMAT ("/IN FLUSH2 Z(I) ARE = ",10(F7.5,2X))
CALL KCALC2
ISW=1
IF (NC .GT. 2) GO TO 26
C
CALL TWCLG

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IF (LDBG .GT. 2)THEN
    WRITE (NPRT,7)
7 FORMAT (/" CHECK ON PARAMETER VALUES IN FLUSH2 SMT # 7"
    CALL PRCHK
    END IF
    CALL KCALC2
    DO 11 I=1,NC
11 Y(I)=EK1(I)*X1(I)
    IF (YDLV .EQ. 0) GO TO 240
    GO TO 13
    CALL KCALC2
    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
    DO 17 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 20 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)
20 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
28 IF (LDBG*GE.1) WRITE(NPRT,28) T,U,V
28 FORMAT ('OFASH2 T+U-V", F12.4,2*E14.5)
    IF (LDBG*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
DFF1UU=0.0  
C DFF1UV=0.0
C DFF2UU=0.0
C
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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
D           SSDU=SDU
D           SSDV=SDV
D           SDU=DU
D           SDV=DV
D           TOP=SSDU**2+SSDV**2+(SDU**2+SDV**2)
D           BTM=(SSDU**2+SSDV**2)*(SDU**2+SDV**2)
D           COSANG=TOP/SQRT(BTM)
D           BETA=1.0+COSANG
D           DU=BETA*DU
D           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
      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)=HCLD
           HCLD=XX(I,1)
           XX(I,1)=XX(I,2)
           XX(I,2)=HCLD
           HCLD=SX(I,1)
           SX(I,1)=SX(I,2)
           SX(I,2)=HCLD
           HOLD=XC(I,1)
           XC(I,1)=XC(I,2)
           XC(I,2)=HCLD
           HCLD=EK1(I)
           EK1(I)=EK2(I)
           EK2(I)=HOLD
           RKS(I)=EK1(I)/EK2(I)
           HCLD=GM1(I)
           GM1(I)=GM2(I)
      91  GM2(I)=HCLD
C
      94  IF (V.LT.1.0E-10) GO TO 231
      94  IF (V.GT.0.99999) GO TO 231
           IF (ABS(CSU).LT.CONV1 .AND. ABS(CSV).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 120 DO 180 I=1,NC
     IF (Z(I).LT.1.0-12) GO TO 170
     IF (L(I)) 130,140,150
     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
     NONCONDENSIBLE
     140 YY(I)=Z(I)/U
         XX(I,1)=0.0
         XX(I,2)=0.0
         GO TO 180
     NORMAL AND SUPERCRITICAL
     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
     IF (ABS(X1(I)+GAM1(I)-X2(I)+GAM2(I))/(X2(I)+GAM2(I)) .GT. 
         * 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

C 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
     HCLD=X1(I)
     X1(I)=X2(I)
     232 X2(I)=HCLD
     WRITE(NPRT,238)
     238 FORMAT (/5X, 'LIQUID HAS GONE TO A ONE PHASE SYSTEM' //</N)
              NLIG=1

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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=SUM+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 (IDL.EQ.0) GO TO 320
DO 290 N = 1,2
DO 290 I =1,NC
290 XCI(N)=XX(I,N)
SUM=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 (IDLY.EQ.0) GO TO 350
SUM=0.0
DO 330 I=1,NC
SY(I)=Y(I)
YCI(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 (IDL.EQ.0) GO TO 400
DO 390 N=1,2
SUM1=0.0
SUM2=0.0
DO 370 I=1,NC
IF (LCI.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))
370 GO TO 400
400 CONTINUE
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
C SUBROUTINE AFLSM2
C
C A DIABATIC FLASH
C
C COMMON /BLANK/ NCR, NPRT, NSTART, KUNITS, TITLE(20)
C COMMON /CMPRO/ NC, NCM1, NCP1, IDLL, IDLV, IDH, LDBUG, ISW,
* NDIM, ZNAME(2,10), L(10), NTCOMP(10), HLQ, IPSET
C COMMON /IDATA/ CPLC(10,4), CPVC(10,4), ENP(10,10), ANT(6,10),
* WC(10), AX, BX, OMEGA(10), AVAL(10), BVAL(10),
* AK(10,10), R(10), Q(10), QP(10), XL(10),
* VQ(10), G(180), ALPHA(45), VCC(10), TC(10),
* PC(10), ZC(10), THDP(10), QA(10), QB(10),
* AC(10,10), G(10,10), ZRA(10), R(10), DMU(10),
* ETA(10)
C COMMON /STRM/ T, P, Z(10), Y(10), X(10), FRACV, ZVAP,
* EK(10), VP(10), FUG(10), GAM(10), SVAP,
* HOFZ, HVAP, HLIQ, DMV, XSH, NDBUB, NDEW
C COMMON /CONTRL/ ITF, IPF, N, NTYPE, JCODE
C COMMON /TWOLQ/ X1(10), X2(10), GAM1(10), GAM2(10), EK1(10),
* EK2(10), DMLC(2), MDLC(2), MHRALL(2), FRACL,
* IE, IR, XMAX, XMN
C COMMON /IFEEDZ/ PF, TF, FEED(10), FMOL, TREF, HI
C COMMON /SUMMY/ XX(10,2), XXL(10,2), XXC(10,2), YY(10), SY(10), YC(10),
* RMAX, RMIN
C
C DATA KMAX, STEP, TINC, CONV /300, 20.0, 1000.0, 1.5E-3/
C DATA STEPMX / 20.0 /
C
C ID = 1
S = T
KOUNT = 0
K T E N = 1
STEP=STEPMX
TSUB=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
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
HREAL(1)=MLIQ
HDL(1) =MLIQ-XSH
IF (NLIQ .NE. 2) GO TO 18
DO 16 I=1,NC
16 X(I)=X2(I)
CALL LIQH
HREAL(2)=MLIQ
HDL(2) =MLIQ-XSH
18 CALL VAPH
HTOT=HVAP*FRACV+HREAL(1)*(1.0-FRACV)*FRACL+
% HREAL(2)*(1.0-FRACV)*(1.0-FRACL)
H=HTOT-MI
IF (ABS(H/HI)-CONV) 70,20,20
20 NLIQ=2
GO TO (30,40), ID
30 T=S-SIGN(TINC,H)
HD=H
ID=2
GO TO 63
40 SLOPE=(HD-M)/(S-T)
DT=-H/DT
S=T
IF (ABS(DT)-STEP) 60,60,50
50 DT=SIGN(STEP,DT)
60 T=T+DT
HD=H
63 T=A_MIN1(T,TDEW-0.5)
T=A_MAX1(T,TSUB+0.5)
IF (LDBG .GE. 1) WRITE (NPRT,55) KGUNT,HTOT,HI,H
55 FORMAT ('IN AFLSH2 : KGUNT-HTOT-HI-DIFF ',I4,3(3E12.5,2X))
KGUNT=KGUNT+1
IF (KDUNT .EQ. KTEN) THEN
KTEN=KTEN+1

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STEP=0.935*STEP
STEP=AMAX1(STEP, 0.0005)
END IF
IF (KOUNT .GE. KMAX) THEN
  WRITE (NPRT, 68) KOUNT
  IS = "PROGAM TERMINATED IN AFLSH2 AFTER ",
  CALL EXIT
END IF

GO TO 10

WRITE (NPRT, 80)
FORMAT ("0FOLLOWING IS THE RESULT OF AN ADIABATIC FLASH.")
RETURN

END

SUBROUTINE KCALC2

ROUTINE TO CALCULATE K VALUES

COMMON /BLANK/ NC, NPRT, NSTART, KUNITS, TITLE(20)
COMMON /CMPOG/ NC, NCMI, NCPI, IDLL, IDLV, IDH, LOBUG, ISW,
  NDIM, ZNAME(2,10), L(10), NTCOMP(10), NLIQ, IPSET
COMMON /ZDATA/ CPL(10, 10), CPV(10, 10), ENP(10, 10), ANTE(10),
  W(10), AX, BX, OMEGA(10), AVAL(10), BVAL(10),
  AK(10, 10), RC(10), Q(10), QP(10), XL(10),
  VOL(10), C(160), ALPHA(45), V(10), TC(10),
  PC(10), ZC(10), TNBP(10), OA(10), OB(10),
  AC(10, 10), GC(10), ZRA(10), RC(10), DMU(10),
  ETA(10)
COMMON /STRM/ T, P, Z(10), Y(10), X(10), FRACV, ZVAP,
  EK(10), VPC(10), FUG(10), GAM(10), SVAP,
  HQFZ, HVAP, HLIQ, DHLV, XSH, NOEB, NODGW
COMMON /CONTRL/ ITF, IPF, N, NTYPE, TCODE
COMMON /TWDLQ/ X1(10), X2(10), GAMA(10), GAM2(10), EK(10),
  EK2(10), DHL2(2), MID(2), MALL(2), FRA, IE,
  IR, XMAX, XMIN
COMMON /DFEED/ PF, TF, FEED(10), FMCL, TREF, HI
COMMON /DUMMY/ XX(10, 2), SX(10, 2), XC(10, 2), YY(10), SY(10), YC(10),
  RMAX, RMIN

IF (T .LE. 0.0) T=273.16
DHV=0.0
IF (ISW .NE. 0) GO TO 40
IF (LOBUG .GE. 2) THEN
  WRITE (NPRT, 5) T, ISW, L(1), I=1, NC
  WRITE (NPRN, 7) (ANTE(I, 1), I=1, NC)
  FORMAT("0SUB KCALC2 ANTONES ", 10(*3E12.5/))
END IF

GO30 I=1, NC
IF (L(I))30, 30, 20
VP(I)=EXP(ANTE(I, 1)+ANTE(2, I)/(T+ANTE(3, I)))*ANTE(4, I)*ALG(T)+
  ANTE(5, I)*T+ANTE(6, I)*T=T
CONTINUE

GO 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,DMV)
   DO90I=1,NC
   IF (L(I))90,90,80
80  EK1(I)=EK1(I)/FUG(I)
90  CONTINUE
C
100  IF (IDLV.EQ.0) RETURN
   CALL ACTVY (T,P,X1,GM1)
   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,GM2)
   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
C
END
SUBROUTINE PRINT2
C
COMMON /BLANK/ NCR, NPRT, NSTART, KUNITS, TITLE(20)
COMMON /CMPRO/ NC, NC1, NCP1, IDL, IDLV, IDM, LDBUG, ISW,
               NDBM, ZNAME(2,10), LC10, NTCOMP(10), NLIG, IPSET
COMMON /DATA/ CPL(10,4), CPV(10,4), ENP(10,10), ANTE(6,10),
               W(10), AX, BX, OMEGA(10), AVAL(10), BVAL(10),
               AK(10,10), RC(10), Q(10), QP(10), XC(10),
               VCL(10), GC(10), ALPH(45), VC(10), TC(10),
               PC(10), ZC(10), TNP(10), GA(10), QB(10),
               AC(10,10), G(10,10), ZRA(10), RDC(10), DMUC(10),
               ETA(10)
COMMON /STRA/ T, P, Z(10), Y(10), X(10), FRACV, ZVAP,
               EK(10), VP(10), FUG(10), GM(10), SVAP,
               HOFZ, HYP, HLIG, DMV, XSH, NDBUB, NODEW
COMMON /CTRL/ ITF, IPF, N, NTYP, JCODE
COMMON /TGL/ X1(10), X2(10), GAM1(10), GAM2(10), EK1(10),
               EK2(10), DMLC(2), HIDLL(2), HREST(2), FPACL,
               IE, IR, XMAX, XMIN
COMMON /ZFEED/ PF, TF, FEEDC(10), FMG, TREF, MI
COMMON /DUMMY/ XX(10,2), SY(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)
   DO 80 N=1, NL1Q
      WRITE(NPRT, 5) N
   5 FORMAT ("OMVLEM DATA FOR VAPOR AND LIQUID PHASE ", I3)
      WRITE(NPRT, 1) (ZNAME(J, I), J=1, 2), I=1, NC
   1 FORMAT ("/2S", 9(2A4, 2X))
      WRITE(NPRT, 6) (Y(I), I=1, NC)
   6 FORMAT (" VAP MOL 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 MOL 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
   16 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, 60, 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)", 5X, 10F10.4)
   80 CONTINUE
   RETURN
C
   END
SUBROUTINE FOFX (ICPT, XVAR, ADJUST, YYY, ZZZ)

THIS SUBPROGRAM IS USED IN CONJUNCTION WITH NLFITS
(MARQUARDT'S NON-LINEAR REGRESSION) PROGRAM.

VERSION # 2 ... MARCH 1984, PROGRAMMED BY HARPREET CHAWLA
VERSION # 3 ... AUGUST 1984, PROGRAMMED BY HARPREET CHAWLA

THE ARGUMENTS IN THE CALL LIST ARE:

ICPT  - INTEGER; THE DATA POINT NUMBER
XVAR  - ARRAY; CONTAINS THE COMPOSITION VALUES
ADJUST - ARRAY; CONTAINS THE CURRENT VALUES OF THE
          ADJUSTABLE PARAMETERS
YYY   - REAL; CONTAINS THE DESIRED RESULT
ZZZ   - REAL; CONTAINS THE CALCULATED RESULT ON RETURN

COMMON /BLANK/ NCR, NPRT, NSTART, KUNITS, TITLE(20)
COMMON /CMPRO/ NC, NCML, IDLL, IDLV, IDM, LDBUG, ISW, NDI,
               ZNAMEC(2,10), L(10), NTCOMP(10)
COMMON /ZCDATA/ CPL(10,4), CPV(10,4), ENP(10,10), ANTC(6,10),
               W(10), AX, BX, OMGEA(10), AVAL(10), BVAL(10),
               AK(10,10), R(10), G(10), QFC(10), XLC(10),
               VDL(10), C(180), ALPA(45), VC(10), TC(10),
               PC(10), ZC(10), TNBP(10), CA(10), OBQ(10),
               AC(10,10), G(10,10), ZRA(10), RD(10), DMU(10),
               ETA(10)
COMMON /STRM/ TFP, ZC(10), Y(10), X(10), FRACY, ZVAP,
              EK(10), VP(10), FUG(10), GAM(10), SVAP,
              HGFP, HVAP, MLIQ, DHL, XSH, NOBUB, NDEW
COMMON /CGNTRL/ ITF, IP, N, NTYPE, JCDEP, NLIQ
COMMON /TWCLQ/ X1C(10), X2C(10), GAM1C(10), GAM2C(10),
               EK1(10),
               EK2(10), DHL(2), MIDLL(2), HREALL(2), FRACL,
               IE, IR, XMAX, XMIN
COMMON /ZFEEDZ/ PF, TF, FEED, FMCL, TREF, H1, NK1, NFEED
COMMON /DUMMY/ XXC(10,2), SX(10,2), XC(10,2), YY(10), SY(10), YC(10),
               RMAX, RMN
COMMON /FOEX/ X1EXP(10), X2EXP(10), GAM1C(10), GAM2C(10),
               GAM1IC(10), GAM2IC(10), ACT1C(10), ACT2C(10),
               ACT1EC(10), ACT2EC(10),
               KE(10), KC(10), KIE(10), KIC(10), W1(10),
               W2(10), YEXP(10), TEXP, PEXP, W1, W1, VLEFN,
               LLEFN, VLLFN, NVLPT, NLLPT, NCVLE, NCLLE,
               NMODEL, INX, RECODE, NDTALE(15,10), NDSET
COMMON /OUTPUT/ X1EC(10,200), X2EC(10,200), X1C(10,200),
                 X2C(10,200), G1EC(10,200), G2EC(10,200),
                 G10C(10,200), G20C(10,200), G1ECG(10,5),
                 G2ECG(10,5), G1ECG(10,5), G2ECG(10,5),
                 KE(10,200), KCG(10,200), KIEG(10,5),
                 KICG(10,5), YEC(10,200), YCG(10,200),
                 TEC(200), PEC(200), TCG(200), PCG(200),
                 ACT1EC(10,200), ACT2EC(10,200), ACT1EC(10,200),
                 ACT2EC(10,200)

DIMENSION DEWC(10), BUBC(10), IJK(7), MLIQD(2)
DIMENSION XVAR(9), ADJUST(20), ALPHAS(3), PICKUP(400)

REAL FD(11), BUBVAP(10), DEWLIQ(10), KE, KC, KIE,
      KIC, KEQ, KCG, KIEQ, KICG
REAL=8 ADJUST
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VLEFN  CODE FOR OBJECTIVE FUNCTION IN VLE
LLEFN  CODE FOR OBJECTIVE FUNCTION IN LLE
VLLFN  CODE FOR OBJECTIVE FUNCTION IN VLLE
IE   COMPONENT #: COMPONENT IE RICH PHASE
IR   COMPONENT #: COMPONENT IR RICH PHASE
     (IF IE AND/OR IR = 0, PROGRAM FINDS IT)
XMAX  INITIALIZATION VALUE; MOLE FRACTION OF
     IE OR IR IN EXTRACT OR RAFFINATE PHASE RESPECTIVELY
     (IF XMAX <= 0.0, IT DEFAULTS TO 0.98)
XMIN  INITIALIZATION VALUE; MOLE FRACTION OF
     IR OR IE IN EXTRACT OR RAFFINATE PHASE RESPECTIVELY
     (IF XMIN <= 0.0, IT DEFAULTS TO 0.02)

RECORD # 2  IF NSKIP<0
ISKIP  READ (IN ANY ORDER) ALL THE DATA POINT NUMBERS
       TO BE SKIPPED FOR THE REGRESSION

RECORD # 3,4,...
NDTAL(E(I,J)) MATRIX IS READ, J = DATASET NO.
FOR EACH VALUE OF J:
I=1: J,
I=2: DATA TYPE CODE,
I=3: CONDITION CODE,
I=4: # OF COMPONENTS,
I=5: # OF DATA POINTS,
I=6-9G=5+NC ... COMPID'S OF ALL COMPONENTS
NOTE: IN TOTAL 4 REC. RECORDS ARE TO BE READ

READ (NCR,*) NMODEL, NTYPE, ITDEP, NOSET, 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,*) (NDTAL(E(I,J),I=1,N+NC)

VARIOUS SETTINGS ARE MADE

NCVLE=NC
NCLLE=NC
NVLPT=0
NLLPT=0
DO 4 J=1,NDSET
    IF (NDTAL(E(2,J) == EQ. 1) THEN
        NVLPT=NVLP+NDTAL(E(5,J)
    NCVLE=NDTAL(E(4,J)
    END IF
    IF (NDTAL(E(2,J) == EQ. 2) THEN
        NLLPT=NLLPT+NDTAL(E(5,J)
    NCLLE=NDTAL(E(4,J)
    END IF
4  CONTINUE

WRITE(NPR,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,

IF (NSKIP .NE. 0) WRITE (NPRT,9) (ISKIP(I),I=1,NSKIP)

9 FORMAT ("0","THE FOLLOWING DATA POINTS HAVE BEEN IGNORED")

ITDEP=ITDEP+1
IF (IDATA .NE. 0) GO TO 11
CALL CDATA
GO TO 15

C NMODEL CODES FOR CDATA TO BE USED WITH FOFX, FOR REGRESSION.

1 - VAN LAAR EQUATION                  (2 PARAMETER)
2 - 3 SUFIX MARGULES EQUATION         (2 PARAMETER)
3 - 4 SUFIX MARGULES EQUATION         (3 PARAMETER)
4 - 5 SUFIX MARGULES EQUATION         (4 PARAMETER)
5 - MODIFIED 5 SUFIX MARGULES EQUATION (4 PARAMETER)
6 - MODIFIED MARGULES EQUATION        (4 PARAMETER)
7 - WILSON EQUATION                   (2 PARAMETER)
8 - NRTL EQUATION                     (2 PARAMETER)
9 - NRTL EQUATION                     (3 PARAMETER)
10 - UNIQUAC EQUATION                 (2 PARAMETER)
11 - MODIFIED UNIQUAC EQUATION        (2 PARAMETER)
12 - UNIFAC EQUATION                  (2 PARAMETER)
13 - KNEX EQUATION                    (2 PARAMETER)
14 - HENRY'S EQUATION                 (2 PARAMETER)
15 - ANTCINE EQUATION                 (6 PARAMETER)

PRESENTLY PROGRAM TAKES CARE OF NMODEL=7 TO 11 CNLY.

NDALE(I,J) MATRIX CONSISTS OF CODES & NUMBERS FOR ALL DATA SETS
   # OF COLUMNS (VECTORS) = # OF DATA SETS READ IN
   1ST ROW: NC. OF DATASETS TO BE REGRESSED
     1,2,3,4,...ETC.
   2ND ROW: DATA TYPE, VLE/LLE/HE
     1 = VLE, 2 = LLE, 3 = HE
   3RD ROW: DATA CONDITION, CONSTANT T/P
     1 = CONSTANT TEMPERATURE DATA
     2 = CONSTANT PRESSURE DATA
   4TH ROW: # OF COMPONENTS IN THE DATASET
   5TH ROW: # OF POINTS IN THE DATASET
   6TH ROW: ID OF FIRST COMPONENT
   7TH ROW: ID OF SECOND COMPONENT
   & SO ON UPTO THE ID OF THE LAST COMPONENT
   0 = ABSENCE OF THE COMPONENT IN THE DATA SET
EXAMPLE: IN CASE OF REGRESSING BINARY & TERNARY DATASETS
   8 (5+3) ROWS ARE TO BE FILLED
   RESTRICTIONS: 1. ALL VLE DATASETS SHOULD APPEAR BEFORE LLE
                 DATASETS.
   2. CONSTANT T & CONSTANT P VLE DATA NOT
      ALLOWED TO BE REGRESSED TOGETHER.

ACCESS DATA RETRIEVAL PROGRAMS

11 CONTINUE
   CALL ZPV1
   CALL ZNRTL
   WRITE (NPRT,13)

13 FORMAT ("0","COMPONENTS USED ARE:")
* 2X, "#", 2X, "NAME", 6X, "iD#")
WRITE (NPR T, 14) (J, (ZNAME(K, J), K=1, 2), NTCOMP(J), J=1, NC)

14 FORMAT (I3, 2X, 2A4, 4X, I3)

15 READ (NCR, 16, END=1500, ERR=7) TITLE
16 FORMAT (20A4)
   IF (TITLE(C1), 'EC. DELLAR) GO TO 7
   WRITE (NPR T, 17) TITLE
17 FORMAT ("1", 20A4)
   READ (NCR, *, END=1500, ERR=1500) PF, TF, WT, WT1

C
PRES = PF

C
TF = SYSTEM TEMP OR INITIAL T DEG C
PF = SYSTEM PRESSURE OR INITIAL P IN MM HG
WT = WEIGHT USED IN FX2LIQ SUBROUTINE
WT1 = WEIGHT USED IN FX2LIQ SUBROUTINE

C
WRITE (NPR T, 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 (NPR T, 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, TC 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 VPCI(I)=0.0
   EKI(I)= 0.0
   EK2(I)= 0.0
35 CONTINUE

C
50 IF (NTYPE * GT. 0) GC TO 55
   GO TO 1000
55 IF (NTYPE .GT. 5) GO TO 1000

ASSIGNMENT OF ADJUSTABLE PARAMETERS

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

IF (NMODEL .NE. 9) GO TO 90
DO 85 I = 1,NC
   ALPHA(I)=ADJUST(INX)
   INX=INX+1
85 CONTINUE
90 CONTINUE

ASSIGNMENT OF INDEPENDENT VARIABLES.
IN THE CASE OF LLE, Z(I) IS REDEFINED IN SUBROUTINE F2XLIQ

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 XI 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
X1EOC(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, 3000, 3000, 3000, 3000),
* RECODE
3000 READ (NCR,*) (PICKUP(CII), 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
TEG(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

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GO TO 3300
C 3050 CONTINUE
NTEMP=(NCVLE-1)*NVLPT
READ (NCR *) (PICKUP(II),II=1,NTEMP)
IF (LDBG>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(I)
YED(I,J)=PICKUP(I)
II=II+1
3060 CONTINUE
YED(NCVLE,J)=1.0-SUM
SUM=0.0
DO 3065 I=1,NCVLE
3065 SUM=SUM+YED(I,J)
DO 3070 I=1,NCVLE
3070 YED(I,J)=YED(I,J)/SUM
3075 CONTINUE
C WRITE (6,*) (J,YED(I,J),I=1,NCN),J=IST,NPT)
IF (RECQDE*.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(I)
X2EGC(I,J)=PICKUP(I)
II=II+1
3110 CONTINUE
X2EGC(NCLLE,J)=1.0-SUM
SUM=0.0
DO 3115 I=1,NCLLE
3115 SUM=SUM+X2EGC(I,J)
DO 3120 I=1,NCLLE
3120 X2EGC(I,J)=X2EGC(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=TEG(IDPT)+273.16
GO TO 3380
3320 IF (VLEFN .LT. 10) GO TO 3340
PEXP=PEG(IDPT)/760.0
IF (VLEFN .GT. 13) GO TO 3380
3340 DO 3350 I=1,NCVLE
YEXP(I)=YED(I,ICPT)
3350 CONTINUE
3380 IF (VLEFN .LE. 0 .OR. IDPT .LE. NVLPT) GO TO 3400
3380 DO 3360 I=1,NCLLE
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X2EXP(I)=X2EO(I,1DPT)

3360 CONTINUE
3400 CONTINUE

C
IF (LDBG .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 (LDBG .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 FDFX ARE ’,2X,10(F7.5,2X))
WRITE(NPRT,110)(CC(J),J=1,NC4)
110 FORMAT(’0CC(J) VALUES AT STM#110 IN FDFX ARE ’,2X/6E13.5/6E13.5/
#5E10.2)
WRITE(NPRT,112)(ALPHA(J),J=1,NC)
112 FORMAT(’0ALPHA(J) VALUES AT STM#112 IN FDFX ARE ’,2X,5E10.2/
#5E10.2)
WRITE(NPRT,103)
103 FORMAT (/T10,’X1EXP (MCLE %)’,T35,’X2EXP (MCLE %)’/)
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
NCDEW=0
NOBU=0
NOBU=0

C
DO 140 I=1,NC
IF (FD(I)) 140,140,119
119 IF (L(I)) 120,130,140
120 NCDEW=1
GO TO 140
130 NOBU=1
140 CONTINUE

C
ICALL=0
GO TO (150,220,280,220,150), NTYPE

C
CONSTANT TEMPERATURE VLE CALCULATIONS
C
150 if(nlq .eq. 5 .and. idpt .gt. nvlpt) go to 280
    if (ldbug .ge. 2) write(npnt,155)
155 format(0'results of total pressure calculation'
    if (nlq .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)
    PBU=P
    if (ldbug .ge. 1) write(npnt,170) zzz
170 format(0'0zzz or p in fofx is ',f10.5)
    if (nq .eq. 5) go to 220
    go to 200
    if (ldbug .ge. 1) write(npnt,210)
210 format(0'pressure could not be determined'
    go to 2000
C
C *** CONSTANT PRESSURE VLE CALCULATIONS ***
C
220 continue
    if (nq .eq. 4 .and. idpt .gt. nvlpt) go to 280
    if (nq .eq. 5 .and. idpt .gt. nvlpt) go to 280
    if (ldbug .ge. 1) write(npnt,221)
221 format(0'results of bubble point calculation'
    if (nobub .eq. 0) go to 240
    if (ldbug .ge. 1) write(npnt,230)
230 format(0'on bubble point since noncondensible components are prese
    nt'
    tbub=-459.0
    do 235 i=1,nc
235 bubi(i)=0.0
    go to 2000
C
240 if (nlq .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(npnt,250)
250 format(0'feed represents a hypothetical liquid cr is in the retrod
    race region. bubble point calculations terminated'
    go to 231
C
255 tbub=T
    CALL FXVLE (ZZZ)
    TDG=TBUB-273.16
    if (ldbug .ge. 1) write(npnt,250) t, tdeg
260 format(0'bubble point of feed at ',f7.2, ' mmhg is ',f7.2, ' deg c'
    do 265 i=1,nc
265 bubi(i)=yi(i)
    if (ldbug .eq. 2) go to 272
    write(npnt,268) (izname(j,i),j=1,2),i=1,nc)
268 format(25x,10(2a4,2x))
WRITE(NPRT,270) (SUBC(I),I=1,NC)
270 FORMAT (" BUS PT YAP MCLE FRAC", 2X, 10F10.5)
CALL PRINT2
272 GO TO 2000
C
*** CONSTANT TEMPERATURE LLE CALCULATIONS ***
C
280 CONTINUE
T=TF
CALL FX2LIQ (ZZZ)
GO TO 2000
C
1000 IF (LDBG.EQ. 2) WRITE (NPRT,1100)
1100 FORMAT(" EXITING FDFX WITH INCOMPLETE CALCULATIONS")
1500 CALL EXIT
2000 CONTINUE
C
THE FOLLOWING STATEMENT IS ACTIVATED IF THE CONTRIBUTION
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 (LDBG .GE. 1) WRITE (NPRT,1950) IDPT, ZZZ
1950 FORMAT (" IN FDFX AT STMT#1950 :", IDPT="",I3," ZZZ="",E15.7)
C
DOWNLOADING INTO OUTPUT VARIABLES FOR FINAL PRINTOUT
C
IF (LDBG .EQ. 0) GO TO 2004
WRITE(NPRT,2002)TEXP,T,PEXP,P,(X1EXP(I),I=1,NCN)
2002 FORMAT ("AT 2002 IN FDFX 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=TED(IDPT)+273.16
CALL ACTVY (TESV,P,X1EXP,GAME1)
TC0(IDPT)=TBUB-273.16
GO TO 2010
2005 PC0(IDPT)=PBUB*760.0
PESV=PEQ(IDPT)/760.0
CALL ACTVY (T,PESV,X1EXP,GAME1)
2010 DO 2020 I=1,NCN
X10(I,IDPT)=X1(I)
G1EC(I,IDPT)=GAME1(E(I)
G1C(I,IDPT)=GAME1(I)
ACT1EC(I,IDPT)=ACT1E(I)
ACT1CQ(I,IDPT)=ACT1CQ(I)
IF (NTYPE .LT. 3) GO TO 2015
IF (NTYPE .GE. 4 .AND. IDPT .LE. NVLPT) GO TO 2015
X20(I,IDPT)=X2(I)
G2EC(I,IDPT)=GAME2(E(I)
G2O(I,IDPT)=GAME2(I)
ACT2EC(I,IDPT)=ACT2E(I)
ACT2CQ(I,IDPT)=ACT2CQ(I)
KEO(I,IDPT)=KE(E(I)
KCD(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 YCD(I, IDPT) = Y(I)
C G1EO(I, IDPT) = GAM1E(I)
C G1IC(I, IDPT) = GAM1I(I)
IF (NTYPE .LT. 3) GO TO 2020
IF (NTYPE .GE. 4 .AND. IDPT .LE. NVLPT) GO TO 2020
C G2EO(I, IDPT) = GAM2E(I)
C G2IC(I, IDPT) = GAM2I(I)
C KIEO(I, IDPT) = KIE(I)
C KICO(I, IDPT) = KIC(I)
2020 CONTINUE
2500 RETURN
END

**********************************************************************
SUBROUTINE PRINT3
C
C PROGRAMMED BY H.S. CHAWLA ... OCT. 1984
C
C IT GIVES PRINT OUT AFTER THE FINAL SET OF PARAMETERS IS OBTAINED
C
C COMMON /BLANK/ NCR, NPRT, NSTART, KUNITS, TITLE(20)
C COMMON /CMPRO/ NC, NCMI, IDLL, IDLV, IDH, LBUG, ISW, NDIM,
* ZNAME(2,10), L(10), NTCOMP(10)
C COMMON /CONTROL/ ITF, IPF, N, NTYPE, JCODE, NLIO
C COMMON /FEEDZ/ PF, TF, FEED, FMCL, TREF, HI, NK1, NFEED
C COMMON /OFFL/ X1C(10), X2C(10), GAM1E(10), GAM2E(10), EK1C(10),
* EK2C(10), DHL(2), HIDLL(2), HREAL(2), FRACL,
* IE, IR, XMAX, XMIN
C COMMON /FOX/ X1EXP(10), X2EXP(10), GAM1E(10), GAM2E(10),
* GAM1I(10), GAM2I(10), GM(10), GM1(10), GM2(10), ACT1C(10),
* ACT2C(10), ACT1E(10), ACT2E(10),
* KE(10), KC(10), KIE(10), KIC(10), W1C(10),
* W2C(10), YEXP(10), TEXP, PERP, WT, WT1, VLEFN,
* LLEFN, VLLFN, NVLP, NLLPT, NCVLE, NCLLE,
* NMDEL, INX, RECQCE, NOTALE(15,10), NDSET
C COMMON /OUTPUT/ X1EOC(10,100), X2EOC(10,100), X1IC(10,200),
* X2O(10,200), G1EC(10,200), G2EC(10,200),
* G1O(10,200), G2O(10,200), G1IEC(10,5),
* G2IEC(10,5), G1ICO(10,5), G2ICO(10,5),
* KEO(10,200), KOC(10,200), KIEO(10,5),
* KICO(10,5), YEO(10,200), YEC(10,200),
* YEC(200), PEOC(200), TCOC(200), PCB(200),
* ACT1EC(10,200), ACT2EC(10,200), ACT1CC(10,200),
* ACT2CC(10,200)

C INTEGER VLEFN, LLEFN, VLLFN, RECQCE
REAL*4 KE, KC, KE, KCD, KIE, KIC, KIEO, KICO,
* MEAN(11), VMAX(11), VMIN(11), HCLD(20,200),
* SS(1), TCTAL(11), SCD(11)
C
C ALL THE VARIABLE NAMES ENDING WITH LETTER "C" 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 REGRESSION PARAMETERS. THE FOLLOWING CHARACTERS IN THE
C VARIABLE NAMES STAND FOR:
C 1/2 LIQUID PHASE # 1/2

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C          E/C  EXPERIMENTAL/CALCULATED VALUES
C          I  VALUES AT INFINITE DILUTION
C          G  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) GC 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>"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,TC0(J),J=IST,NPT)
115 FORMAT ("CALCULATED TEMPERATURES = "/(NPRT/8+1)(<5(I2,F7.2,1X))/")
WRITE (NPRT,120)
120 FORMAT (" T DEG C","<4*NCN-6>"X," IN MCLE %","<8*NCN-8>"X,
*"Y IN MCLE %","<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 (<12,NCN>"="",I1,"-",5X),3X,NCN>"="",I1,"-",5X),8X,
*NCN>"="",I1,"-",5X)/
C
DO 134 J=1,NPT
DO 134 I=1,NCN
134 HOLDC(I,J)=0.0
DO 160 J=IST,NPT
HOLD(I,J)=TC0(J)-TC0(J)
DO 160 I=1,NCN-1
HOLD(I+1,J)=YECO(I,J)-YECO(I,J)
160 CONTINUE
WRITE (NPRT,150) TED(J),(X1ED(I,J),I=1,NCN),(YED(I,J),I=1,NCN),
*HOLD(I,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) (SC(I),I=1,NCN)
179 FORMAT (<16*NCN-6>"X,"STD. DEVIATION :",3X,F6.2,
*NCN-1>(2PF7.3,1X))
GO TO 250
CONSTANT TEMPERATURE VLE CASE

180 WRITE (NPR1,200)
200 FORMAT ("i", P MM HG", 3X, "X IN MOLE %", 7X, "+Y IN MOLE %", 9X, "P", "+<2\#NCN> X", "Y")
WRITE (NPR1,130) (I,I=1,NCN),(I,I=1,NCN),(I,I=1,NCN-1)
DO 205 J=1,NPT
DO 205 I=1,NCN
205 MCLD(I,J)=0.0
DO 240 J=IST,NPT
MCLD(I,J)=PEDC(J)-PCO(J)
DO 210 I=1,NCN-1
MCLD(I+1,J)=YEC(I,J)-YCO(I,J)
210 CONTINUE
WRITE (NPR1,150) PEDC(J),(X1ED(I,J),I=1,NCN),(YEC(I,J),I=1,NCN), 
&MCLD(I,J),(MCLD(I+1,J),I=1,NCN-1)
240 CONTINUE
CALL TALLY1 (MCLD, SS, TCTAL, MEAN, SD, VMIN, VMAX, IST, NPT, NCN)
WRITE (NPR1,177) (MEAN(I),I=1,NCN)
WRITE (NPR1,178) (VMAX(I),I=1,NCN)
WRITE (NPR1,179) (SD(I),I=1,NCN)

GAMMA VALUES FOR CONSTANT T OR P CASES (VLE)

250 WRITE (NPR1,260)
260 FORMAT ("i", <8\#NCN-12>X,"ACTIVITY COEFFICIENT VALUES", 
*<12\#NCN-6>X,"\% REL DIFF")
WRITE (NPR1,280)
280 FORMAT ("i", <4\#NCN-6>X,"EXPERIMENTAL", <8\#NCN-8>X,"CALCULATED")
WRITE (NPR1,300) (I,I=1,NCN),(I,I=1,NCN),(I,I=1,NCN)
300 FORMAT ("i", T4,<NCN>("-", I1, "-", 5X), 3X, <NCN>("-", I1, "-", 5X), 3X, 
*<NCN>("-", I1, "-", 4X)/)
DO 302 J=1,NPT
DO 302 I=1,NCN
302 MCLD(I,J)=0.0
DO 340 J=IST,NPT
DO 340 I=1,NCN
MCLD(I,J)=100.0*(G1ED(I,J)-G10(I,J))/G1ED(I,J)
305 CONTINUE
WRITE (NPR1,320) (G1ED(I,J),I=1,NCN),(G10(I,J),I=1,NCN), 
*MCLD(I,J),I=1,NCN)
320 FORMAT ("i", <NCN>FS.3,3X,<NCN>FS.3,3X,<NCN><2PG10.3>)
320 FORMAT ("i", <NCN>FS.3,3X,<NCN>FS.3,3X,<NCN><G10.3))
340 CONTINUE
CALL TALLY1 (MCLD, SS, TCTAL, MEAN, SD, VMIN, VMAX, IST, NPT, NCN)
WRITE (NPR1,345) (MEAN(I),I=1,NCN)
345 FORMAT ("i", <16\#NCN-13>X,"MEAN DEVIATION \"", 5X,<NCN> 
"*<2PG10.3,2X>)
WRITE (NPR1,347) (VMAX(I),I=1,NCN)
347 FORMAT ("i", <16\#NCN-13>X,"MAX DEVIATION \"", 5X,<NCN> 
"*<2PG10.3,2X>/)
WRITE (NPR1,348) (SC(I),I=1,NCN)
348 FORMAT ("i", <16\#NCN-13>X,"STD. DEVIATION \"", 5X,<NCN> 
"*<2PG10.3,2X>/)

INFINITE DILUTION GAMMA VALUES FOR CONSTANT T OR P BINARY VLE

IF (NCVLE .GT. 2) GO TO 380
WRITE (NPRT,350)
350 FORMAT(’O”,”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)
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)=X1ED(I,J)
X1C(I)=X1D(I,J)
355 CONTINUE
IF (NTYPE EQ. 1 OR NTYPE EQ. 5) PEXP=PED(JJ)/760.0
IF (NTYPE EQ. 2 OR NTYPE EQ. 4) TEXP=TEC(JJ)+273.16
CALL INFY (IMIN1,IMIN2)
G1IED(IMIN1,JJ)=GAM1IE(IMIN1)
G1ICO(IMIN1,JJ)=GAM1IC(IMIN1)
360 CONTINUE
DO 365 JJ=1,1
365 WRITE (NPRT,320) (G1IED(I,JJ),I=1,NCN),(G1ICO(I,JJ),I=1,NCN),
*’((G1IED(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
2 LIQUID PHASE COMPOSITIONS

450 NCN=NCLLE
DO 1060 III=1,NLLST
IST=NPT+1
NPT=NPT+NDTAE(5,III+NVLST)
WRITE (NPRT,70) III+NVLST
WRITE (NPRT,500)
500 FORMAT(’/T10,”EXPERIMENTAL LIQUID PHASE COMPOSITIONS IN
*MCLE %”)
WRITE (NPRT,530) IE, IR
530 FORMAT(’/”T10,” PHASE RICH IN ”,II,T45,” PHASE RICH IN ”,II/
) WRITE (NPRT,550) (I,I=1,NCN), (I,I=1,NCN)
550 FORMAT(’”5X,<NCN>(””,II,””,7X),5X,<NCN>(””,II,””,7X))
DO 630 J=IST,NPT
WRITE (NPRT,600)X1ED(I,J),I=1,NCN),(X2ED(I,J),I=1,NCN)
600 FORMAT(’”<NCN>(2PF10.4),5X,<NCN>(2PF10.4))
630 CONTINUE
C
WRITE (NPRT,650)
650 FORMAT(’”O”,” CALCULATED LIQUID PHASE COMPOSITIONS IN MCLE %”)
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)X1C(I,J),I=1,NCN),(X2C(I,J),I=1,NCN)
C
C
CALCULATION OF ABSOLUTE DIFFERENCE OF COMPOSITIONS (MCLE %):
C
C
WRITE (NPRT,750)
750 FORMAT(’”#”,”T10,” ABSOLUTE DIFFERENCE OF COMPOSITIONS IN MCLE %”)
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 HCLD(I,J)=0.0
DO 840 J=IST,NPT
DO 820 I=1,NCN
HCLD(I,J)=100.0*(X1ED(I,J)-X1D(I,J))
HCLD(I+NCN,J)=100.0*(X2ED(I,J)-X2D(I,J))
820 CONTINUE
WRITE (NPRT,862) (HCLD(I,J),I=1,2*NCN)
840 CONTINUE

C
NNN=2*NCN
CALL TALLY1 (HCLD,SS,TOTAL,MEAN,SD,VMIN,VMAX,IST,NPT,NNN)
DO 858 I=1,NNN
958 SUM=MEAN(I)
QVMEAN=SUM/NNN
WRITE (NPRT,860)
960 FORMAT ("" MEAN DEVIATION VALUES (EXPT-CALC) IN MOLE %"")
WRITE (NPRT,861) (MEAN(I),I=1,NNN), QVMEAN
961 FORMAT ("",<NCN>(G13.4),5X,<NCN>(G13.4)
* OVERALL MEAN DEVIATION (EXPT-CALC) IN MOLE % =",G13.4)
C
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)
970 FORMAT ("" STD. DEVIATION VALUES (EXPT-CALC) IN MOLE %"")
WRITE (NPRT,862) (SD(I),I=1,NNN)
C
CALCULATION OF % RELATIVE DIFFERENCE OF COMPOSITIONS:
C
WRITE (NPRT,872)
872 FORMAT ("","I10,""% RELATIVE DIFFERENCE OF COMPOSITIONS")
WRITE (NPRT,873) 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 HCLD(I,J)=0.0
DO 875 J=IST,NPT
DO 874 J=1,NCN
HCLD(I,J)=100.0*(X1ED(I,J)-X1D(I,J))/X1ED(I,J)
HCLD(I+NCN,J)=100.0*(X2ED(I,J)-X2D(I,J))/X2ED(I,J)
874 CONTINUE
WRITE (NPRT,862) (HCLD(I,J),I=1,2*NCN)
875 CONTINUE
C
NNN=2*NCN
CALL TALLY1 (HCLD,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. % REL DEVIATION VALUES ""
WRITE (NPRT,862) (SD(I),I=1,2*NCN)
C
ACTIVITY COEFFICIENTS (LLE)
WRITE (NPRINT,880)
830 FORMAT ("1",T10,"ACTIVITY COEFFICIENTS WITH EXPERIMENTAL X
*VALUES")
WRITE (NPRINT,530) IE, IR
WRITE (NPRINT,550) (I,I=1,NCN), (I,I=1,NCN)
DO 920 J=1,NPT
WRITE (NPRINT,910) (G1ED(I,J),I=1,NCN), (G2ED(I,J),I=1,NCN)
910 FORMAT (" ",<CN>/(F10.4),5X,<CN>/(F10.4))
920 CONTINUE
C
WRITE (NPRINT,940)
940 FORMAT ("0",T10,"ACTIVITY COEFFICIENTS WITH CALCULATED X VALUES")
WRITE (NPRINT,530) IE, IR
WRITE (NPRINT,550) (I,I=1,NCN), (I,I=1,NCN)
DO 970 J=1,NPT
970 WRITE (NPRINT,910) (G10(I,J),I=1,NCN), (G20(I,J),I=1,NCN)
C
C CALCULATION OF ABSOLUTE DIFFERENCE OF ACTIVITY COEFFICIENTS:
C
WRITE (NPRINT,975)
975 FORMAT ("1",T10,"ABSOLUTE DIFFERENCE OF ACTIVITY COEFFICIENTS")
WRITE (NPRINT,530) IE, IR
WRITE (NPRINT,550) (I,I=1,NCN), (I,I=1,NCN)
DO 995 J=1,NPT
995 MCLD(I,J)=MCLD(I,J)-G10(I,J)
990 CONTINUE
WRITE (NPRINT,862) (MCLD(I,J),I=1,NCN)
983 FORMAT (" ",<CN>/(F10.3),5X,<CN>/(F10.3))
985 CONTINUE
C
NNN=2*NCN
CALL TALLY1 (MCLD,SS,TOTAL,MEAN,SD,VMIN,VMAX,IST,NPT,NNN)
WRITE (NPRINT,993)
993 FORMAT (" MEAN DEVIATION VALUES (EXPT-CALC)")
WRITE (NPRINT,362) (MEAN(I),I=1,NCN)
WRITE (NPRINT,995)
995 FORMAT (" MAX. DEVIATION VALUES (EXPT-CALC)")
WRITE (NPRINT,862) (VMAX(I),I=1,NCN)
WRITE (NPRINT,997)
997 FORMAT (" STD. DEVIATION VALUES (EXPT-CALC)")
WRITE (NPRINT,862) (SD(I),I=1,NCN)
C
C CALCULATION OF RELATIVE % DIFFERENCE OF ACTIVITY COEFFICIENTS:
C
WRITE (NPRINT,1000)
1000 FORMAT ("0",T10,"RELATIVE % DIFFERENCE OF ACTIVITY COEFFICIENTS")
WRITE (NPRINT,530) IE, IR
WRITE (NPRINT,550) (I,I=1,NCN), (I,I=1,NCN)
DO 1001 J=1,NPT
1001 MCLD(I,J)=0.0
1000 DO 1002 I=1,NCN
1002 MCLD(I,J)=100.0*(G1ED(I,J)-G10(I,J))/G1ED(I,J)
MCLD(I+NCN,J)=100.0*(G2ED(I,J)-G20(I,J))/G2ED(I,J)
1005 CONTINUE

1002 CONTINUE
   WRITE (NPRT, 362) (MCLD(I,J), I=1,2*NCN)
C1003 FORMAT (",",<NCN>(2PF10.3),5X,<NCN>(2PF10.3))
1005 CONTINUE
C
   NNN=2*NCN
   CALL TALLY1 (MOLD, 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, 962) (SC(I), I=1,2*NCN)
C
   CALCULATION OF DIFFERENCE IN ACTIVITIES: LLE SYSTEM
C
   WRITE (NPRT, 1015)
C1015 FORMAT ("1",T10,"DIFFERENCE IN ACTIVITIES (EXPT-CALC)")
   WRITE (NPRT, 530) IE, IR
   WRITE (NPRT, 550) (I,I=1,NCN), (I,I=1,NCN)
   DO 1017 J=IST,NPT
C1017 WRITE (NPRT, 1018) ((ACT1ED(I,J)-ACT1CO(I,J)),I=1,NCN),
   C  *( (ACT2ED(I,J)-ACT2CO(I,J)),I=1,NCN)
   C
   * FORMAT (",",<NCN>F10.6,5X,<NCN>F10.6)
C
   ABSOLUTE EXPT & CALC ACTIVITY DIFFERENCES IN LLE SYSTEM
C
   WRITE (NPRT, 1020)
C1020 FORMAT ("0",<5*NCN-9>,"ABS DIFF IN EXPT ACT",<10*NCN-11>,X,
   C  *"ABS DIFF IN CALC ACT")
   WRITE (NPRT, 550) (I,I=1,NCN), (I,I=1,NCN)
   DO 1025 J=IST,NPT
C1025 WRITE (NPRT, 1018) ((ABS(ACT1ED(I,J)-ACT1CO(I,J))),I=1,NCN),
   C  *( (ABS(ACT2ED(I,J)-ACT2CO(I,J))),I=1,NCN)
C
   DISTRIBUTION COEFFICIENTS IN LLE SYSTEM
C
   WRITE (NPRT, 1030)
1030 FORMAT ("1","EXPERIMENTAL DISTRIBUTION COEFF",7X,"CALCULATED
   C  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
   ABSOLUTE & % RELATIVE DIFF OF DISTRIBUTION COEFFICIENTS IN
   C LLE SYSTEM
C
   WRITE (NPRT, 1040)
C1040 FORMAT ("0",<5*NCN-9>,"DIFF IN DIST COEFF",<10*NCN-15>,X,
   C  "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 MCLD(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.*((KEO(I,J)-KCO(I,J))/KEO(I,J))
1045 CONTINUE
WRITE (NPR,T,1047) (HOLD(I,J),I=1,2#NCN)
1047 FORMAT ("",<NCN>13.4,5X,<NCN>13.4)
1050 CONTINUE
C
CALL TALLY1 (HOLD,SS,TOTAL,MEAN,SD,VMIN,VMAX,IST,NPT,NNX)
WRITE (NPR,T,993)
WRITE (NPR,T,1047) (MEAN(I),I=1,2#NCN)
WRITE (NPR,T,995)
WRITE (NPR,T,1047) (VMAX(I),I=1,2#NCN)
WRITE (NPR,T,997)
WRITE (NPR,T,1047) (SD(I),I=1,2#NCN)
1060 CONTINUE
C
INFINITE DILUTION ACTIVITY COEFFICIENTS (LLE)
C TEMPORARY BYPASS ESTABLISHED BECAUSE INFX 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 (NPR,T,1070)
1070 FORMAT ("QINFINITE DILUTION ACTIVITY COEFFICIENTS WITH
*EXPERIMENTAL X VALUES")
WRITE (NPR,T,530) IE, IR
WRITE (NPR,T,550) (I, I=1,NCN), (I, I=1,NCN)
DO 1100 J=IST,NPT
1100 WRITE (NPR,T,910) (G1IEO(I,J),I=1,NCN), (G2IEO(I,J),I=1,NCN)
C
WRITE (NPR,T,1120)
1120 FORMAT ("QINFINITE DILUTION ACTIVITY COEFFICIENTS WITH
*CALCULATED X VALUES")
WRITE (NPR,T,530) IE, IR
WRITE (NPR,T,550) (I, I=1,NCN), (I, I=1,NCN)
DO 1160 J=IST,NPT
1160 WRITE (NPR,T,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 (NPR,T,1165)
1165 FORMAT ("0",T5,"% RELATIVE DIFFERENCE OF INFINITE DILUTION
* ACTIVITY COEFFICIENTS")
WRITE (NPR,T,530) IE, IR
WRITE (NPR,T,550) (I, I=1,NCN), (I, I=1,NCN)
DO 1175 J=IST,NPT
WRITE (NPR,T,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 (NPR,T,1190)
1180 FORMAT ("0",T15,"INFINITE DILUTION DISTRIBUTION COEFFICIENTS/
*T20,"EXPERIMENTAL",T45,"CALCULATED")
WRITE (NPR,T,530) IE, IR
WRITE (NPR,T,550) (I, I=1,NCN), (I, I=1,NCN)
DO 1220 J=IST,NPT
1220 WRITE (NPRINT,910) (KIED(I,J),I=1,NCN), (KICO(I,J),I=1,NCA)
   DELK=0.0
   DO 1250 I=1,NCN
1230 DELK=DELK+ABS(KIED(I,J)-KICO(I,J))/KI0(I,J)
   DELK=DELK/NPT
   WRITE (NPRINT,1240) I,100.0*DELK
1240 FORMAT ('AAVE % REL DIFF IN DIST COEFF (AT INFINITE DILLTION)
   *OF COMP 111','111.4)
1250 CONTINUE
C
1300 RETURN
C******************************************************************************
   END
   SUBROUTINE TALLY1 (AA,SS,TCTAL,MEAN,SD,VMIN,VMAX,IST,NPT,NV)
C
REAL*4 AA(20,200), SS(1), TCTAL(20), SC(20), MEAN(20),
* VMIN(20), VMAX(20), SCN(20)

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
   TCTAL(K)=0.0
   MEAN(K)=0.0
   SD(K)=0.0
   SCN(K)=0.0
   VMIN(K)=1.0E35
   VMAX(K)=-1.0E35
10 CONTINUE

C CALCULATE TCTAL, 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
   TCTAL(I)=TCTAL(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))
   SC(I)=SD(I)+AA(I,J)*AA(I,J)
60 CONTINUE
70 CONTINUE

C CALCULATE MEANS AND STANDARD DEVIATIONS
C
DO 80 I=1,NV
   IF (SCNT(I) .EQ. 0.0) GC TO 80
   MEAN(I)=TCTAL(I)/SCNT(I)
   SC(I)=SQRT(ABS(SCD(I)-TCTAL(I)*TCTAL(I)/SCNT(I))
   * (SCNT(I)-1.0))
80 CONTINUE

C 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

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RETURN
END

SUBROUTINE FXVLE (ZZZ)

PROGRAMMED BY H.S. CHAWLA ... OCT. 1994.
THIS SUBPROGRAM CALCULATES THE OBJECTIVE FUNCTION FOR
VLE REGRESSION

COMMON /BLANK/ NCR, NPRT, NSTART, KUNITS, TITLE(20)
COMMON /CMPRO/ NC, NCM1, IDLL, IDLV, IDH, LDEBUG, ISW, NDIM,
  * ZNAMEC(2,10), LC(10), NTCOMP(10)
COMMON /STRM/ T, P, Z(10), Y(10), X(10), FRACTZ, ZVAP,
  * EK(10), VP(10), FUGIC(10), GAMC(10), SVAP,
  * MDFZ, HVAP, HLIQ, DHV, XSH, NOSUB, NOSUB
COMMON /CTRL/ ITF, IFP, N, NTYPE, JCODE, NLIQ
COMMON /TWCLQ/ X1(10), X2(10), GAM1C(10), GAM2C(10), EK1(10),
  * EK2(10), DHL(2), HIDL(2), HREALL(2), FRACT,
  * IE, IR, XMAX, XMIN
COMMON /ZFEED/ PF, TF, FEED, FMOL, TREF, MI, 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),
  * KEC(10), KEC(10), KIE(10), KIC(10), WIC(10),
  * W2(10), YEXP(10), TEXP, PEXP, WT, WT1, VLEFN,
  * LLEFN, VLLFN, NVLPT, NLPT, NCVE, NCLLE,
  * NMODEL, INX, RECODE, NDTALE(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 C500,505,600,650,700,750,800,850,900,950,1000,1050,
*1100,1150,1200,1250,1300,1350,1400,1450,1500,1550), VLEFN

C
FUNCTION # 1: ABSOLUTE DIFFERENCE OF INFINITE DILUTION
C ACTIVITY COEFFICIENTS
C TO BE FIXED
C CALL INFY (IMIN1,IMIN2)
DC 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
FUNCTION # 2: RELATIVE DIFFERENCE OF INFINITE DILUTION
C ACTIVITY COEFFICIENTS
C TO BE FIXED
C CALL INFY (IMIN1,IMIN2)
DC 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

FUNCTION # 3: RELATIVE DIFFERENCE OF LOGRITHM OF INFINITE
DILUTION ACTIVITY COEFFICIENTS

TO BE FIXED
600 CALL INFY (IMIN1,IMIN2)
610 DO 610 I=1,NCVLE
IF (XIEXP(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

FUNCTION # 4: ABSOLUTE DIFFERENCE OF ACTIVITY COEFFICIENTS

650 DO 660 I=1,NCVLE
IF (XIEXP(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

FUNCTION # 5: RELATIVE DIFFERENCE OF ACTIVITY COEFFICIENTS

700 DO 710 I=1,NCVLE
IF (XIEXP(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

FUNCTION # 6: RELATIVE DIFFERENCE OF LOGRITHM OF ACTIVITY
COEFFICIENTS

750 DO 760 I=1,NCVLE
IF (XIEXP(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

FUNCTION # 7: ABSOLUTE DIFFERENCE OF Y'S

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
FUNCTION # 8: RELATIVE DIFFERENCE OF Y's

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

FUNCTION # 9: DIFFERENCE OF LOGRITHM OF Y's

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

FUNCTION # 10: ABSOLUTE DIFFERENCE OF Y's AND RELATIVE DIFFERENCE OF TOTAL P's

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

FUNCTION # 11: RELATIVE DIFFERENCE OF Y's AND RELATIVE DIFFERENCE OF TOTAL P's

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

FUNCTION # 12: DIFFERENCE OF LOGRITHM OF Y's AND DIFFERENCE OF LOGRITHM OF TOTAL P's

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

FUNCTION # 13: ABSOLUTE DIFFERENCE OF TOTAL P's
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SUM = SUM + ABS(YEXP(I) - Y(I))

CONTINUE
BBB = SUM / (NCVLE - INC)
ZZ = AAA + BBB

C
2000 ZZZ = ZZ
RETURN
END

SUBROUTINE FX2LIQ (ZIZ)

C
PROGRAMMED BY H.S. CHAWLA ... OCT., 1984
C
CALCULATE THE OBJECTIVE FUNCTION FOR THE LLE REGRESSION.

C
COMMON /BLANK/ NCR, NRPT, NSTART, KUNITS, TITLE(20)
COMMON /CMAPD/ NC, NCM1, IDLL, IDLV, IDH, LDBUG, ISW, NOIM,
* ZNAME(2,10), L(10), NTCOMP(10)
COMMON /ZDATA/ CPL(10,4), CPV(10,10), ENPC(10,10), ANT(6,10),
* M(10), AX, BX, OMEGAC(10), AVAL(10), BVAL(10),
* AK(10,10), RC(10), QC(10), QP(10), XL(10),
* VCL(10), CC(180), ALPHAC(45), WC(10), TC(10),
* PC(10), ZZ(10), TNBP(10), CA(10), CB(10),
* AC(10,10), GC(10,10), ZRAC(10), RDC(10), DM(10),
* ETA(10)
COMMON /STRM/ T, P, Z(10), Y(10), X(10), FRACV, ZVAP,
* EK(10), VP(10), FUG(10), GAM(10), SWAP,
* HGDZ, HVAP, HLIQ, CV, XSH, NOBUB, NDEW
COMMON /CCTRL/ IF, IPF, K, NTYP, JCODE, NLIQ
COMMON /TWCCL/ X1(10), X2(10), GAM1(10), GAM2(10), EK1(10),
* EK2(10), DHL(2), MIDL(2), HREALL(2), FRACL,
* IE, IR, XMAX, XMIN
COMMON /FOX/ X1EXP(10), X2EXP(10), GAM1E(10), GAM2E(10),
* GAM1E1(10), GAM2E1(10), GAM1E1(10), GAM2E1(10),
* ACT1(10), ACT2C(10), ACT1E(10), ACT2E(10),
* KE(10), K(10), KIE(10), KIC(10), W1(10),
* W2(10), YEXP(10), TEXP, PEXP, WT, WT1, VLEFN,
* LLEFN, VLLFN, NNLPT, NLLPT, NCVLE, NCLLE,
* NMODEL, INX, RECODE, NDATA(15,10), NDSET
C
REAL KE, K, KIE, KIC
INTEGER VLEFN, LLEFN, VLLFN, RECODE

NLIQ = 2
FRACL = 0.5
SUM = 0.0
DO 10 I = 1, NCLLE
I(I) = X1EXP(I) * FRACL + X2EXP(I) * (1.0 - FRACL)
SUM = SUM + I(I)
10 CONTINUE
DO 20 I = 1, NCLLE
I(I) = I(I) / SUM
20 CONTINUE
CALL INTLIZ (I0)
IF (LDBUG .GE. 2) WRITE (NVRT, 30) (I(I), I = 1, NCLLE)
30 FORMAT (' IN FX2LIQ : I(I) = ', I10, 'E13.7,2X')
C
IF (LDBUG .GE. 2) WRITE (NVRT, 35) (X1(I), I = 1, NCLLE)
35 FORMAT (' X1(I) GUESSES = ', I10, 'E13.5,2X')
IF (LDBUG .GE. 2) WRITE (NVRT, 38) (X2(I), I = 1, NCLLE)
38 FORMAT (' X2(I) GUESSES = ', I10, 'E13.5,2X')
C
CALL TWCCL
IF (NLIG .GT. 1) GO TO 39
IZ=10.0
GO TO 1000
C
C CALCULATION OF WEIGHTING FACTORS W1(I), W2(I).
W1(I)=W2(I)=1.0 IF W=0.0
C
39 DO 40 I=1,NCLLLE
IF (X1EXP(I) .EQ. 0.0) GO TO 40
W1(I)=ABS(1.0+W*I)/(ABS(X1EXP(I)-X1(I))/X1EXP(I))
IF (X2EXP(I) .EQ. 0.0) GO TO 40
W2(I)=ABS(1.0+W*I)/(ABS(X2EXP(I)-X2(I))/X2EXP(I))
40 CONTINUE
C
C CALCULATION OF EXPERIMENTAL AND CALCULATED ACTIVITIES IN BOTH THE LIQUID PHASES.
C
DO 50 I=1,NCLLLE
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,NCLLLE
ACT1E(I)=GAM1E(I)*X1EXP(I)
ACT2E(I)=GAM2E(I)*X2EXP(I)
60 CONTINUE
C
C CALCULATION OF SOLUTE DISTRIBUTION COEFFICIENTS
KE(I) : EXPERIMENTAL ; KC(I) : CALCULATED
C
DO 70 I=1,NCLLLE
KE(I)=GAM2E(I)/GAM1E(I)
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
IN=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,NCLLLE
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
IZ=SUM/(NLIG*(NCLLLE-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) GC 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
FUNCTION # 3 : RELATIVE ACTIVITIES

200 DO 210 I=1,NCLLE
    IF (X1EXP(I) .NE. 0.0 .OR. X2EXP(I) .NE. 0.0) GC 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
THE FOLLOWING OBJECTIVE FUNCTION EMPHASIZES THE REGION IN
THE VICINITY OF THE PLAIT POINT

FUNCTION # 4 : RELATIVE ACTIVITIES

250 DO 260 I=1,NCLLE
    IF (X1EXP(I) .NE. 0.0 .OR. X2EXP(I) .NE. 0.0) GC TO 255
    INC=INC+1
    IINC=INC
    GO TO 260
255 IF (I.EQ. IE .OR. I.EQ. IR) GC 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) GC 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
THE FOLLOWING OBJECTIVE FUNCTIONS ARE IN TERMS OF CCNC::
ABSOLUTE & RELATIVE

FUNCTION # 5 : ABSOLUTE CONCENTRATIONS

300 DO 310 I=1,NCLLE
    IF (X1EXP(I) .LT. 0.0 .OR. X2EXP(I) .NE. 0.0) GC 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
FUNCTION # 6 : RELATIVE CONCENTRATIONS.
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=M1(I)*ABS(ALCG(X1EXP(I))-ALOG(X1(I))))
    TEMP2=M2(I)*ABS(ALCG(X2EXP(I))-ALOG(X2(I))))
    SUM=SUM+TEMP1+TEMP2
360 CONTINUE
    ZZ=SUM/(NLIG*(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=M1(I)*ABS((X1EXP(I)-X1(I))/X1EXP(I))
    TEMP2=M2(I)*ABS((X2EXP(I)-X2(I))/X2EXP(I))
    SUM=SUM+TEMP1+TEMP2.
410 CONTINUE
    ZZ=SUM/(NLIG*(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=M1(I)*ABS((X1EXP(I)-X1(I))/(X1EXP(I)+X1(I))))
    TEMP2=M2(I)*ABS((X2EXP(I)-X2(I))/(X2EXP(I)+X2(I))))
    SUM=SUM+TEMP1+TEMP2
460 CONTINUE
    ZZ=SUM/(NLIG*(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
505 IF (I .EQ. IE .OR. I .EQ. IR)GO TO 510
505 AAA=AAA+ABS((KE(I)-K(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=M1(I)*ABS((X1EXP(I)-X1(I))/X1EXP(I))
    TEMP2=M2(I)*ABS((X2EXP(I)-X2(I))/X2EXP(I))
    SUM=SUM+TEMP1+TEMP2
520 CONTINUE
    ZZ=SUM/(NLIG*(NCLLE-INC))+AAA/(NCLLE-IINC-2)
    ZZ=SUM/(NLIG*(NCLLE-INC))+AAA/(NCLLE-IINC)
    GO TO 1000
C
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FUNCTION # 10 : RELATIVE CONC & DISTRIBUTION RATIOS
ONLY FOR MULTICOMPONENT SYSTEM

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
   AAA=AAA+ABS(ALOG(ABS(KE(I)/KC(I))))
C 510 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 620
   TEMP1=W1(I)*ABS(ALOG(X1EXP(I)))-ALOG(X1(I))
   TEMP2=W2(I)*ABS(ALOG(X2EXP(I)))-ALOG(X2(I))
   SUM=SUM+TEMP1+TEMP2
C 520 CONTINUE
   ZZ=SUM/(NLIQ*(NCLLE-INC))+AAA/(NCLLE-INC-2)
   ZZ=SUM/(NLIQ*(NCLLE-INC))+AAA/(NCLLE-INC)
   GO TO 1000
C
FUNCTION # 11 : RELATIVE CONC & DISTRIBUTION RATIOS
ONLY FOR MULTICOMPONENT SYSTEM

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
   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
C 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
   AAA=AAA+ABS((KE(I)-KC(I))/(KE(I)+KC(I)))
C 670 CONTINUE
   ZZ=SUM/(NLIQ*(NCLLE-INC))+AAA/(NCLLE-INC-2)
   ZZ=SUM/(NLIQ*(NCLLE-INC))+AAA/(NCLLE-INC)
   GO TO 1000
C
FUNCTION # 12 : RELATIVE CONC, PARAMETER VALUES & DISTRIBUTION
RATIO AT INFINITE DILUTION
ONLY FOR MULTICOMPONENT SYSTEM
THE FOLLOWING OBJ FUNCTION TAKES INTO ACCOUNT THE DISTRIBUTION
COEFFICIENTS OF THE SOLUTE AT INFINITE DILUTION
INX = # OF PARAMETERS BEING REGRESSED
WT1 = WEIGHT

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
      CONTINUE
   CALL 710
C 705 IF (I .EQ. IE .OR. I .EQ. IR) GO TO 710
C 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) GC 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/(NLIC*(NCLLE-INC))+BBB+AAA/(NCLLE-INC-2)
C ZZ=SUM/(NLIC*(NCLLE-INC))+BBB+AAA/(NCLLE-INC)
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) GC 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) GC 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/(NLIC*(NCLLE-IINC))+AAA/(NCLLE-IINC-2)
C ZZ=SUM/(NLIC*(NCLLE-IINC))+AAA/(NCLLE-IINC)
C
1000 ZZZ=ZZ
NLIC=2
C IF (LDBUG .LT. 2) GC TO 1300
WRITE (NPRINT,1200)
1200 FORMAT (" IN FX2LIC AT STMT # 1200 */")
WRITE (NPRINT,1220)(X1EXP(I),I=1,NCLLE)
1220 FORMAT (" X1EXP(I) = ",10(E13.5,2X))
WRITE (NPRINT,1230)(X1(I),I=1,NCLLE)
1230 FORMAT (" X1(I) = ",10(E13.5,2X))
WRITE (NPRINT,1240)(X2EXP(I),I=1,NCLLE)
1240 FORMAT (" X2EXP(I) = ",10(E13.5,2X))
WRITE (NPRINT,1250)(X2(I),I=1,NCLLE)
1250 FORMAT (" X2(I) = ",10(E13.5,2X))
1300 CONTINUE
C RETURN
END
C***********************************************************************************
SUBROUTINE IVFY (IMIN1,IMIN2)
PROGRAMMED BY M.S. CHAWLA  .... OCT, 1984.
THIS SUBPROGRAM COMPUTES THE INFINITE DILUTION ACTIVITY
COEFFICIENTS FOR 1/2 LIQUID PHASES AND DISTRIBUTION
COEFFICIENTS FOR 2 LIQUID PHASE SYSTEM. IT EVALUATES THE ABOVE
VALUES FOR EXPERIMENTAL AND CALCULATED X VALUES. CALCULATIONS
ARE PERFORMED ON THE FIRST AND THE LAST DATA POINTS. IT
EVALUATES THE GAMMA/K'S OF I WHOSE X IS APPROACHING ZERO.

COMMON /BLANK/ NCR, NPRT, NSTART, KUNITS, TITLE(20)
COMMON /CMRD/ NC, NCM1, IDLL, ICMD, IDH, LOBUG, ISW, NDIM,
* ZNAMEC(2,10), L(10), NTCOMP(10)
CGMON /ZDATA/ CPL(10,4), CPV(10,4), ENP(10,10), ANB(6,10),
* W(10), AX, BX, OMEGA(10), AVAL(10), BVAL(10),
* AK(10,10), RC(10), Q(10), QFC(10), XL(10),
* VD(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), RC(10), DMU(10),
* ETA(10)
CGMON /STRM/ T, P, Z(10), Y(10), X(10), FRACV, ZVAP,
* EK(10), W(10), FCCV, H(10), TX, VFCV, SWAP,
* HCQZ, HVAP, MLIQ, DHV, XS, NDBUB, NODEW
COMMON /CONTRL/ ITF, IPF, N, NTYPE, JCDFE, NLIQ
COMMON /TWCQL/ X1C(10), X2C(10), GAM1C(10), GAM2C(10), EK1C(10),
* EK2(10), DMLC(2), HISC(2), HREALC(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),
* KC(10), KCC(10), KIC(10), KIE(10), W1(10),
* W2(10), YEXP(10), TEXP, PEXP, WT, W1, VLEFN,
* LLLEN, VLLFN, NVLPT, NLLPT, NCVLE, NCLLE,
* NMODEL, INX, RECODE, NDPLEX(15,10), NDSET

REAL XS1(10), XS2(10), G1TEMP(10), G2TEMP(10),
* ISAVE(6), KE, KC, KIE, KIC
INTEGER VLEFN, LLLEN, VLLFN, RECODE
LCICAL FLAG

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 (MLIQ .GE. 2) GC TC 300
IF (NCVLE .GT. 2) GC TC 1000

SINGLE LIQUID PHASE CASE (BINARY SYSTEM ONLY)

IMIN1=1
XMIN=1.0
SUM1=0.0
SUM2=0.0
DO 70 I=1,NCN

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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) GC 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=TNP3P(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(I)=1.0
    XS1(I)=0.0
    XS2(I)=1.0
    XS2(I)=0.0
    CALL ACTVY (T,P,XS1,GAM1IC)
    CALL ACTVY (T,P,XS2,GAM2IC)
    KIC(I)=GAM2IC(I)/GAM1IC(I)
    KIC(I)=GAM2IC(I)/GAM1IC(I)
    GO TO 1000
C
C    TWO LIQUID PHASES CASE
C    CALCULATIONS WITH EXPERIMENTAL X VALUES
C
400 DO 420 J=1,NCLLE-2
420 ISAVEC(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
    DO 400 I=1,NCLLE
C    INNER LOOP FOR INFINITE VALUES CF 1 COMPONENT IN THE SYSTEM
    IF (FLAG .EQ. .TRUE.) GC TO 470
    IF (I .EQ. IE .OR. I .EQ. IR) GO TO 470
C
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IFLAG=0
K=K+1
GO 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 .CR. 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
570 CONTINUE
XS1(I)=X1(I)
XS2(I)=XS2(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
    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 (ICDATA,MFEED,MCASES,*)

KEY INTEGER CODES ARE INITIALIZED FOR VAPCR PHASE
DIMERIZATION THE ASSOCIATED TEMPERATURE DEPENDENT
CONSTANTS ARE DEFINED.
RETURN 1 USED FOR END OF FILE AND ERROR RETURN.
FEBRUARY 1985 ... ADDITION OF OPTION FOR TWO SETS OF ACTIVITY
COEFFICIENT PARAMETERS

COMMON /BLANK/ NCR, NPRT, NSTART, KUNITS, TITLE(20)
COMMON /CMPRD/ NC, NCM1, NCP1, IDLL, IDLV, IDH, LDBUG, ISW,
+ NDIM, ZNAME(2,10), L(10), NTCOMP(10), NLIG, IPSET
+ SW1(10), X1(10), X2(10), GAM1(10), GAM2(10), EK1(10),
+ EK2(10), DHL(2), MIDLL(2), MREALL(2), FRACL,
+ IE, IR, XMAX, XMIN

DEC Error-Set Routines Activated
Errset 72 = Floating Point Overflow
Errset 73 = Divide Check
Errset 74 = Floating Point Underflow
Errset 77 = Subscript Out Of Range

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)

NCR=5
NPRT=6

*** BASIC CONTROL PARAMETERS ... RECORD # 1 (11 ENTRIES)

<table>
<thead>
<tr>
<th>NC</th>
<th>NUMBER OF COMPONENTS (1 THRU 10)</th>
</tr>
</thead>
<tbody>
<tr>
<td>IDLL</td>
<td>LIQUID PHASE CLASSIFICATION CODE</td>
</tr>
<tr>
<td>0</td>
<td>IDEAL</td>
</tr>
<tr>
<td>1</td>
<td>VAN LAAR</td>
</tr>
<tr>
<td>2</td>
<td>MARGULES</td>
</tr>
<tr>
<td>3</td>
<td>WILSON</td>
</tr>
<tr>
<td>4</td>
<td>NRTL</td>
</tr>
<tr>
<td>5</td>
<td>UNIQUAC</td>
</tr>
<tr>
<td>6</td>
<td>UNIQUAC ... MODIFIED</td>
</tr>
<tr>
<td>7</td>
<td>UNIFAC</td>
</tr>
<tr>
<td>8</td>
<td>****</td>
</tr>
<tr>
<td>9</td>
<td>*****</td>
</tr>
<tr>
<td>10</td>
<td>****</td>
</tr>
<tr>
<td>11</td>
<td>BWRF</td>
</tr>
<tr>
<td>12</td>
<td>PENG-ROBINSON (PR)</td>
</tr>
<tr>
<td>IDLV</td>
<td>VAPOR PHASE CLASSIFICATION CODE</td>
</tr>
<tr>
<td>0</td>
<td>IDEAL</td>
</tr>
<tr>
<td>1</td>
<td>VIRIAL ... HAYDEN - O'CONNELL</td>
</tr>
<tr>
<td>2</td>
<td>VIRIAL ... TSONOPOULOS' CORRELATION</td>
</tr>
<tr>
<td>3</td>
<td>REDLICH-KWONG (RK)</td>
</tr>
<tr>
<td>4</td>
<td>SOAVE-REDLICH-KWONG (SRK)</td>
</tr>
</tbody>
</table>

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**C**

5  *****
6  *****
7  *****
8  *****
9  *****
10  *****
11  BWR-F
12  PENG-ROBINSON (PR)

**IDH**

ENTHALPY CORRECTION
0  CORRECT BOTH PHASES
1  CORRECT VAPOR PHASE ONLY
2  NO CORRECTION

**LDBUG**

DEBUG CODE
0  MINIMUM PRINT OUT OF SEPARATION SYSTEM
1  COMPONENT DATA AND FINAL COLUMN PROFILES PRINTED
2  CODE 1 + INTERMEDIATE COLUMN PROFILES PRINTED

**IDATA**

DATA LIBRARY SWITCH
0  READ VLE DATA FROM "CDATA"
1  OBTAIN DATA FROM "ZIPVICINRTL"

**NDIM**

DIMERIZATION CODE ... VAPOR PHASE
0  NO DIMERIZATION IN VAPOR PHASE
#  COMPONENT NUMBER UNDERGOING DIMERIZATION

**NLIQ**

NUMBER OF LIQUID PHASES
0/1  ONE PHASE
2  TWO PHASES

**IPSET**

PARAMETER SETS CORRESPONDING TO IDLL
0  GLOBAL SET OF PARAMETERS
1  ONE SET OF PARAMETERS ... VLE VALUES
2  TWO SETS OF PARAMETERS ... VLE VALUES FOLLOWED BY LLE VALUES
3  NOT YET DEFINED

NOTE: IPSET IS USED IN CDATA, TWCLIC AND SWITCH SUBROUTINES

**MFEED**

UNITS CODE FOR FEED VAPORIZATION ... FOR COLUMN SIMULATION
0  FEED VAPORIZATION IS SPECIFIED
1  FEED PRESSURE SPECIFIED ...
   FEED IS FLASHED BOTH AT BATTERY LIMITS (ISOTHERMALLY) AND THEN AT THE FEED STAGE (ADIABATICALLY)
*** FEED HEAT ADDITION PERMITTED ***

ALTERNATE USE IS BY SINGLE STAGE SIMULATION PROGRAM(S) ... This option is not yet activated.
0/1  A SINGLE STREAM IS TO BE ANALYZED
#  NUMBER OF STREAMS TO BE COMBINED PRIOR TO PERFORMING THE EQUILIBRIUM SEPARATION

**MCASES**

PROCESS COMPUTATION DATA SWITCH
ONLY BASE CASE IS TO BE EVALUATED
NUMBER OF ADDITIONAL PROCESS VARIANTS
TO BE EVALUATED ... INTERNAL RETURN
TO EVALUATE VARIANTS IS ACCOMPLISHED

READ (NCR,12) NC,IDLL,IDLV,IDM,LDBUG,IDATA,NDIM,NLIQ,IPSET,
* MFEED,MCASES
12 FORMAT (20I2)
READ (NCR,=) NC,IDLL,IDLV,IDM,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

*** BASIC PARAMETERS -- DIMERIZATION CONSTANTS ... RECORD # 2
Optional Record
FOR "NDIM" NOT EQUAL TO ZERO READ IN THE DIMERIZATION CONSTANTS
IF (NDIM.NE.0) READ (NCR,=) AX,BX

IF (IDLL.LT.0 .OR. IDLL.GT.8) IDLL=0
IF (IDLV.LT.0 .OR. IDLV.GT.5) IDLV=0

IF (IDATA.EQ.1) IDLL=4
IF (IDATA.EQ.1) IDLV=3

WRITE (NPRT,13) NC
13 FORMAT ("NUMBER OF COMPONENTS =", I3)
WRITE (NPRT,14) IDLL,IDLV,IDM
14 FORMAT ("VAPOR-LIQUID EQUILIBRIUM DATA Cycles:"//
* 5X, "LIQUID =", I4 /
* 5X, "VAPOR =", I5 /
* 5X, "ENTHALPY =", I2//)

WRITE (NPRT,15) LDEBUG,IDATA,NDIM,MFEED,MCOLS
15 FORMAT ("DEFINED CODE VALUES:"//
* 5X, "PRINT/DEBUG =", I17/
* 5X, "VLE DATA =", I17//
* 5X, "NDIM =", I17/
* 5X, "FEED VAPORIZATION =", I11/
* 5X, "# OF PROCESS ALTERNATES =", I5//)

VAPOR PHASE DIMERIZATION CONSTANTS ARE DEFINED
IF (NDIM.NE.0) WRITE (NPRT,17) AX,BX
17 FORMAT ("VAPOR PHASE DIMERIZATION CONSTANTS:"//
* 5X, "A =", G20.5/
* 5X, "B =", G20.5)
GO TO 50

30 WRITE (NPRT,35)
35 FORMAT ("ZERO, ONE, OR MORE THAN TEN COMPONENTS SPECIFIED.")
GO TO 100

*** BASIC PARAMETERS -- COMPONENT IC NUMBERS ... RECORD # 3
Optional Record
COMPONENT IDENTIFICATION NUMBERS ARE DEFINED FOR USE BY
THE DATA LIBRARY SUBPROGRAMS
50 IF (IDATA.EQ.1) READ (NCR,*) (NTCOMP(I),I=1,NC)
C
WRITE (NPRT,65) NLIQ, IPSET
65 FORMAT ("DEFINED CODES AND VALUES:")
   * 5X, "NO. OF LIQ PHASES =", I9/
   * 5X, "# PARAMETER SETS =", I10/
90 WRITE (NPRT,91)
91 FORMAT ("NOTE: 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
ROUTINE DEFINES THE PHYSICAL AND THERMODYNAMIC DATA FOR UP
TO A TEN (10) COMPONENT SYSTEM. INCLUDED ARE THE ACTIVITY
COEFFICIENT MODEL PARAMETERS, WHICH ARE SYSTEM DEPENDENT.
C
COMMON /BLANK/ NCR, NPRT, NSTART, KUNITS, TITLE(20)
COMMON /CMRDP/ NC, NC1, NC2, IDLL, IDLV, IDM, LDBUG, ISW,
   * NDIM, INAME(2,10), C(10), NTCOMP(10), NLIQ, IPSET
C COMMON /ZNAME/ ZNAME
C COMMON /ZDATA/ CPLC(10,4), CPVC(10,4), ENP(10,10), ANTC(6,10),
   * WC(10), AM, BM, OMEGA(10), AVAL(10), BVAL(10),
   * AK(10,10), RC(10), Q(10), QP(10), XL(10),
   * VCLC(10), CC(180), ALPHA(45), VCC(10), TCC(10),
   * PC(10), ZC(10), TNAP(10), GA(10), OB(10),
   * AC(10,10), G(10,10), ZRAC(10), RD(10), DMU(10),
   * ETAP(10)
C COMMON /SWITCH/ CSTORE(180,2), ASTORE(45,2), ISTORE(2)
C COMMON /CONTRL/ IF, IPF, N, NTYPE, JCODE
C
INTEGER ID(10)
REAL TREF(10), HVAP(10), EK(10), ETM(10,10)
C
EQUIVALENCE THE SOLVATION PARAMETERS (ETM) OF THE VIRIAL
EQUATION OF STATE ... HAYDEN-O'CONNELL VERSION WITH THE
CHARACTERISTIC BINARY CONSTANTS (AK) OF THE VIRIAL EQUATION
OF STATE ... TSIGNOPUOLOS VERSION
C
EQUIVALENCE (ETM(1,1),AK(1,1))
C
DOUBLE PRECISION ECNV, EQNM, EQUW, EQNR, EQNU, EQNU2, ECNF
CHARACTER=8 ECNV, EQNM, EQUW, EQNR, EQNU, EQNU2, ECNF
DATA ECNV */VANLAAR*/
DATA ECNM */MARGULES*/
DATA EQUW */WILSON*/
DATA EQNR */RENON*/
DATA ECNU */UNIQUAC*/
DATA ECNU2*/M-UNIQUAC*/
DATA ECNF */UNIFAC*/

DATA DMA, CMB /0.42748, 0.09664/

C
C BASIC CONTROL PARAMETERS ... DEFINED IN START
C
NC       NUMBER OF COMPONENTS

IDLL    LIQUID PHASE CLASSIFICATION CODE
  0    IDEAL
  1    VAN LAAR
  2    MARGULES
  3    WILSON
  4    NRTL
  5    UNIQUAC
  6    UNIQUAC ... MODIFIED
  7    UNIFAC
  8    ****
  9    ****
 10    ****
 11    BWR-F
 12    PENG-ROBINSON (PR)

IDLV    VAPOR PHASE CLASSIFICATION CODE
  0    IDEAL
  1    VIRIAL ... HAYDEN - O'CONNELL CORRELATION
  2    VIRIAL ... TSONOPoulos' CORRELATION
  3    REDLICH-KWONG (RK)
  4    SOAVE-REDLICH-KWONG (SRK)
  5    ****
  6    ****
  7    ****
  8    ****
  9    ****
 10    ****
 11    BWR-F
 12    PENG-ROBINSON (PR)

IDM     ENTHALPY CORRECTION
  0    CORRECT BOTH PHASES
  1    CORRECT VAPOR PHASE ONLY
  2    NO CORRECTION

LDEBUG  DEBUG CODE
  0    MINIMUM PRINT OUT OF SEPARATION SYSTEM
  1    COMPONENT DATA AND FINAL COLUMN PROFILES PRINTED
  2    CODE 1 + INTERMEDIATE COLUMN PROFILES PRINTED

IDATA   DATA LIBRARY SWITCH
  0    READ VLE DATA FROM "CDATA"
  1    OBTAIN DATA FROM "ZPVTSINRTL"

NDIM    DIMERIZATION CODE ... VAPOR PHASE
  0    NO DIMERIZATION IN VAPOR PHASE
* COMPONENT NUMBER UNDERGOING DIMERIZATION

NLIQ    NUMBER OF LIQUID PHASES
  1    ONE PHASE
  2    TWO PHASES

IPSET   PARAMETER SETS CORRESPONDING TO IDLL
  0    GLOBAL SET OF PARAMETERS
  1    ONE SET OF PARAMETERS ... VLE VALUES
C TWO SETS OF PARAMETERS ...VLE VALUES
C FOLLOWED BY LLE VALUES
C NOT YET DEFINED
C NOTE: IPSET IS USED IN CDATA, TWCLIQ AND 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 PURE COMPONENT DATA ... EIGHT (8) RECORDS NEEDED PER COMPONENT
C
C INPUT RECORD #1 ... A Format is used
C INAME 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 NGN 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 VML 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 Db UNIQUAC PARAMETERS -- VOLUME ... molecular volume
C Q --- SURFACE AREA ... molecular area
C QP --- INTERACTION AREA ... molecular area
C AVAL TSOPPOPOULOS' PARAMETERS FOR VIRIAL EQUATION
C BVAL
C IRA 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, C3, C4
C C1=a, C2=b, C3=c, C4=d
C cal per gm vs Deg K
C C0 = 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 C INPUT TYPE INTERNAL
C -1 NON-VOLATILE -1
C 0 NON-CONDENSIBLE 0
C 1 NORMAL 1
C 2 SUPERCRITICAL 2
C
C DO 10 I=1,2
C ISTORE(I)=0
C DO 7 J=1,160
C 7 CSTORE(J,I)=0.0
C DO 10 K=1,45
C 10 ASTORE(K,I)=0.0
C
C DO 110 I=1,NC
C
C *** INPUT RECORD #1 ... A Format is used
C READ (NCR,30) (ZNAME(J,I),J=1,2)
C 30 FORMAT (2A4)
C
C *** INPUT RECORD #2 ... Integer Values / Real Values are used
C READ (NCR,*) LCI,I,W(I),TN5P(I),TC(I),PC(I),VC(I),ZC(I),
C * VOL(I)=OEGAC(I)
C IF (W(I).LE.0.0) W(I)=1.0
C
C *** INPUT RECORD #3 ... Real Values are used
C READ (NCR,*) DA(I),DB(I),R(I),Q(I),QP(I),AVAL(I),BVAL(I),
C * ZRAC(I)
C XL(I)=10.0/2.0*(CR(I)-Q(I))-(R(I)-1.0)
C IF (QP(I).LE.0.0) QP(I)=Q(I)
C
C *** INPUT RECORD #4
C READ (NCR,*) RD(I),DMU(I),ETA(I)
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
60 L(I) = 0
   GO TO 100
90 L(I) = -1
100 CONTINUE

C C
C *** INPUT RECORD #5  ENTHALPHY DATA
C READ (NCR,*)  (MVAP(I), TREF(I))
C
C *** INPUT RECORD #6
C READ (NCR,*)  (CPL(I,J), J = 1, 4)
C
C *** INPUT RECORD #7
C READ (NCR,*)  (CPV(I,J), J = 1, 4)
C
C *** INPUT RECORD #8
C READ (NCR,*)  (ANT(J,I), J = 1, 6)
110 CONTINUE

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-O'CONNELL VERSION, THEN THE
C SOLVATION PARAMETERS MUST 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 ... TSOPONPOULOS
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 (LDBG .EQ. 0) GO TO 430
C
C WRITE (NPRT,250)
C 250 FORMAT ("1")
C
C WRITE (NPRT,251)
C 251 FORMAT (2(/))
C
C DJ 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

WRITE (NPRINT,260) (J,J=J1,J2)
   260 FORMAT ('1COMPONENT NO', 2IX, 9(I2,8X),I2)
WRITE (NPRINT,270) ((ZNAME(I,J),I=1,2),J=J1,J2)
   270 FORMAT (' NAME', 27X, 9(ZA4,2X),ZA4)
WRITE (NPRINT,275) (L(J),J=J1,J2)
   275 FORMAT (' COMPONENT TYPE', 19X, 9(I2,8X),I2)

WRITE (NPRINT,280) (W(J),J=J1,J2)
   280 FORMAT ('OMGEOCLAR WEIGHT', 15X, 9(F6.2,4X),F6.2)
WRITE (NPRINT,281) (TNBP(J),J=J1,J2)
   281 FORMAT (' NORMAL BOILING POINT (Deg K)', 2Y,
* 9(F7.1,3X),F7.1)

WRITE (NPRINT,285) (TCC(J),J=J1,J2)
   285 FORMAT (' CRITICAL PROPERTIES'/1X,' TEMPERATURE (Deg K)',
* 9X, 9(F7.1,3X),F7.1)
WRITE (NPRINT,290) (PCC(J),J=J1,J2)
   290 FORMAT (1X,' PRESSURE (Atm)', 10X, 9(F7.1,3X),F7.1)
WRITE (NPRINT,295) (VCC(J),J=J1,J2)
   295 FORMAT (1X,' VOLUME (cc/gmol)', 7X, 9(F7.1,3X),F7.1)
WRITE (NPRINT,297) (ZCC(J),J=J1,J2)
   297 FORMAT (' COMPRESSIBILITY FACTR', 7X, 9(F7.3,3X),F7.3)

WRITE (NPRINT,300)
   300 FORMAT (' LIQUID MOLAR VOLUME')

WRITE (NPRINT,390) I,(VOL(J),J=J1,J2)
   390 FORMAT (' LIQUID VOLUME (R)', 19X, 9(F7.4,3X),F7.4)
WRITE (NPRINT,395) (GMEGA(J),J=J1,J2)
   395 FORMAT (' ACENTRIC FACTR', 15X, 9(F7.3,3X),F7.3)

IF (IDLL.NE.5 .OR. IDLL.NE.6) GO TO 345
   345 WRITE (NPRINT,346) (RC(J),J=J1,J2)
   346 FORMAT (' ONORMALIZED UNIQAC PARAMETERS'/
* 1X,' VOLUME (R)', 19X, 9(F7.4,3X),F7.4)
WRITE (NPRINT,347) (CC(J),J=J1,J2)
   347 FORMAT (1X,' SURFACE AREA (Q)', 13X, 9(F7.4,3X),F7.4)
WRITE (NPRINT,348) (CQP(J),J=J1,J2)
   348 FORMAT (1X,' INTERACTION AREA (Q''''', 8X, 9(F7.4,3X),F7.4)

WRITE (NPRINT,350) (ZRA(J),J=J1,J2)
   350 FORMAT (' RACKETT PARAMETER', 13X, 9(F7.3,3X),F7.3)
WRITE (NPRINT,356) (RO(J),J=J1,J2)
   356 FORMAT (' RADIUS OF GYRATION, A', 9X, 9(F7.3,3X),F7.3)
WRITE (NPRINT,357) (CMU(J),J=J1,J2)
   357 FORMAT (' DIPOLE MOMENT, DEBYES', 9X, 9(F7.4,3X),F7.4)
WRITE (NPRINT,358) (ETA(J),J=J1,J2)
   358 FORMAT (' ASSOCIATION PARAMETER', 9X, 9(F7.4,3X),F7.4)
WRITE (NPRT,360) (HVAP(J),J=J1,J2)
360 FORMAT ("ENTHALPY 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("I",")", 21X, 1P10G10.6)
C 390 FORMAT (2X," C("I",")", 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(J,I),J=J1,J2)
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("I",")", 21X, 10F10.3)
C
IF (J2.EQ.NC) GO TO 430
425 CONTINUE
C
CONVERT ALL DATA TO MOLAR UNITS AND THEN GENERATE THE
C ENTHALPY POLYNOMIAL COEFFICIENTS ... FOR BOTH THE
C VAPOR AND LIQUID PHASES
430 DO 440 I=1,NC
C The following statement converts mm Hg to atm.
C ANT(1,I)=ANT(1,I)-LOG(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
345 CPL(I,J)=CPL(I,J)*W(I)
C 345 CPL(I,J)=CPL(I,J)*W(I)
C 345 CPL(I,J)=CPL(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)
T=TREF(I)
ENP(I,1)=-(CC*ENP(I,5)*T*ENP(I,4)*T*ENP(I,3)*T*ENP(I,2))*T*
* 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)-(CC*ENP(I,10)*T*ENP(I,9)*T*ENP(I,8)*T+*
* ENP(I,7))*T
440 CONTINUE
C
WRITE (NPRT,250)
IF (IDLV.EQ.0) GO TO 455
C
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IF (IDLV.EQ.1) WRITE (NPRT,431)

431 FORMAT ('OSCLAVATION PARAMETERS FOR THE VIRIAL EQUATION CF" / 
  " STATE ... HAYDEN-Q"CONNELL VERSION")
IF (IDLV.EQ.2) WRITE (NPRT,432)

432 FORMAT ('OCHARACTERISTIC BINARY CONSTANTS FOR THE VIRIAL" / 
  " EQUATION OF STATE ... TSNOPOULOS 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
NOTE: SOLVATION PARAMETERS AND CHARACTERISTIC BINARY
  CONSTANTS SHARE THE SAME STORAGE SPACE ... ETM(,*),
  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),AKCI,IJ),IJ=1,2)
445 FORMAT (3X, 2("K",I4,F9.4,3X))
GO TO 450
446 WRITE (NPRT,447) (ID(IJ),AKCI,IJ),IJ=1,3)
447 FORMAT (3X, 3("K",I4,F9.4,3X))
GO TO 450
448 WRITE (NPRT,449) (ID(IJ),AKCI,IJ),IJ=1,4)
449 FORMAT (3X, 4("K",I4,F9.4,3X))
450 CONTINUE
WRITE (NPRT,451)
451 FORMAT (///)
C
LIQUID-LIQUID BINARY INTERACTION PARAMETERS ...
... IDLL DEFINES THE ACTIVITY COEFFICIENT MODEL
C
  0  IDEAL
  1  VAN LAAR
  2  MARGULES
  3  WILSON
  4  NRTL
  5  UNIQUAC
  6  UNIQUAC ... MODIFIED
  7  UNIFAC
  8  ****
  9  ****
 10  ****
 11  EWR-F
 12  PENG-ROBINSON (PR)
C
RENEN ALPHA PARAMETERS
  ALPHA  NRTL CONSTANTS
455 IF (IDLLEQ.0) GO TO 520
C IF IDLLEQ.7 CALL RUNFAC FOR READING AND WRITING UNIFAC CONSTANTS
C IF (IDLLEQ.7) THEN
CALL RUNFAC
GO TO 520
END IF
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*NCH#2
C *** INPUT RECORD #10 --- ACTIVITY COEFFICIENT CODE --- Used
C *** Only If IDLLEQ.1 and for the second set of data.
C IF (NREAD.NE.0) READ (NCR#*) IDLLEQ.0 IDLL=ISTORE(1)
C *** INPUT RECORD #11 --- ACTIVITY COEFFICIENT PARAMETERS --- Used
C *** Only If IDLLEQ.1
DO 465 I=1,J,9
I2=II+7
IF (I2.GT.J) I2=J
465 READ (NCR#*) (C(I),I=I1,I2)
C 467 IF (LDBG.EQ.0) GO TO 495
IF (IDLLEQ.1) WRITE (NPRT,470) EQNV
IF (IDLLEQ.2) WRITE (NPRT,470) EQNM
IF (IDLLEQ.3) WRITE (NPRT,470) EQNW
IF (IDLLEQ.4) WRITE (NPRT,470) EQNR
IF (IDLLEQ.5) WRITE (NPRT,470) EQUU
IF (IDLLEQ.6) WRITE (NPRT,470) EQUU2
IF (IDLLEQ.7) WRITE (NPRT,470) EQNF
470 FORMAT (',', A8, ', CONSTANTS (ca/s/g-mol')
K=0
DO 490 I=1,NCH1
II=I+1
DO 490 J=II,NC
K=K+4
C 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*I+J
IF (I.GE.10) ID(2)=100*I+J
WRITE (NPRT,480) ID(1),CC(K-3),ID(1),CC(K-2),ID(2),CC(K-1),ID(2),
*C
490 CONTINUE
C 495 IF (IDLLEQ.4) GO TO 517
WRITE (NPRT,496)
496 FORMAT ('')

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**INPUT RECORD #12 ... NRTL ALPHA PARAMETERS --- Used Only If IDLL = 4**

```c
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 (LDBG.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(C"ALPHA",I4,"=""F7.4,4X))
  KK=1
510 CONTINUE
  IF (KK.EQ.1) GO TO 517
    KK=KK-1
    WRITE (NPRT,500) (ID(I),EK(I),I=1,KK)
    IF (KK.EQ.1) WRITE (NPRT,512) ID(1),EK(1)
512 FORMAT (3X,4(C"ALPHA",I4,"=""F7.4,4X))
  IF (KK.EQ.2) WRITE (NPRT,514) (ID(I),EK(I),I=1,2)
      IF (KK.EQ.3) WRITE (NPRT,516) (ID(I),EK(I),I=1,3)
516 FORMAT (3X,3(C"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
ON EXIT FROM "CDATA" GAMMA PARAMETERS IN "ICATA" ARE THE FIRST
PARAMETERS READ.
IF (NREAD.EQ.2) THEN
  IPSET=1
  CALL SWITCH
  GO TO 520
END IF
```

```c
GO TO 460
```

```c
DEFINE THE MODIFIED R-K CONSTANTS
520 IF (IDLV.EQ.0) GO TO 600
DO 590 I=1,NC
  IF (DA(I).NE.0.0) GO TO 550
590 DA(I)=OMA
550 IF (DB(I).NE.0.0) GO TO 570
```
**NOTE:** THE EQUATIONS FOR ENTHALPY AND VAPOR PRESSURE ARE:

1. **ENTHALPY DATA**/
   - HEAT OF VAPORIZATION \( \text{cal per gm} \) / \( \text{Deg K} \)/
   - SPECIFIC HEAT CONSTANTS LIQUID/
     - \( C_1 = a, C_2 = b, ..., C_4 = d \) / \( \text{cal per gram vs Deg K} \) /
     - \( C_p = a + bT + cT^2 + dT^3 \) /
   - SPECIFIC HEAT CONSTANTS VAPOR/
     - \( C_1 = a, C_2 = b, ..., C_4 = d \) / \( \text{cal per g-mole vs Deg K} \) /
     - \( C_p = a + bT + cT^2 + dT^3 \) /
   - VAPOR PRESSURE CONSTANTS/
     - \( C_1, C_2, ..., C_6 \) /
     - \( C_1 = a, C_2 = b, ..., C_6 = f \) /
     - \( \text{Atm versus Deg K} \) /
     - \( \ln(P) = a + b/(c + T) + d*ln(T) + e*T + f*T^2 \) /

END

SUBROUTINE RUNFAC

THIS SUBROUTINE READS UNIFAC DATA (R, Q AND GROUP INTERACTION PARAMETERS) FROM A DATA FILE ... LOGOCAL UNIT 10

COMMON /BLANK/ NCR, NPRT, NSTART, KUNITS, TITLE(20)
COMMON /CMRPRO/ NC, NCM1, NCP1, IDLL, IDLV, IDM, LDBG, ISW,
                NDIM, ZNAME(2,10), L(10), NTCOMP(10), NLIQ, IPSET
COMMON /IDATA/
       CPLC(10,4), CPVC(10,4), ENP(10,10), ANTC(5,10),
       W(10), AX, BX, OMEGA(10), AVALC(10), BVALC(10),
       AK(10,10), AK(10,10), Q(10,10), QPC(10), XL(10),
       V(10), C(10), ALPHAC(45), VHC(10), TC(10),
       PC(10), ZC(10), TNBP(10), GA(10), Q(10),
       A(10,10), G(10,10), ZR(10), RC(10), DMU(10),
       ETA(10)

COMMON /UNIFAC/ XMCL(11), COMLN(11), RESLN(11), ALGAC(11),
                ACTCF(11), IDPG(6,11), NQGPG(6,11), NQGMOL(11), AL(11),
                RI(11), QIC(11), HQPG(6,11), QGP(11), PARML(11,11),
                TIDC(11), GSUM(11), GG(11), TANAM(3,11)
COMMON /UNIFAC/ GNAM(3,80), QQ(80), RR(80), PARAM(42,42), NKTAB(80),
                KODE(42,42), NGPT, NSPS

CHARACTER*4 ZNAME, LNK, MOL(5,11), CARDC(20)
INTEGER ID(10)
REAL TREF(10), HVAP(10), EK(10)

NOTE: DIMENSION OF KODE AND PARAM HAVE BEEN SET TO 42X42
BECAUSE OF INPUT BY AN IMPLIED DO-LOOP AND FORMAT
# 4003.
INPUT FOR UNIFAC
1. READ DATA BANK FROM THE TAPE/DISK

2. READ COMPONENT AND NO. OF GROUPS PER COMP.
   * ONE RECORD FOR EACH CMP. (NC<11)
   NGMGL = NO. OF DIFFERENT GROUPS IN THE MOLECULE, (<=6)
   MGL = NAME OF THE COMPONENT.
   * BLANK RECORD AFTER THIS SET OF INPUT.
3. READ GROUP SPECIFICATION RECORDS
   * FOR EACH COMPONENT
   * A SEPERATE RECORD FOR EACH MOLECULE
   NDGP = NO. OF TIMES THE GROUP APPEARS IN THE MOLECULE
   IDGP = ID NO. OF THE GROUP (SECONDARY GROUP NO. FOUND
   IN THE TABLE IV IN THE REFERENCE STATED BELOW)

REF: 1. GHMLING, J., ET AL., IND. ENG. CHEM. PROCESS DES.
     DEV. 21, 118-127 (1982).

READ DATA BANK.

LUD=10

OPEN (UNIT=LUD, STATUS="OLD", ACCESS="SEQUENTIAL",
       FILE="C\CHAWLA\THERMOJ\BANKUNIF.DAT")

READ DATA BANK ... FILE LUD=10

NMG = # OF MAIN GROUPS
NSG = # OF SECONDARY GROUPS

QQ = GROUP AREA PARAMETER
RR = GROUP VOLUME PARAMETER
NKTAB = MAIN GROUP * TO WHICH THE SECONDARY GROUP BELONGS
GNAM = GROUP NAME

KODE = CODE FOR SOURCE OF DATA
PARAM = GROUP INTERACTION PARAMETERS

READ (LUD, 4000) CARD
466 READ (LUD, 4001) NMG,NSG
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)
WRITE (6,1)
1 FORMAT ("1")
WRITE (6,*) NSG
DO 10 I=1, NSG
WRITE (6,5) I, QQ(I), RR(I), NKTAB(I), (GNAM(J, I), J=1, 3)
5 FORMAT (15, 5X, 2F10.4, I10, 10X, 2A4, A2)
10 CONTINUE
WRITE (6,1)
WRITE (6,*) NMG
DO 15 I=1, NMG
WRITE (6,*) I
READ (LUD, 4003) (KODE(I, J), PARAM(I, J), J=1, NMG)
15 CONTINUE
WRITE (6,*) J, KODE(I, J), PARAM(I, J)
CONTINUE
4000 FORMAT (20A4)
4001 FORMAT (2I2)
4002 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
LNK = 10H
J = 1
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)
40 READ (5,1002) (NDGP(I,J),IDGP(I,J),I=1,NN)
40 READ (5,*) (NGGP(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
IDP(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
63 READ (5,1003) NMIX
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 = NGMCL(J)
DO 61 I=1,K
L1 = IDGP(I,J)
LI = IID(L1)
M = NXTAB(LI)
NUM = NGP(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 (KODECK(LI),EQ.0) GO TO 64
WRITE (6,2009)
IF (KODECK(LI),EQ.1) WRITE (6,2010) K,LI,IID(I),IID(J)
IF (KODECK(LI),EQ.2) WRITE (6,2011) K,LI,IID(I),IID(J)
IF (KODECK(LI),EQ.3) WRITE (6,2012) K,LI,IID(I),IID(J)
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
PRINT GROUP INTERACTION PARAMETER DATA.

C
DO 70 I=1,NGPT
K = IID(I)
DO 70 J=1,3
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
75 WRITE (6,2006) TNAM(I),PARAM(I,J),J=1,NGPT
75 WRITE (6,2006) (TNAM(J,I),J=1,3),(PARAM(I,J),J=1,NGPT)
C1001 FORMAT (2A10,I2)
1001 FORMAT (I12,4A6)
C1002 FORMAT (16I5)
C1003 FORMAT (F10.0,I5)
C1004 FORMAT (9F10.0)
2001 FORMAT (1H1,"UNIFAC CALCULATION OF ACTIVITY COEFFICIENTS")
2002 FORMAT (1H0,5A4//8X,"GROUP","4X","PRI","2X","SEC","3X","NUM","7X",1 ","9X,"R")
2003 FORMAT (6X,2A4,A2,"("","I2",""),",1X,"("","I2",""),",4X,I2,4X,F6.4,F6.4,F6.4)
2005 FORMAT (14X,11C2A4,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 10BAINED FROM METHANOL DATA, SEE REF. 3",/,
27X,"THES PARAMETERS ARE USED FOR THE ",I2,"-",I2," SECONDARY GROUP 3P INTERACTION")/)
2011 FORMAT(7X,"PARAMETERS FOR THE ",I2,"-",I2," INTERACTION MAY NOT BE 1 RELIABLE IN WHOLE CONCENTRATION RANGE, SEE REF. 3",/,
27X,"THES PARAMETERS ARE USED FOR THE ",I2,"-",I2," SECONDARY GROUP 3P INTERACTION")/)
2012 FORMAT(7X,"PARAMETERS FOR THE ",I2,"-",I2," INTERACTION WERE OBTAI NED FROM GAS CHROMATOGRAPHIC DATA, SEE REF. 4",/,
27X,"THES PARAMETERS ARE USED FOR THE ",I2,"-",I2," SECONDARY GROUP 3P INTERACTION")/)
C
RETURN
SUBROUTINE SWITCH

SUBROUTINE IS USED BY SETTING IPSET TO EITHER 1 OR 2
AND THEN CALLING SWITCH.

IF IPSET=1 LOAD FIRST SET OF DATA (VLE PARAMETERS)
IF IPSET=2 LOAD SECOND SET OF DATA (LLE PARAMETERS)

THIS SUBROUTINE LOADS AND UNLOADS PROPER PARAMETERS
RESTORE VLE PARAMETERS IN THE C ARRAY
LOAD LLE PARAMETERS IN THE C ARRAY

COMMON /BLANK/ NCR, NPRT, NSTART, KUNITS, TITLE(20)
COMMON /CMPRO/ NC, NCM1, NCP1, IDLL, IDLV, IDH, LBUG, 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),
* WC(10), AX, BX, OMEGA(10), AVAL(10), BVAL(10),
* AK(10,10), R(10), Q(10), QP(10), XL(10),
* VDL(10), C(180), ALPHA(45), VC(10), TC(10),
* PC(10), ZC(10), TNBP(10), JAC(10), OB(10),
* AC(10,10), G(10,10), ZRA(10), RDC(10), DMUC(10),
* ETA(10)
COMMON /SWITCH/ CSTORE(180,2), ASTORE(45,2), ISTORE(2)

IPSET = 0 ... NO ENTRY TO THIS SUBROUTINE
IPSET = 1 ... VLE PARAMETERS TO BE LOADED
IPSET = 2 ... LLE PARAMETERS TO BE LOADED
IPSET = 3 ... NOT YET DEFINED

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

ISTORE PRESERVES VALUES OF IDLL.
CSTORE AND ASTORE KEEP THE C AND ALPMA VALUES IN THE VECTORS
CORRESPONDING TO THE IPSET VALUE AS COLUMN NUMBER.

IDLL = ISTORE(IPSET)

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
  C(I)=CSTORE(I,IPSET)
620  CONTINUE
  IF (IDLL .NE. 4) GO TO 650
  J=NC#NCM1/2
  DO 650 I1=1,J,3
    I2=I1+7
    IF (I2.GT.J) I2=J
    DO 630 I=I1,I2
    ALPHA(I)=ASTORE(I,IPSET)
630  CONTINUE
RETURN
END

SUBROUTINE VIRFG1(T,P,Y,VP,FUG,DN,V)
VIRIAL EQUATION OF STATE USING THE HAYDEN - O'CONNELL METHOD

COMMON /CMPRO/ NC, NCM1, NCP1, IDLL, IDLV, IDH, LDBUG, ISW,
* NDIM, ZNAME(2,10), L(10), NTCOMP(10), NLIQ, IPSET
* COMMON /DATA/ CPL(10,4), CPV(10,4), ENP(10,10), ANT(6,10),
* W(10), AX, BX, DMEGA(10), AVAL(10), BVAL(10),
* AK(10,10), R(10), Q(10), QT(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)

REAL Y(1), VP(1), FUG(1), B(10,10)

DATA RPVT/82.055/, EXPN/0.333333/

-----------------------------------------------
OBTAIN THE VIRIAL COEFFICIENTS FROM "BCALC"
-----------------------------------------------

CALL BCALC (T,B)

OBTAIN B=MIX

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

SQARG=0.25*BMIX*PORT
IF (SQARG) 22,25,25

OBTAIN THE FUGACITY COEFFICIENT

IF BMIX*P/R/T IS MORE NEGATIVE THAN 0.25, THE PRESSURE SERIES
EQUATION MUST BE USED ... FTN STM #22. THE ALTERNATE IS TOO USE
THE VOLUME SERIES ... FTN STM #25.

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

PHI IS THE FUGACITY OF THE VAPOR & PHIS IS THE FUGACITY OF
THE SATURATED LIQUID EVALUATED AT THE VAPOR PRESSURE

PHI=EXP(C2.0*SUMB-BMIX)*PORT
PHIS=EXP(C(I,I)*VP(I)/RT)
PGNTY=EXP((P-VP(I))*VCL(I)/RT)
FUG(I)=PHIS*QNTY/PHI

PRINT 300,I,PHIS,PONTY,PHI,FUG(I),Y(I),VP(I)
24 CONTINUE
GO TO 50
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)*A(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(C(B(I,I))*VP(I)/RT)
PONTY=EXP((P-VP(I))*VQ(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
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
VIRIAL EQUATION OF STATE USING THE HAYDEN - O'CONNELL METHOD
C
COMMON /CMPRO/ NC, NCMI, NCP1, IDLL, IDLV, IDH, LDBG, ISW,
* COMMON /ZDATA/ CPL(10,4), CPV(10,4), ENP(10,10), ANT(6,10),
* W(I), AX, BX, OMEGA(I), AVAL(I), BVAL(I),
* AK(10,10), RC(10), GC(10), QPC(10), XL(10),
* VCL(10), C(180), ALPHA(45), VC(10), TC(10),
* PC(10), ICC(10), TNBP(10), QA(10), OB(10),
* A(10,10), G(10,10), IRA(10), R(I), DMU(10),
* ETA(T)
C
REAL Y(I), B(I)
C
DATA RPVT/82.055/, EXPN/0.333333/
C
CALL BSEC (T,9)
C
OBTAIN THE VIRIAL CGEFFECTS FROM "BCALC"
C
CALL BCALC (T,9)
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)
15 SUMY=SUMY+Y(I)
DO 10 J=1,NC

10 BMIX = BMIX + Y(I) * Y(J) * 9(I,J)
15 CONTINUE
   BMIX = BMIX / SUMY ** 2
C
   SQARG = 0.25 * BMIX / PORT
   IF (SQARG) 22, 25, 25
C
   IF BMIX * P/R/T IS MORE NEGATIVE THAN 0.25, THE PRESSURE SERIES
   EQUATION MUST BE USED ... FTN STM #22. THE ALTERNATE IS TOO USE
   THE VOLUME SERIES ... FTN STM #25.
C
   PRESSURE SERIES FORM OF THE VIRIAL EQUATION OF STATE
22 VMIX = BMIX + 1.0 / PORT
   ZMIX = PORT * VMIX
   GO TO 50
C
   VOLUME SERIES FORM OF THE VIRIAL EQUATION OF STATE
25 VMIX = (0.5 + SQRT(SQARG)) / PORT
   ZMIX = PORT * VMIX
C
50 RETURN
END
C
SUBROUTINE BCALC (T, S)
C
THIS PROGRAM BUILDS A MATRIX OF PURE COMPONENT AND
CROSS VIRIAL COEFFICIENTS, BC(I, J) FOR UP TO 10
C COMPONENTS
C
COMMON /CMPRO/ NC, NCM1, NCP1, IDL1, IDLV, IDH, LDBUG, ISW,
   NDIM, NAME(2,10), LI(10), NTCOMP(10), NLIG, ISP.
   COMMON /2DATA/ 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), RC(10), Q(10), QP(10), XL(10),
   VOL(10), CC(180), ALPHM(45), VC(10), TC(10),
   PPC(10), ZC(10), TNBP(10), OA(10), OB(10),
   AC(10,10), GC(10,10), ZR(10), RC(10), DMUC(10),
   ETA(10)
C
REAL PPC(2), RR(2), DDMUC(2), EETA(3), TTC(2),
   ZZC(2), BB(3), BB(10,10), ETM(10,10)
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 ... TSDNOPOLUS VERSION
C
EQUIVALENCE (ETM(1,1), AK(1,1))
C
THE PROGRAM CALLS SUBROUTINE SVIR ... FOR ACTUAL
C GENERATION OF THE B-VALUES
C
PPC = CRITICAL PRESSURE IN ATMOSPHERES
TTC = CRITICAL TEMPERATURE IN K
RRD = MEAN RADIUS OF UNIQUATION IN A
DMUC = DIPOLE MOMENT IN DEBYE
EETA = ASSOCIATION PARAMETER FOR COMPONENT I
ZZC = CRITICAL COMPRESSIBILITY FACTOR
ETM = SCLVATION PARAMETERS. EACH CARD CONTAINS
THE SOLVATION PARAMETERS BETWEEN A
GIVEN I = 1, NC-1 AND ALL J = I+1, NC

IN=NCM1
DO 11 I=1, IN
II=I+1
DO 11 J=II, NC
11 ETM(J, I)=ETM(I, J)
DO 12 I=1, NC
12 ETM(I, I)=EETA(I)
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)
ZIC(K)=ZC(M)
IF (K.EQ.2) GO TO 24
K=2
M=J
GO TO 23
24 ETA(3)=ETM(I, J)
CALL SVIR (N, TEMP, BB, PPC, RRD, DDMU, EETA, TTC, ZIC)
B(I, I)=BB(1)
B(J, J)=BB(2)
B(I, J)=BB(3)
32 B(J, I)=B(I, J)
RETURN
END
SUBROUTINE SVIR (N, TEMP, BB, PPC, RRD, DDMU, ETA, TTC, ZIC)

CALCULATION OF PURE COMPONENT AND CROSS VIRIAL COEFFICIENTS
FOR TWO COMPONENTS AT TEMPERATURE T FROM HAYDEN AND O'CONNELL
... IEC PROC. DES. DEV. 14(3)209(1975)

N = NUMBER OF COMPONENTS (1 OR 2)
BF = BFREE
BB = B TOTAL
NC = # OF COMPONENTS
PC = CRITICAL PRESSURE, ATM
RD = MEAN RADIUS OF GYRATION, A
DMU = DIPOLE MOMENT IN DEBYE
ETA(1) AND ETA(2) = ASSOCIATION PARAMETERS (PURE COMPONENTS)
ETA(3) = SOLVATION PARAMETER (CROSS INTERACTION)
TC = CRITICAL TEMPERATURE , DEG K
ZC = CRITICAL COMPRESSIBILITY FACTOR

REAL BF(3), BB(3), w(3), EPSI(3), RDUM(3), SIGM3(3),
*  RDM(3), A(3), DELK(3), O(3), BO(3)
REAL PC(1), RD(1), DMU(1), ETA(1), TC(1), ZC(1)
DATA EXPN /0.33333/

CALCULATION OF COMPONENT PARAMETERS
EQ'S 15,30,17,24,25,23,21,22,10

103 N=16.0+400.0*W(I)
C=2.882-1.882*W(I)/(0.03+W(I))
XI=DMU(I)**4/(C*EPSI(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*X1/(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

NONPOLAR-NONPOLAR, EQ'S 32,33,34
PARAMETERS FOR MIXTURE CALCULATION

401 EPSI(C)=0.7*SQRT(EPSI(1)*EPSI(2))+0.5/((1.0/EPSI(1)+1.0/EPSI(2))
SIGM3 (3)=SQRT(SIGM3(1)**SIGM3(2))
W(C)=0.5*(W(1)+W(2))
IF (DMU(1)*DMU(2)) 500,5,1,500

POLAR-NONPOLAR, EQ'S 38,24,36,37

501 IF (DMU(1)+DMU(2)-2.0) 500,500,19
19 XI38=(DMU(1)**2*EPSI(2)**2*SIGM3(2)**2*EXPN*SIGM3(2)+DMU(2)**
2*EPSI(1))**2*SIGM3(1)**2*EXPN*SIGM3(1)/EPS(3)*SIGM3(3)**2)
PN=16.0+400.0*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))

POLAR-PCLAR, EQ'S 35,37

500 RDMU(3)=7243.8*DMU(1)*DMU(2)/EPSI(3)**SIGM3(3))
301 DD 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 RDMCI=0.0
GO TO 600
17 RDMCI=RDMU(I)-0.25
600 CONTINUE

LAST PARAMETERS, EQ'S 7,8,9,29

DD 609 I=1,J
C CALCULATION OF VIRIAL COEFFICIENTS, EQUATIONS 14, 13, 26, 6, 29
C
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
BF=(0.75-3.0*TSTR+2.1*TSTR**2+2.1*TSTR**3)*RDME(I)
BF(I)=(BFN-BF)*BD(I)
BB(I)=BF(I)+BD(I)*A(I)*EXP(DELM(I)*EPSI(I)/TEMP)
IF (ETA(I)) 651, 651, 653
653 BBHEM=BD(I)*EXP(ETA(I)*(CT(I)-4.27))+(1.0-EXP(1500.*ETA(I)/TEMP))
BB(I)=BB(I)+BBHEM
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 COMPONENTAL 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
C COMMON /CMPRO/ NC, NCMI, NCP1, IDLL, IDLV, IDMH, DBUG, ISW,
* COMMON /ZDATA/ CPL(10,6), CPV(10,4), ENP(10,10), ANT(6,10),
* W(10), AX, BX, OMEGA(10), AVAL(10), BV(10),
* AK(10,10), RC(10), Q(10), QPC(10), XL(10),
* VOL(10), C(180), ALPHC(45), VC(10), TC(10),
* PCC(10), ZC(10), TNAP(10), CA(10), GB(10),
* A(10,10), G(10,10), IRC(10), RC(10), DMU(10),
* ETA(I)
C
C REAL X(I), GAM(I), THETA(I), THS(I), PHIC(I),
1 THETAP(I)
C
C IF (ISW .NE. 0) GO TO 20
C
C RT=1.9972*T
K=0
DO 10 I=1,NCMI
IP1=I+1
DO 10 J=IP1,NC
K=K+4
G(I,J)=EXP(-CC(K-3)+C(K-2)*T)/T
G(J,I)=EXP(-CC(K-1)+C(K)*T)/T
10 CONTINUE
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
      THETAP(I)=Q(I)*X(I)/THETS
      THETAP(I)=QP(I)*X(I)/THETPS
40   PHI(I)=X(I)*R(I)/PHS

   TAU(I,J)=G(I,J)=EXP((A+8*T)/T)
   DO 50 I=1,NC
      THS(I)=0.0
      DO 50 J=1,NC
      GB=1.0-ALOG(THS(I))
      DO 60 J=1,NC
      GB=GB-THETAP(J)*G(I,J)/THS(J)
60   GB=GB-THETAP(J)*G(I,J)/THS(J)
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)-RL(I)/PHS*XL
      GB=1.0-ALOG(THS(I))
    DO 60 J=1,NC
70   GAM(I)=EXP(GA+QP(I)*GB)

RETURN
END

SUBROUTINE XHUNQ2(T,X,XSH)

THIS ROUTINE USES THE MODIFIED UNIQUAC EQUATION AS DEVELOPED
BY ANDERSON (1978). EQUATION USES MOLECULAR PARAMETERS R,
Q, AND Q", FLUS BINARY COMPONENTAL PARAMETERS A(I,J) AND
A(J,I).

REFERENCE: "COMPUTER CALCULATIONS FOR MULTICOMPONENT
V-L AND L-L SYSTEMS" ... BY J. PRAUSNITZ ET. AL. (1990)

COMMON /CMPRO/ NC, NCM1, NCPI, IDL1, IDLV, IDM, LDBUG, ISW,
  NDIM, ZNAME(2,10), L(10), NTCOMP(10), NLIQ, IPSET
COMMON /ZDATA/ CPL(10,4), CPV(10,+), ENP(10,10), ANT(6,10),
  w(10), AX, BX, OMEGA(10), AVAL(10), BVAL(10),
  AK(10,10), RK(10), Q(10), QP(10), XL(10),
  VOL(10), C(180), ALPMA(45), VCI(10), TCI(10),
  PC(10), ZC(10), TNBP(10), OA(10), DB(10),
  A(10,10), G(10,10), IRAC(10), RC(10), DMU(10),
  ETA(10)

REAL X(1), THETAP(10), HFAC(10), HMFA(10), HM(10)

C IF (ISW.NE.0) GO TO 20
C
RGC=1.9872
K=0
DO 10 I=1,NCM1
   IP1=I+1

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DO 10 J=1,P1,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

ARG=TAU(I,J)=G(I,J)=EXP((A+B*T)/T)

C

DO 50 I=1,NC
HFAC(I)=0.0
HMFA(I)=0.0
DO 50 J=1,NC
ARG=G(J,I)
HFAC(I)=HFAC(I)+THETAP(J)*ARG+ALDG(ARG)
50 HFAC(I)=HMFA(I)+THETAP(J)*ARG
DO 60 I=1,NC
60 HMCI=QP(I)*X(I)*HFAC(I)/HMFA(I)
DO 70 I=1,NC
70 XSH=XSH-RGC*HMCI

C

RETURN
END

SUBROUTINE UNIFAC (T,X,GAM)

C COMMON /UNFAC/ XMOL(11),QOMLN(11),RESLN(11),ALGAC(11),
1 ACTCF(11),IDGP(6,11),NOGP(6,11),NGMOL(11),AL(11),
2 RI(11),QIC(11),QGPIC(5,11),QGP(11),PARAM(11,11),
3 IID(11),GSUM(11),GC(11),TNAM(3,11)

C COMMON /UNFAC1/

C REAL X(1), GAM(1)

C CHARACTER,*4 MCL(5,11)

C

DO 10 J = 1, NSPS
XMCL(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 COMPUTE COMBINATORIAL PORTION AND RELATED SUMS.

C

RSUM = 0.
QSUM = 0.
DO 80 I=1,NGPT

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80 QGP(I) = 0.
   DO 95 J=1,NSPS
   RIC(J) = 0.
   QI(J) = 0.
   K = NGMGL(J)
   DO 85 I=1,K
   A = NGOPI(I,J)
   L = IDGP(I,J)
   M = IID(L)
   RIC(J) = RIC(J) + A*RR(M)
   QI(J) = QI(J) + A*QQ(M)
   QGPI(I,J) = A*QQ(M)
85   QGPP(L) = QGPP(L) + QGPI(I,J)*XMDL(J)
   RSUM = RSUM + RIC(J)*XMDL(J)
   QSUM = QSUM + QI(J)*XMDL(J)
   DO 90 I=1,K
   90   QGPI(I,J) = QGPI(I,J)/QI(J)
   CONTINUE
   DO 100 I=1,NGPT
100  QGP(I) = QGP(I)/QSUM
   SUML = 0.
   DO 105 J=1,NSPS
   AL(J) = 5.*(RIC(J) - QI(J)) - RIC(J) + 1.
   105   SUML = SUML + AL(J)*XMDL(J)
   DO 120 J=1,NSPS
   CON1 = RIC(J)/RSUM
   CON2 = QI(J)/QSUM
   DO 120 CONM(J) = ALOG(CON1) + 5.*QI(J)*ALOG(CON2/CON1)
120   + 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
   SUM = SUM + QGP(K)*PARM(I,K)/GSUM(K)
135   GG(I) = 1. - ALOG(GSUM(I))/SUM
   DO 155 J=1,NSPS
   RESL(J) = 0.
   K = NGMGL(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)
   CCONST = FLOAT(NGOPI(I,J)) + QQ(JJ) + QQ(M) - (1. - ALOG(GSUM(I))-SUM)
150   RESL(J) = RESL(J) + CCONST
   ALGAC(J) = COMLNC(J) + RESL(J)

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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), XMCL(J), ALGAC(J), ACTCF(J)
 C 160 WRITE (6,2008) (MCL(K,J), K=1,5), XMCL(J), ALGAC(J), ACTCF(J)
 CC
 C 999 CALL EXIT
 C   STOP
 C   RETURN
 C   END
SELECTED BIBLIOGRAPHY


W. Germany, 1977.


