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THE ENTRAINER EFFECT ON AZEOTROPIC DISTILLATION COLUMN DESIGN

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THE ENTRAINER EFFECT ON AZEOTROPIC DISTILLATION COLUMN DESIGN

by

CHARLES MING-HSIAO TSAI

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
1982

APPROVAL SHEET

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ABSTRACT

Title of Dissertation: The Entrainer Effect on Azeotropic Distillation Column Design

Charles Ming-Hsiao Tsai, Doctor of Engineering Science, 1982

Dissertation directed by:

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

A rigorous multistage distillation model was developed for use with non-ideal multicomponent systems. A subsidiary computer program was also developed to handle the problem of two liquid phases after condensation of a vapor.

Using the program developed, entrainer entry location and rate effects have been investigated via computer simulation for azeotropic distillation columns. The specific example used to verify the procedure was an ethanol dehydration column using benzene as the entrainer. The results indicate that the entrainer should enter the column two to five theoretical stages above the feed. The optimum entrainer rate was also determined.

The overhead vapor product from the azeotropic column, upon condensing to a subcooled liquid, forms two liquid phases in the accumulator. A two-liquid phase separation model was used to deal with the liquid phase splitting. This model has been validated using published data for nonideal ternary and quaternary systems. A study of the accumulator temperature effect on liquid phase splitting was also accomplished for the ethanol

dehydration column. The results indicate that at lower accumulator temperatures the benzene loss in the heavy phase can be reduced.

Finally, the azeotropic distillation model and the two-liquid phase flash model were included in a representation of a complete industrial ethanol purification plant. Incorporated in the plant simulation is the azeotropic column, two-liquid phase accumulator, a benzene stripping column and an ethanol recovery/water purge column. The ability of this model to converge on the benzene entrainer stream was verified.

PREFACE

Azeotropic distillation refers to those processes where a component is used to modify the relative volatility of the key components to some value greater than or less than unity. The added component is called an entrainer, and forms an azeotrope with one or more of the feed components. The azeotrope is removed as part of the desired overhead product. The entrainer is recovered to a significant degree with the distillate or the overhead product.

It is commonly accepted that the entrainer in azeotropic distillation forms a minimum boiling azeotrope with one of the key components and not with the other, or it forms a ternary azeotrope having a widely different composition from that of an azeotrope with one of both of the keys. The change of the relative volatility is due to the tendency toward immiscibility of the entrainer and the associated key component with respect to the other key component. If immiscibility does occur or is approached, one phase will contain the entrainer and light key, and the other the heavy key. The entrainer in this case will act as a stripping agent.

If a heterogeneous phase azeotrope (second liquid phase) is formed upon condensing the overhead vapor, a decanter (liquid gravity separator) which also serves as the distillate accumulator can be used to separate the entrainer from the key component. The entrainer rich layer is recycled back to the column as the second feed. The other liquid (net overhead product) is processed further to separate the light key from the entrainer. The loss of the entrainer in the heavy key rich stream, if it can not be recovered, will require a make up stream to maintain the proper concentration level of the entrainer to the azeotropic column. The recycled entrainer stream can mix with the feed to column, either above or below the feed entry. The entrainer entry point and rate plays an important role in the operation of the azeotropic distillation column.

This research proposes to study the entrainer effect on the azeotropic distillation process which forms two liquid phases when the column overhead vapor is condensed. The optimum entrainer rate, composition, and entry location are the main subjects of this dissertation.

DEDICATION

Dedicated to Cheryl,
my lovely and intelligent daughter.

ACKNOWLEDGEMENT

The author wishes to express his sincere appreciation to his faculty advisor, Dr. Edward C. Roche, Jr. for his guidance and help. The management of the Bayway Refinery of Exxon Company, USA has been very supportive of this work. The author is in debt to his family for the encouragement and support he received during the preparation of this work.

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CHAPTER 1

INTRODUCTION

This research proposes to study the entrainer effect on azeotropic distillation from the standpoint of rate, composition, and entry location. A ternary system, ethanol-water-benzene, with benzene as the entrainer was chosen for the in depth analysis.

The selection of the entrainer is not included in this study, this having been discussed by Ewell and Berg (1944). The entrainer rate effect was investigated by Hachmuth (1952) for the ternary system, MEK-n-heptane-toluene, with MEK used as the entrainer. Hachmuth concluded that the entrainer must be presented in an appreciable concentration, at least as much as 30 mole percent and preferably more than 50 mole percent of the feed rate. Recently, Black (1980) evaluated the entrainer selection, and entrainer to feed ratio for the ethanol dehydration process. Black concluded that pentane was superior to either benzene or diethyl ether as the entrainer in the ethanol dehydration process. Unfortunately, the detailed approaches used to arrive at the conclusion were not revealed in the publication.

Rubin and Benedict (1945) studied the entrainer entry location using a graphical method for the ternary system, toluene-n-heptane-methanol (entrainer). They concluded that the entrainer can be added with, above or below the feed depending upon the volatility of the entrainer with respect to the non-entrainer components.

The two-liquid phase handling in a distillation column has been reported by Block and Hegner (1976), Ross and Seider (1979), and Shah-Boston (1979). Since in this research, the two-liquid phase distillate is the primary concern, the two-liquid phase flash calculation methods by Deam (1969), and Roche (1977) were used to determine the distillate splitting.

To facilitate the azeotropic distillation simulation, the algorithm of Fredenslund (1977) was modified and enhanced for the reboiled absorber stripper type simulation. In Chapter 2, this azeotropic distillation model, which is the first part of this research, is discussed. As part of the initial phase of this research, the effect of entrainer location and rate was evaluated. This is the first accomplishment of this dissertation.

The next focal point in this research endeavor is the two-liquid phase flash which occurs in the distillate accumulator. In Chapter 3, a two-liquid phase flash model was utilized for this purpose. The simulation is based on Deam (1967) and Roche (1977). The sub-cooling effect on liquid phase splitting is investigated in this segment of the study. This is the second accomplishment of this research.

The third part of the research effort was the combining of the previously mentioned models using a specific executive. The details of this executive are discussed in Chapter 4, where the entrainer rate and composition are converged to yield the desired separation. The ability to converge the entrainer rate and composition is the third accomplishment of this research.

Finally, the conclusions reached as a result of this research and the recommendations for further studies are presented in Chapter 5.

CHAPTER 2

THE AZEOTROPIC DISTILLATION MODEL

In this chapter, the azeotropic distillation model used in this research is described. The model is presented by Fredenslund et al. (1977) which is based on the work of Naphtali and Sandholm, and has been extensively modified and enhanced for this research. Since the systems which form a heterogeneous azeotrope in the overhead distillate are the primary subject of this research, the two-liquid phase condition is assumed to occur only in the overhead accumulator upon condensation and subcooling. The capabilities of the azeotropic distillation model are summarized as follows:

1. Multiple feeds (maximum, 10 feed streams)
2. Vapor and liquid sidestreams (maximum, 10 streams of each phase)
3. Multicomponent system (maximum, 10 components)
4. Multiple stages (maximum, 50 stages)
5. Vapor-liquid equilibrium package can handle ideal and most non-ideal vapor-liquid systems.
6. Multiple stage heat exchangers (maximum, 10 heat exchangers).

With the multistage vapor liquid model validated in its various forms, the reboiled absorber mode was used to conduct the entrainer location study. The ethanol-water-benzene system was verified using the developed model with information published by the Chem Share Corporation (1980) on the design of the ethanol recovery section of a 'Gasohol Process.' With continuing interest in gasohol as a gasoline octane improver, the ethanol-water-benzene (entrainer) system was used to conduct the entrainer effect study. The results of this study are discussed in Section 2.5.

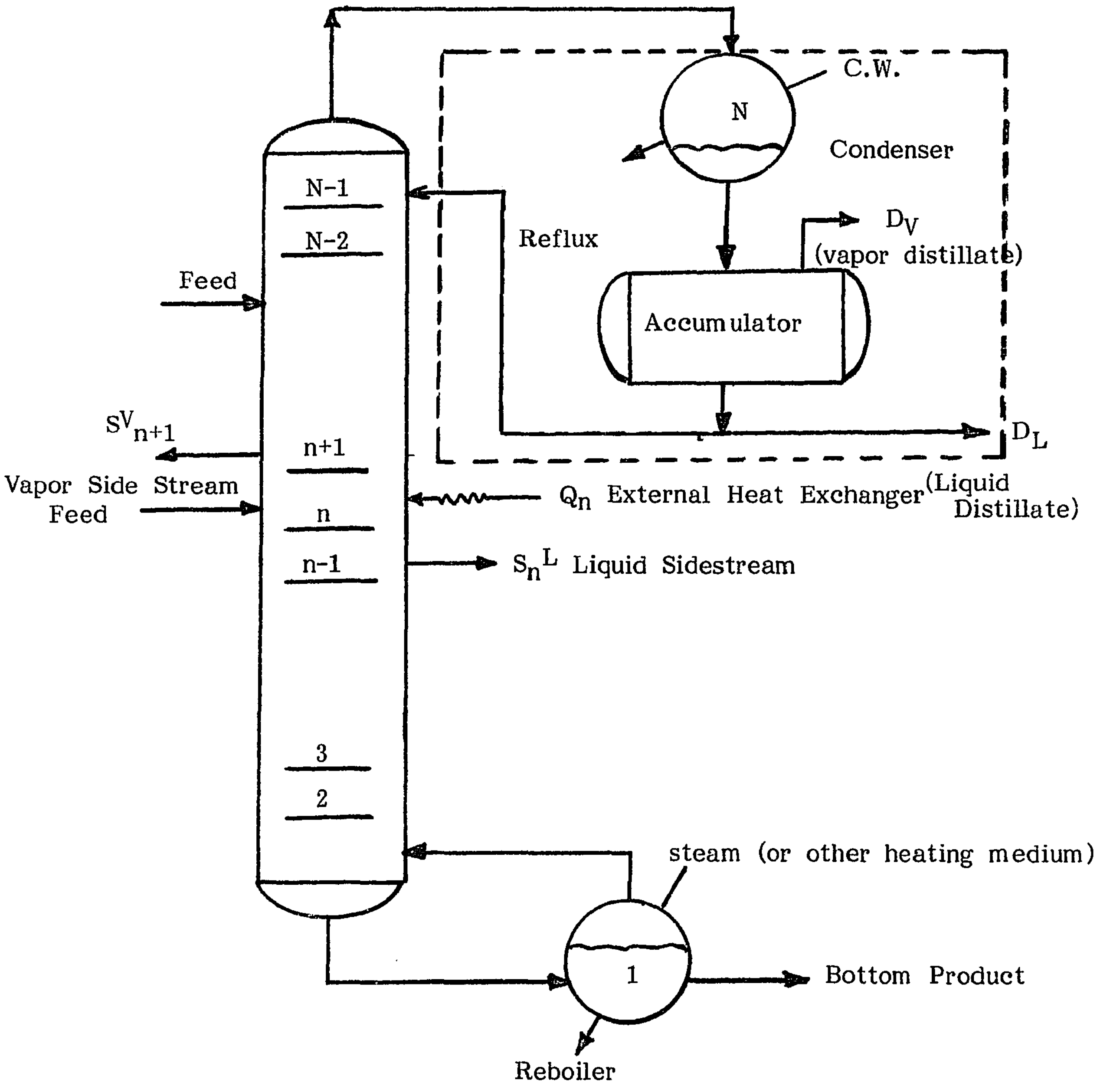
2.1 Equations and Column Configuration

The model developed by Fredenslund et al. (1977), is based on the Naphtali-Sandholm algorithm (1971) and has been enhanced to accommodate the strong non-ideal behavior of the systems chosen for this research. Modifications proposed by Roche (1978) were used in this work. The newer Vapor-Liquid-Equilibrium (VLE) correlations by Prausnitz et al. (1977, 1980, 1981) and Tsonopoulos (1972) have been incorporated in the model and used in this investigation. These newer correlations are chosen since the topic of interest is a low pressure separation involving polar compounds. In addition, the stagewise Newton-Raphson convergence technique has been enhanced.

The distillation column for this research is illustrated in Figure 2.1 and the following column specifications must be specified to execute the rigorous multicomponent stage to stage calculations.

1) The number of stages, with the reboiler designated as the first stage, while the partial condenser (with vapor and liquid distillates) is the Nth.
2) Murphree stage efficiencies (default value is 100%).
3) Sidestream location and withdrawal rate.

Figure 2.1 Distillation Column Configuration



Note: For reboiled absorber type operations the overhead stream contains only the vapor distillate, condensor and accumulator are not included.

4) Feed composition, rate, thermal state, and location.
5) Total overhead flow rate.
6) Reflux ratio or boilup ratio.
7) Column pressure distribution.

This model with appropriate specifications can be applied to the following simulations:

a) Absorber/stripper (end feed column).
b) Reboiled absorber/refluxed stripper.
c) Distillation column with product rate and reflux ratio.
d) Distillation column with product rate and boilup ratio.

The product distillate can be either dew point vapor, bubble point liquid, subcooled liquid, or an equilibrium vapor/liquid mixture. All but the dew point vapor require the presence of a condenser.

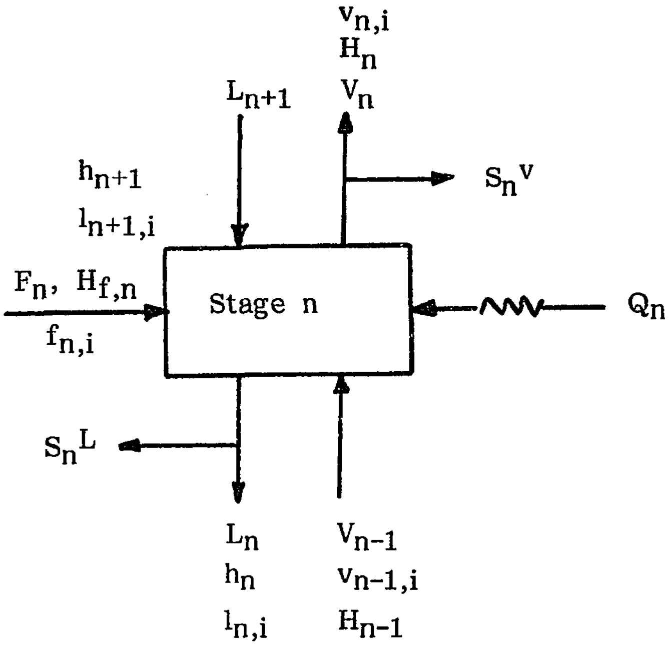
For an arbitrary stage n, the configuration and nomenclature are given in Figure 2.2.

The threefold set of discrepancy functions describing stage n are listed below:

Component Material Balance (one for each component)

$$F_1(n,i) = (1 + \frac{S_n^L}{L_n}) l_{n,i} + (1 + \frac{S_n^V}{V_n}) v_{n,i} - v_{n-1,i} - l_{n+1,i} - f_{n,i} = 0 \tag{2-1}$$

Equilibrium Condition coupled with the Murphree stage efficiency, η_n



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

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

H = vapor phase enthalpy

h = liquid phase enthalpy

H_f = feed enthalpy

V = total vapor flow

v = component vapor flow

L = total liquid flow

l = component liquid flow

F = total feed

f = component feed

S^L = liquid sidestream

S^V = vapor sidestream

Q_n = external heat exchanger

Figure 2.2 Stage Configuration

$$F_2(n,i) = \eta_n \frac{K_{n,i}\, V_n}{L_n} l_{n,i} - v_{n,i} + (1 - \eta_n) \frac{V_n}{V_{n-1}} = 0 \quad (2\text{-}2)$$

Where the Murphree stage efficiency is defined by

$$\eta_n = \frac{y_{n,i} - y_{n-1,i}}{K_{n,i} x_{n-1,i} - y_{n-1,i}} \quad (2\text{-}3)$$

and the Equilibrium Constant is defined by

$$K_{n,i} = \left(\frac{y_i}{x_i}\right)_n = \left(\frac{\gamma_i f_i^o}{\phi_i \pi}\right)_n \quad (2\text{-}4)$$

Equation 2-4 will be discussed in more detail in Section 2.3.

Energy Balance

$$F_3(n) = \left(1 + \frac{S_n^L}{L_n}\right) h_n + \left(1 + \frac{S_n^V}{V_n}\right) H_n - H_{n-1} -$$

$$h_{n+1} - h_n^F - Q_n + h_{n+1}^{mix} = 0 \quad (2\text{-}5)$$

The enthalpy calculations associated with Eq. 2-5 are calculated as follows:

Liquid Enthalpy

$$h_n = l_i \int_{T_{ref}}^{T} C_{p_L}(T)dT + h_n^{mix} \quad (2\text{-}5A)$$

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

T_{ref} = the reference time used in enthalpy calculations, normal boiling point is used.

h_n^{mix} = the heat of mixing, which is described in Appendix B.

Vapor Enthalpy

$$H_V = v_i\{\lambda_i + \int_{T_{ref}}^{T} C_{p_v}(T)dt + \Delta H\} \qquad (2\text{-}5B)$$

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

λ = the component heat of vaporization

ΔH = the enthalpy correction due to temperature, pressure effects

2.2 Iteration Algorithm

The discrepancy functions, $F_i(N_i)$, are a quantitative measure of the failure of the independent variable, $l_{n,i}$,$v_{n,i}$, and T_n to satisfy the physical condition of the column.

These relationships comprise a vector of test functions,

$$\underline{F}(\underline{x}) = \begin{Bmatrix} \underline{F}_1 \\ \underline{F}_2 \\ \underline{F}_3 \end{Bmatrix} = 0 \qquad (2\text{-}6)$$

Which can be solved for equally many unknowns:

$$\underline{x} = \begin{Bmatrix} \underline{l} \\ \underline{v} \\ \underline{T} \end{Bmatrix} \qquad (2\text{-}7)$$

Where the vector $\underline{l}$ contains all the elements $l_{n,i}$, $\underline{v}$ all the elements $v_{n,i}$, and $\underline{T}$ all the elements T_n. Once all $l_{n,i}$, $v_{n,i}$, and T_n's are known, the product flow rates, composition, and concentration profile can be evaluated.

Eq. (2-6) is solved by utilizing the Newton-Raphson method which employs the simultaneous convergence of all the independent variables $\underline{x}$.

In a Newton-Raphson iteration, a new set of values of the independent variables, $\underline{x}_r$, is generated from a previous estimate, $\underline{x}_{r-1}$, in the following fashion:

$$\underline{x}_r = \underline{x}_{r-1} - \underline{F}_{r-1}(\underline{x}_{r-1}) \left(\frac{\partial \underline{F}}{\partial \underline{\underline{x}}}\right)^{-1} \Bigg|_{\underline{x}_{r-1}} \qquad (2\text{-}8)$$

When $(\underline{X}_r - \underline{X}_{r-1})$ is sufficiently small, the correct set of values of $\underline{X}$ has been found, and the iteration stops.

The variations between subsequent iterations are arbitrarily limited as follows:

1) Negative component molar flow rates are not permitted.
2) Componential flow rates exceeding L_n are set equal to L_n.
3) The maximum change in the temperature at each stage, T_n is 10^{o}K.

The linearization of the discrepancy function, evaluation of Jacobian correction matrix, $(\partial F/\partial \underline{X})$, the structure of the Jacobian, and the iteration algorithm proposed by Roche (1977) are described in Appendix A.

2.3 VLE Predication Method

Vapor-liquid equilibrium requires that the fugacity of a component in the vapor be equal to the fugacity of that component in the liquid. The vapor-liquid equilibrium has been discussed by Prausnitz (1967, 1980) and Gmehling et al. (1977) in detail for systems involving separations at or below essentially atmospheric pressure.

$$f_i^V = f_i^L \tag{2-8}$$

The vapor phase fugacity can be represented by:

$$f_i^V = \phi_i y_i \pi \tag{2-9}$$

Where

y_i = is the component mole fraction in the vapor phase.

π = is the system pressure.

ϕ_i = is the fugacity coefficient of the component in the multicomponent vapor phase.

The fugacity in the liquid phase can be represented by:

$$f_i^L = \gamma_i X_i f_i^{oL} \tag{2-10}$$

where

X_i = is the component mole fraction in the liquid phase.

γ_i = is the activity coefficient at the system temperature.

f_i^{oL} = is the standard state fugacity of the pure component at system temperature and pressure.

$$f_i^{oL} = f_i^S \operatorname{Exp} \int_{p_i^S}^{\pi} \frac{\overline{V}_i dp}{RT} = \phi_i^S p_i^S \operatorname{Exp} \int_{p_i^S}^{\pi} \frac{\overline{V}_i dp}{RT} \tag{2-11}$$

Where

$\int_{p_i^S}^{\pi} \overline{V}_i dp$ = is the poynting correction factor.

f_i^S = fugacity of component at saturation ($p = p_i^S$)

$\overline{V}_i$ = partial molar volume of component.

$\phi_i{}^s$ = fugacity coefficient of component at saturation pressure.

$p_i{}^s$ = saturation pressure of component.

For convenience, $\overline{V}_i$ is assumed to be independent of pressure, and if system conditions are remote from the critical, then $\overline{V}_i$ is set equal to $V_i{}^L$, the molar volume of component.

Combine Eqs. 2.10 and 2.11 and eliminate the subscript L for simplicity, then

$$f_i{}^L = \gamma_i X_i p_i{}^s \phi_i{}^s \text{ Exp } \left[\frac{(\pi - p_i{}^s)V_i}{RT}\right] \qquad (2\text{-}12)$$

Substituting Eqs. 2-9 and 2-11 into Eq. 2-8 one obtains

$$K_i = \frac{y_i}{x_i} = \frac{\gamma_i p_i{}^s \phi_i{}^s \text{ Exp}\left[\frac{(\pi - p_i{}^s)V_i}{RT}\right]}{\phi_{i\pi}} \qquad (2\text{-}13)$$

For a system with an ideal vapor, Eq. 2-13 becomes

$$K_i = \frac{\gamma_i p_i{}^s}{\pi} \qquad (2\text{-}14)$$

The saturation pressure or the vapor pressure data are most conviently related to temperature by an equation having the general form

$$\ln p_i{}^s = c_1 + \frac{c_2}{c_3 + T} + c_4 T + c_5 T^2 + c_6 \ln T \qquad (2\text{-}15)$$

The empirical constants, c_1, c_2, c_3, c_4, c_5, and c_6, as reported by Gmehling et al. (1977) have been used for the systems involved with in this investigation.

Systems chosen for this research contain polar components like ethanol which exhibit strong non-ideality in the vapor phase and this requires special handling in the fugacity coefficient calculations. The Tsonopoulos' (1972) correlation is therefore used for the virial coefficient predictions in this study.

The fugacity coefficient obtained from the virial equation of state turncated after the second virial coefficient is

$$\ln \phi_i = [2 \sum_j^m y_j B_{ij} - B_{mix}]\frac{\pi}{RT} \qquad (2\text{-}16)$$

Where

B_{ij} = the second cross virial coefficient for binary i-j.

B_{mix} = the second virial coefficient of the vapor mixture.

$$B_{mix} = \sum_{i=1}^{m} \sum_{j=1}^{n} y_i y_j B_{ij}$$

For a pure component, the equation (2-16) becomes

$$\phi_i{}^s = \text{Exp}\,\frac{B_{ii} P_i{}^s}{RT} \qquad (2\text{-}17)$$

The fugacity coefficient can be expressed in either a pressure or a volume series, the existence of real root in the following expression is the determining factor for selecting which method to use.

$$\text{Root} = (0.25 + B_{mix}\frac{\pi}{RT})^{1/2}$$

For a negative root the following pressure series must be used:

$$\phi_i = \text{Exp}\{[2 \sum_j^m y_i B_{ij} - B_{mix}]\}\frac{\pi}{RT} \qquad (2\text{-}18)$$

For a positive root the following volume series is used:

$$\phi_i = \text{Exp}\left[\frac{2}{V_{mix}} \left(\sum_{j=1}^{m} y_i B_{ij} \right)\right] - Z_{mix} \tag{2-19}$$

Where

$$V_{mix} = B_{mix} + \frac{RT}{\pi}$$

$$Z_{mix} = \frac{V_{mix}}{RT}$$

The calculation of the fugacity coefficient of a component in the vapor phase precipitates the problem of obtaining the second virial coefficients. Tsonopoulos (1972) extended the well known Pitzer-Curl correlation for polar compounds' second virial coefficients predictions. This method is discussed in Appendix B together with other thermodynamic property calculation methods used.

The liquid phase activity coefficient for components with strong non-ideal behavior must be handled carefully. Also, due to the two-liquid formation in the hetergeneous azeotropic distillate reflux accumulator. The NRTL by Renon et al. (1968) and UNIQUAC by Abrams et al. (1975) were used in this research. For a solution of m components, the activity coefficient for a given component can be calculated using:

NRTL Equation

$$\ln \gamma_i = \frac{\sum_{j=1}^{m} \tau_{ji} G_{ji} X_j}{\sum_{l=1}^{m} G_{l,i} X_l} + \sum_{j=1}^{m} \frac{X_j G_{ij}}{\underset{j=1}{\overset{m}{}} B_{ij} X_l} \left(\tau_{ij} - \frac{\sum_{n=1}^{m} X_n \tau_{nj} G_{nj}}{\sum_{l=1}^{m} G_{lj} X_l} \right) \tag{2-20}$$

UNIQUAC Equation

$$\ln \gamma_i = \ln \gamma_i^C + \ln \gamma_i^R \tag{2-21}$$

$$\ln \gamma_i^C = \ln \frac{\phi_i}{x_i} + \frac{z}{2} q_i \ln \frac{\theta_i}{\phi_i} + l_i - \frac{\phi_i}{x_i} \sum_{j=1}^{m} x_j l_j \tag{2-22}$$

$$\ln \gamma_i^R = q_i [1 - \ln(\sum_{j=1}^{m} \theta_j \tau_{ji}) - \sum_{j=1}^{m} \frac{\theta_j \tau_{ij}}{\sum_{k=1}^{m} \theta_k \tau_{kj}}] \tag{2-23}$$

The details of the above equations are described in Appendix B.

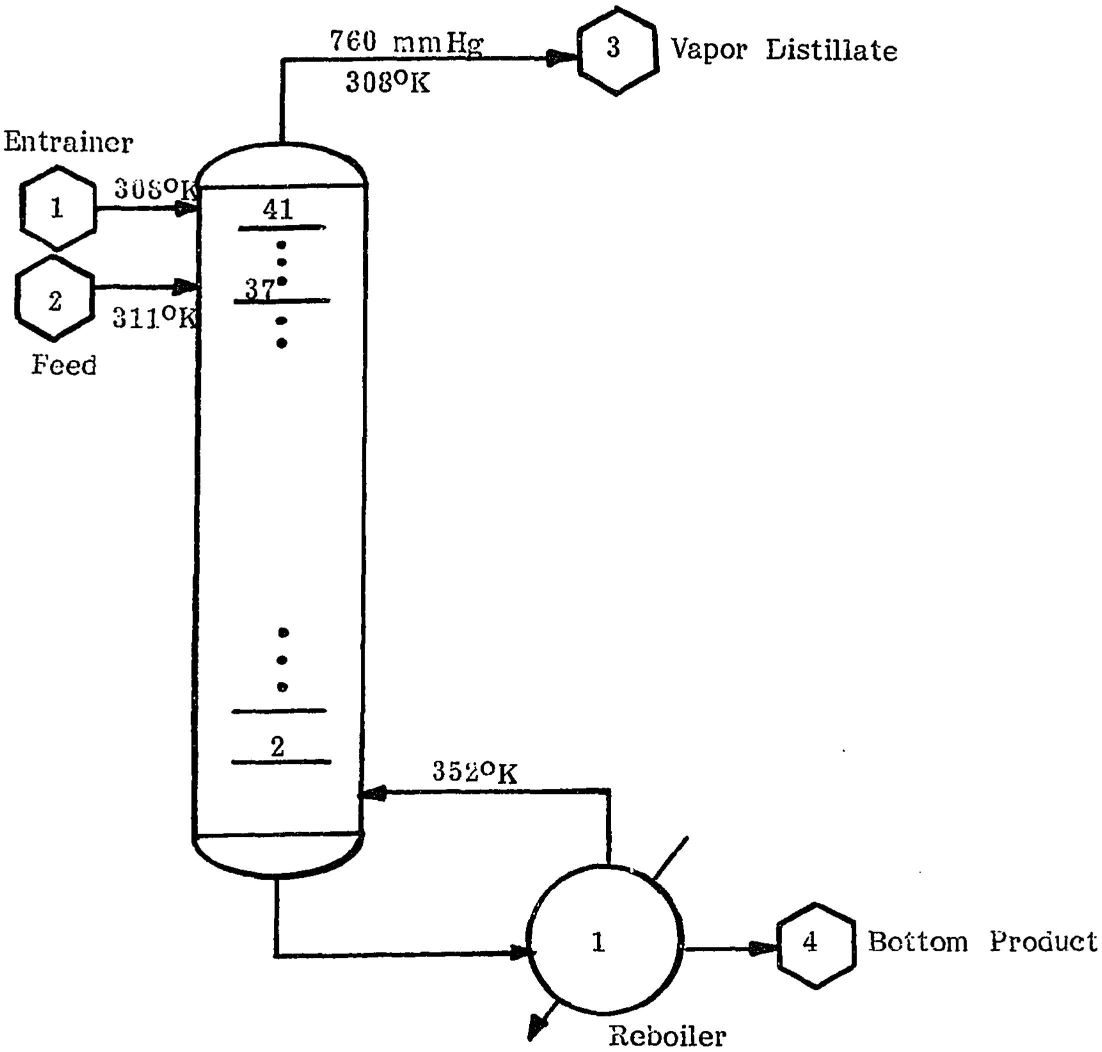
2.4 Research Problem Definition

It has been known that during the concentrating process of ethanol, an entrainer is required to break the ethanol-water azeotrope to achieve high purity ethanol for both industrial and Gasohol uses. Black (1980) evaluated different entrainers for the ethanol dehydration process, however, the details used in his work are unavailable to the general public. Recently, the Chem Share Corporation used its Design 2000 flowsheet simulation for commercial representation of the Gasohol dehydration process. Chem Share (1980) used a system with benzene as the entrainer in their publication entitled "GASOHOL."

In this research, a system similar to Chem Share's is illustrated in Figure 2.3. This problem, as described, has been studied using the extended Naphthali-Sandholm algorithm. In this segment of the research, the two-liquid phase handling in the distillate accumulator has been ignored intentionally. The

Figure 2.3 The Research Problem Configuration (Reboiled Absorber Type)

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



Component	1	2	3	4
Ethanol	28.6 mol %	74.2 mol %	32.7 mol %	99.8 mol %
Water	3.8	25.8	12.3	0.15
Benzene	67.6	0.0	55.0	$3\text{x}10^{-5}$
Total moles/hr	591.85 mole/hr	727.0 mole/hr	727.0 mole/hr	123.35 mole/hr

entrainer rate and location have been adjusted manually to enable the studies of its effects on the azeotropic distillation.

2.3.1 The Dehydration of Ethanol Using Benzene as the Entrainer

The Chem Share azeotropic distillation column consists of 41 stages which can be configured as the conventional distillation column with very small reflux ratio or as a reboiled absorber. The feed stream contains 74.2 mol percent of ethanol and 25.8 mol percent of water as obtained from an ethanol concentrator of crude biomass ethanol. It is desired to produce a bottom stream which is 99.8 mol percent ethanol. The entrainer stream enters the top of the column containing 67.6 mol percent benzene, 28.6 mol percent water and 3.8 mol percent ethanol. In Chapter 3, the overhead vapor stream from the azeotropic column will be used as the feed to a two-liquid phase flash model to generate the entrainer stream (organic rich) as used above. In Chapter 4, the complete azeotropic model is used to study the entrainer rate and composition, coupled with a make up stream to compensate for benzene losses in the water rich overhead product and the small amount of benzene removed with the ethanol product.

The thermodynamic data of the components of the research problem are indicated in Table 2.1 and Table 2.2.

2.5 Results of Simulation--The Research Problem

The research problem, an ethanol dehydration column with

TABLE 2.1

Research Problem

Component Physical Properties and Thermodynamic Data

Part I

1. Vapor pressure equation constants:

temperature in °K
pressure in mmHg
from Gmehling et al. (1977)

	c_1	c_2	c_3
ETOH	18.912	-3803.98	-41.68
Water	18.304	-3816.44	-46.13
Benzene	15.901	-2788.51	-52.36

2. Tsonopoulos' K_{ij}, and A_i, B_i for Polar Component from Tsonopoulos (1972)

$K_{ii} = 0$

	A_i	B_i	K_{ij}	K_{ji}
ETOH	0.0878	0.0572	0.20	0.15
Water	0.0279	0.0229	0.20	0.40
Benzene	0.0	0.0	0.15	0.40

3. NRTL binary parameters:

from Gmehling (1977)

ETOH(1) - Water(2) - Benzene(3)

ij	A_{ij}	A_{ji}	α_{ij}
12	-86.76	1289.91	0.270
13	282.33	1096.90	0.295
23	3820.95	2213.35	0.267

Note: A_{ij} and A_{ji} in cal/gmole; $\alpha_{ij} = \alpha_{ji}$

TABLE 2.2

Research Problem

Component Physical Properties and Thermodynamic Data

Part II

UNIQUAC Equation parameters:

Binary Parameters: cal/gmole

ij	A_{ij}	A_{ji}
12	110.01	200.05
13	-156.57	850.61
23	428.45	1072.79

Pure Component Parameters:

	r_i	q_i
ETOH	2.1055	1.9720
Water	0.9200	1.4000
Benzene	3.1878	2.4000

benzene as the entrainer has been simulated using the azeotropic distillation model completed in this segment of this research. Three different cases are investigated. The first two cases employing the NRTL equation for component activity coefficient calculations using two different operational modes, a reboiled absorber mode, and a conventional distillation with small reflux ratio. The third case used the UNIQUAC equation for activity coefficient calculation in a conventional distillation column with small reflux ratio is also investigated. The input and output data for the above three cases is attached in Appendix C.

2.5.1 Comparison of the Research Problem and Chem Share's Example

This research problem uses the reboiled absorber solution and is compared with the Chem Share Gasohol example. The configuration of both columns is similar, a 41-stage column with vapor distillate as the overhead product and operated under atmospheric pressure. The feeds (normal feed and entrainer feed) are identical in rate, composition, location, and thermal condition. In the vapor-liquid equilibrium prediction method, the research problem uses the virial equation for fugacity coefficient calculation, while Chem Share assumed ideal vapor and failed to correct the non-ideal behavior of the polar components, water and ethanol in the vapor phase. The NRTL equation is used in both. The following important simulation results are compared and tabulated:

1) Mainstream Composition--Table 2.3

2) Column Temperature Profile--Table 2.4
3) Selected Stage Component Equilibrium Constant--Table 2.5
4) VLE Prediction Methods--Table 2.6.

Also, the column composition profiles of the research problem is shown in Figure 2.4.

2.5.2 Simulation Using UNIQUAC Equation

The UNIQUAC equation is used as an alternative to calculate the liquid phase activity coefficients in addition to the previously mentioned NRTL equation. To achieve the same degree of separation as in the NRTL case, the pressure drop per stage in the simulation was assumed to be 45 mmHg which is excessive for a column operation. As a result, the bottom temperature is 33^{o}K higher than that obtained by using the NRTL equation. Also, from the standpoint of convergence, the NRTL case required only nine iterations, while in the UNIQUAC twelve iterations were necessary.

The computer input and output of the UNIQUAC case run with stage ΔP = 45 mmHg is attached in Appendix C. Another investigation with stage ΔP set equal to zero was conducted, the converged results are tabulated in Table 2.7. From this table of main stream composition, it is obvious that the bottom and distillate product qualities were all off spec. Also, 40 iterations were required to converge the simulation.

One explanation for this is that with two interaction

TABLE 2.3

Main Stream Composition Comparison

Stream: (1) Entrainer
(2) Feed
(3) Vapor Distillate
(4) Bottom Product

Composition: in mole percent

	Research Problem				Chem Share's			
Component/Stream	(1)	(2)	(3)	(4)	(1)	(2)	(3)	(4)
Ethanol	28.588	74.236	32.724	99.869	28.588	74.236	32.736	99.76
Water	3.827	25.764	12.276	3×10^{-4}	3.827	25.764	12.278	5.1×10^{-4}
Benzene	67.584	0.0	54.998	0.13	67.585	0.0	54.986	0.27

By comparing the compositions of the bottom product and the overhead distillate, Table 2.3 indicates that it is an average deviation of 0.15%.

TABLE 2.4

Column Temperature Profile (^{O}K)

Stage No.	Research Problem	Chem Share
41 (Distillate)	338.0	338.8
37	339.4	338.8
33	340.8	340.1
29	342.2	340.7
25	343.6	340.5
21	345.0	340.5
17	346.4	340.5
13	347.8	340.6
11	348.5	340.7
9	349.2	341.3
5	350.6	343.3
3	351.3	349.7
1 (Reboiler)	352.0	351.3

Note: Chem Share's problem with stages numbered from top down.

TABLE 2.5

Selected Component Equilibrium Constants

		Research Problem	Chem Share	Dev.
(1)	Stage No. 1 (Bottom)			
	Ethanol	0.99649	0.99325	0.3%
	Benzene	3.6817	3.7697	2.3
	Water	1.1510	1.1802	2.4
(2)	Stage No. 2			
	Ethanol	0.987	0.9778	0.9
	Benzene	3.679	3.681	0.05
	Water	1.145	1.169	2.0
(3)	Stage No. 39			
	Ethanol	1.119	1.115	0.3
	Benzene	0.8311	0.8327	0.2
(4)	Stage No. 41 (Vapor Distillate)			
	Ethanol	1.1249	1.1175	0.6
	Benzene	0.82846	0.8309	0.3
	Water	2.7155	2.7098	0.2

TABLE 2.6

VLE Prediction Method

	Research Problem	Chem Share
Vapor phase - ϕ_i	Virial Eq.-- Tsonopoulos Correlation	Ideal--Antoine Eq.
Liquid phase - γ_i	NRTL & UNIQUAC	NRTL Eq.

Note: (1) In most azeotropic distillation publications, the ideal vapor phase is assumed. In this research the Tsonopoulos method is applied to the virial equation to calculate the vapor fugacity coefficient of component. This is believed to be a better approach due to the polar compound's existence in the system.

(2) In the liquid phase activity coefficient calculation, the newer UNIQUAC prediction was also used on a separate run. The results indicated that the NRTL equation is superior to the UNIQUAC equation in both the predictions and convergence.

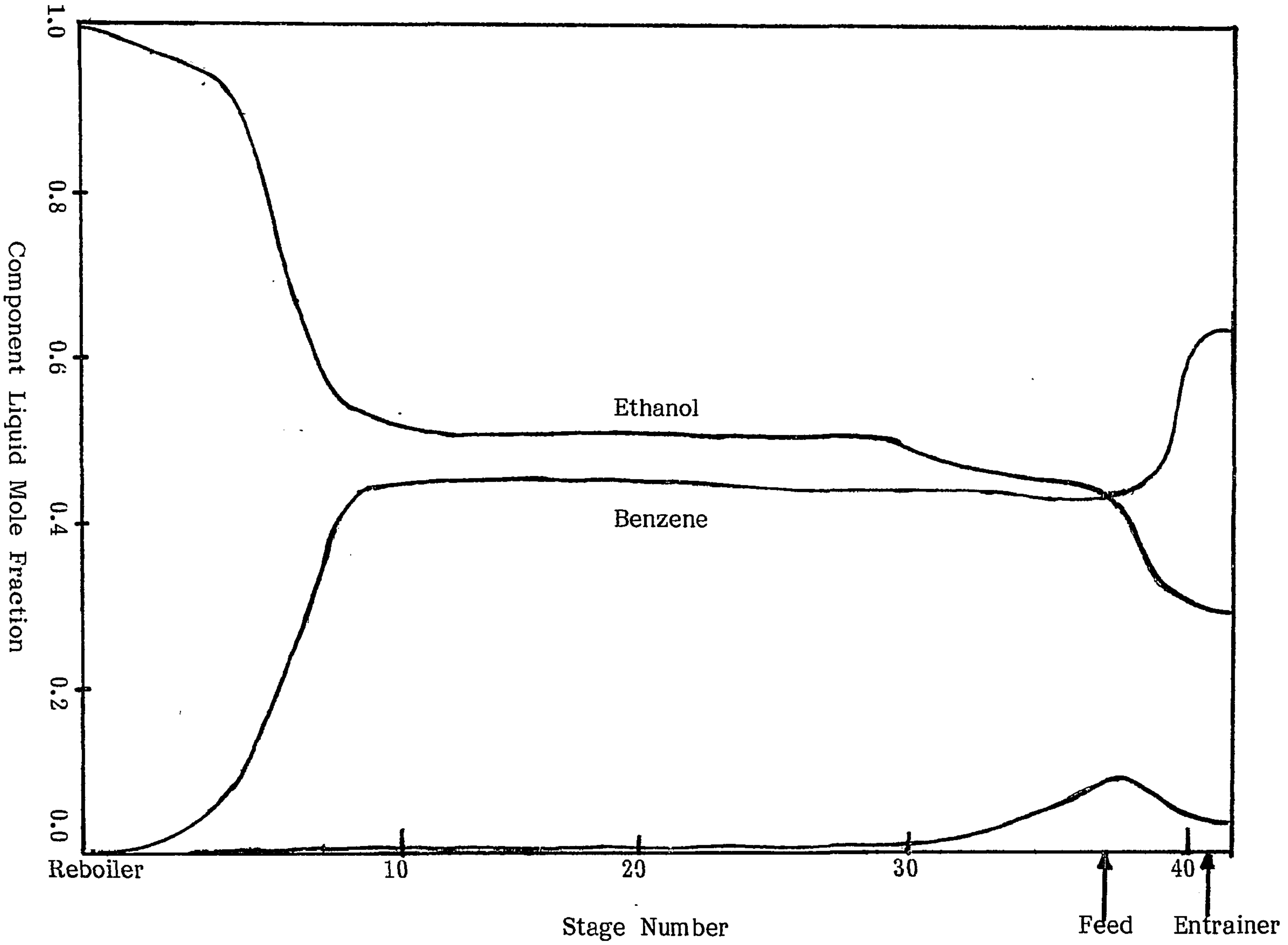


Figure 2.4 Column Composition Profiles--The Research Problem

TABLE 2.7

Main Stream Composition Using UNIQUAC

Stream (1) Entrainer (2) Feed (3) Vapor Distillate (4) Bottom Product

	Research Problem using NRTL				Research Problem using UNIQUAC			
Component/Stream	(1)	(2)	(3)	(4)	(1)	(2)	(3)	(4)
Ethanol	28.588	74.236	32.724	99.869	28.588	74.236	38.18	78.23
Water	3.827	25.764	12.276	3×10^{-4}	3.827	25.764	4.26	21.77
Benzene	67.585	0.0	54.998	0.13	67.585	0.0	57.55	0.0

Note: Composition in mol percent

parameters per binary for the UNIQUAC Equation versus three parameters per binary as required by the NRTL Equation. The NRTL equation will predict the VLE better.

2.6 Results of Studies on Entrainer Effect

With the azeotropic distillation model for this research segment validated, the entrainer entry and rate effects on the separation of the research problem were evaluated. The results confirm the previous study by Rubin et al. (1945).

2.6.1 The Entrainer Entry Effect

The entry of an entrainer to the column, especially its location in relation to the feed is of importance in this study. The results indicated that the entrainer must be introduced above the feed, and at least two, preferably three, stages above the feed. Table 2.8 indicates that in this research, since the entrainer, benzene is more volatile than one of the key components--water; it should be introduced above the feed. During the evaluation of the entrainer entry effect, the feed location was fixed at the 37th stage of the column. This study confirms the report by Rubin et al. (1945) that a volatile entrainer should be introduced above the feed. Mixing the entrainer with feed or introducing it at a point below the feed will result in either poorer separations or failure in program convergence.

Also, studies were made by varying the feed introducing point while the entrainer entry is fixed at the 41st stage.

In all cases, the entrainer stays above the feed. If the

TABLE 2.8

The Entrainer Entry Effect--Entrainer Location Varied

Feed enters at 37th stage in all cases

Entrainer Entry Stage No.	Ethanol Mol % in Bottoms	Benzene Mol % in Bottoms	H_2O Mol % in Bottoms
41 (base case)	99.86	0.139	0.00003
40 (3 above feed)	99.85	0.148	0.0003
39 (2 above feed)	99.76	0.237	0.00003
38 (1 above feed)	98.93	1.0687	0.00001
37 (mixed with feed)	90.52	9.4837	0
36 (below feed)	48.03	51.96	0
35 (below feed)	35.0	65.0	0
32 (below feed)	15.6	84.0	0

number of stages between the feed and entrainer is reduced to less than two, the benzene concentration level in the bottom product will begin to increase to an unacceptable level as indicated in Table 2.9.

The entrainer entry effect was further evaluated by varying both entrainer and feed locations with the entrainer always above the feed. This study confirms the previous findings in that the entrainer must stay at least two stages above the feed irregardless of the feed point. The results are indicated in Table 2.10.

2.6.2 The Entrainer Rate Effect

The next focal point is the entrainer rate effect on the separation. The benzene rate in the entrainer stream of the research problem was varied, however, the entrainer and feed locations remain unchanged.

The research problem with 400 moles/time benzene rate seems to yield the best separation. Increasing the benzene rate does not improve the separation further. Decreasing the benzene rate more than 10 moles/time resulted in very poor separations as evidenced in Table 2.11.

2.7 Conclusions

The azeotropic distillation model for this research was completed and validated in various forms. A research problem was defined and simulated using the stagewise model in a reboiled absorber mode. The results compared favorably with the Gasohol

TABLE 2.9

The Entrainer Entry Effect--Feed Location Varied

Entrainer enters at 41th stage in all cases

Feed Introduced Stage No.	Ethanol Mol % in Bottoms	Benzene Mol % in Bottoms	H_2O Mol % in Bottoms
40	98.9314	1.685	0.00003
39	99.129	0.8701	0.00002
38	99.859	0.140	0.0002
37 (base case)	99.86	0.139	0.00003
36	99.861	0.1392	0.0004
35	99.862	0.1379	0.00005
30	99.862	0.1375	0.00006
24	99.855	0.1359	0.00007
20	99.85	0.1487	0.00008

TABLE 2.10

The Entrainer Entry Effect--Feed and Entrainer Locations Varied

Case	Bottom Product Ethanol Mol %	Bottom Product Benzene Mol %	Bottom Product H_2O Mol %
(1) Feed = 37 Entrainer = 41 (Base) Δ Stage = 4	99.86	0.139	0.00003
(2) Feed = 39 Entrainer = 39 Δ Stage = 0	90.52	9.48	0.0000
(3) Feed = 38 Entrainer = 39 Δ Stage = 1	98.93	1.068	0.0001
(4) Feed = 35 Entrainer = 38 Δ Stage = 3	99.85	0.1487	0.00008
(5) Feed = 33 Entrainer = 38 Δ Stage = 5	99.86	0.138	0.00019
(6) Feed = 26 Entrainer = 36 Δ Stage = 10	99.86	0.137	0.00373

TABLE 2.11

The Entrainer Rate Effect

Feed at 37th Stage

Entrainer at 41st Stage

Entrainer Rate	Bottom Product Ethanol Mol %	Bottom Product Benzene Mol %	Bottom Product H_2O Mol %
400 moles/time (base case)	99.86	0.139	0.00003
405	98.34	1.660	0.00001
410	96.83	3.170	0.00001
420	93.87	6.128	0.0000
395	96.75	3.24	0.0001
390	97.64	0.1211	2.2398
385	96.75	3.247	0.0001
380	77.208	0.5223	12.269

design simulation of Chem Share, and, in fact, is a better process representation since the simulation model is capable of correcting non ideal vapor behavior in the vapor-liquid equilibrium.

The in-depth studies of entrainer entry effect on the azeotropic distillation leads to the conclusion that the entrainer must always enter the column above the feed with at least two stages separating the feeds. Better separation is achievable only if three or more stages are provided between the feed and entrainer. If the entrainer enters the column below the feed or mixes with the feed, poor separations will result.

The entrainer rate for this research is probably at its optimum, 400 moles/time, for the research problem. Further increase in the entrainer rate will theoretically drive the water out of the bottom product stream, however, the benzene concentration will begin to buildup in the bottom ethanol product.

Reducing the entrainer rate to the column will result in poor separations as indicated by the water concentration level increase in the bottoms, since less than the required amount of entrainer is presented in the column to break the water-ethanol azeotrope to accomplish the separation.

CHAPTER 3

THE TWO-LIQUID PHASE FLASH MODEL

In this chapter, the second part of the research dealing with the two-liquid phase separation in the overhead distillate accumulator is discussed. The literature concerning "Three-Phase Flash" (or Two-Liquid Phase Separation) have been covered by Deam et al. (1969), Osbrone (1964), Heidemann (1974), Leach (1977), and Roche (1977). A stand alone model has been developed to study the two-liquid phase separation that results when the overhead vapor from the reboiled absorber column is condensed.

3.1 Background and Theory

The two-liquid phase flash model is illustrated in Figure 3.1. Feed enters the accumulator which is at constant temperature and pressure. Depending on the conditions and the compositional structure, a single liquid phase or two liquid phases can exist in the accumulator.

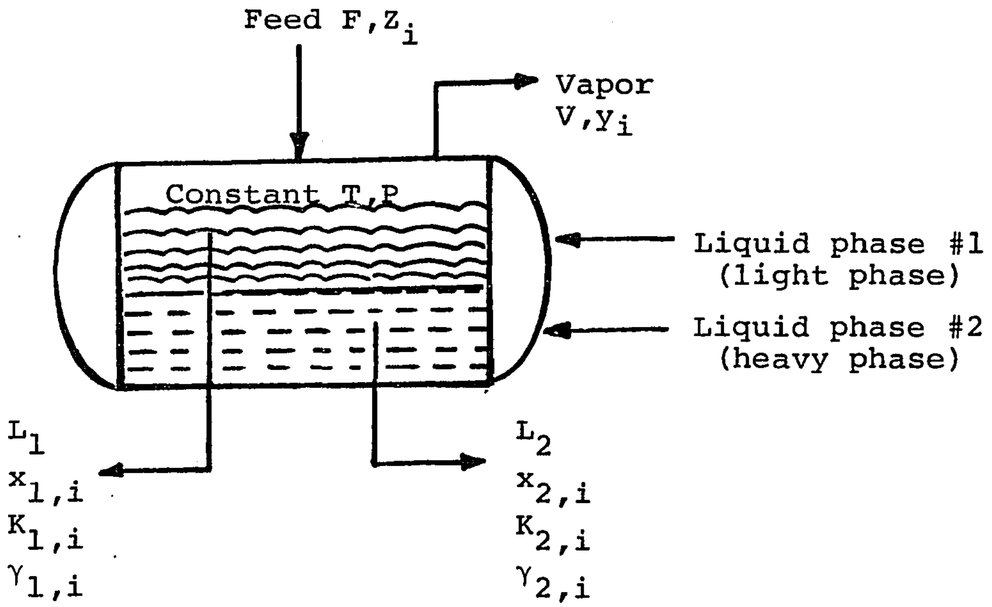
3.1.1 Dew Point Temperature

The temperature at which a gas mixture begins to condense is the dew point, and is established using the following relationship

$$F = \sum_i \frac{y_i}{K_i} - 1.0 = 0.0 \qquad (3.0)$$

where y_i is the given vapor feed composition. The vapor liquid equilibrium constant, K_i, is functionally dependent on the

Figure 3.1 Two-Liquid Phases Flash Model



where,

F - Total Feed moles/time

Z_i - Component mole fraction in feed

L_1 - Liquid phase #1 rate, moles/time

$x_{1,i}$- Component mole fraction in liquid phase #1

$K_{1,i}$- Component vapor and liquid phase #1 equilibrium constant

$\gamma_{1,i}$- Component activity coefficient in liquid phase #1

L_2 - Liquid phase #2 rate, moles/time

$x_{2,i}$- Component mole fraction in liquid phase #2

$K_{2,i}$- Component vapor and liquid phase #2 equilibrium constant

$\gamma_{2,i}$- Component activity coefficient in liquid phase #2

V - Vapor phase rate, moles/time

y_i - Component mole fraction in vapor phase temperature, the equilibrium liquid composition, X_i, and the vapor phase composition. Because of the functional dependence of the VLE constant, the evaluation of the dew point temperature, T_{DP}, is iterative. The solution method requires the use of the Secant Method to solve Eq. (3-0). Wegstein's algorithm is used to enhance the convergence of liquid composition. The details of solution is described in Appendix D.

3.1.2 Bubble Point Temperature--Two Liquid Phases

With the two-liquid phase, the unknowns associated with the bubble point temperature are two fold, namely the temperature, T_{BP}, and the relative amount of material in the two liquid phases. The basic relationships governing two-liquid phase equilibrium are:

Material Balance:

$$F = L_1 + L_2 + V \quad (3\text{-}1a)$$

$$(L_1 + L_2)Z_i = L_1X_{1,i} + L_2X_{2,i} \quad (3\text{-}1b)$$

$$V \equiv 0 \quad (3\text{-}1c)$$

Equilibrium Relationship:

$$\gamma_{1,i}X_{1,i} = \gamma_{2,i}X_{2,i} \quad (3\text{-}2a)$$

$$Y_i = K_{1,i}X_{1,i} = K_{2,i}X_{2,i} \quad (3\text{-}2b)$$

Constraints:

$$\sum_i X_{1,i} = 1.0 \quad (3\text{-}3a)$$

$$\sum_i X_{2,i} = 1.0 \quad (3\text{-}3b)$$

$$\sum_i Y_i = 1.0 \quad (3\text{-}4)$$

When Eq. 3-3a and Eq. 3-3b are combined

$$F_1 = \sum_i (X_{2,i} - X_{1,i}) = 0 \qquad (3\text{-}5)$$

From Eq. 3-1a

$$Z_i = \frac{L_1}{L_1 + L_2} X_{1,i} + \frac{L_2}{L_1 + L_2} X_{2,i} \qquad (3\text{-}6)$$

Let $R = \frac{L_1}{L_1 + L_2}$ be the liquid distribution factor (3-7)

then $$1 - R = \frac{L_2}{L_1 + L_2} \qquad (3\text{-}8)$$

Combining Eq. 3-6, Eq. 3-7, and Eq. 3-8, then

$$Z_i = R\,X_{1,i} + (1 - R)X_{2,i}$$

or

$$Z_i = [R + (1 - R)\frac{X_{2,i}}{X_{1,i}}]X_{1,i} \qquad (3\text{-}9)$$

Substituting Eq. 3-2b into Eq. 3-9

$$Z_i = [R + (1 - R)\frac{\gamma_{1,i}}{\gamma_{2,i}}]X_{1,i} \qquad (3\text{-}10)$$

let $W_i = R + (1 - R)$

the resulting phase compositions are then defined by

$$X_{1,i} = \frac{Z_i}{W_i}$$

$$X_{2,i} = \frac{Z_i}{W_i}\frac{\gamma_{1,i}}{\gamma_{2,i}}$$

$$y_i = \frac{Z_i}{W_i} K_{1,i}$$

Substituting $X_{1,i}$ and $X_{2,i}$ into Eq. 3-5, then

$$F_1 = \sum_i (X_{1,i} - X_{2,i}) = \sum_i \frac{Z_i(1 - \frac{\gamma_{1,i}}{\gamma_{2,i}})}{W_i} = 0 \qquad (3\text{-}11)$$

Eq. 3-11 and the bubble point temperature condition,

$$F_2 = \sum_i (X_{1,i} - y_i) = \sum_i \frac{Z_i(1 - K_{1,i})}{W_i} = 0 \qquad (3\text{-}12)$$

In Eq. 3-11, the liquid phase distribution factor R, is one of the unknown and has the following range of value:

$$0.0 < R < 1.0 \qquad (3\text{-}13)$$

The solution of Eqs. 3-11 and 3-12 is described in Appendix D. The solution method requires the use of the Secant and Newton methods to solve the functions F_1 and F_2. Wegstein's algorithm is used to converge the phase compositions.

3.1.3 Bubble Point Temperature--Single Liquid Phase

The temperature at which a liquid mixture begins to boil at a fixed pressure is the bubble point, and is obtained from

$$F = \sum_i K_i X_i - 1.0 = 0.0 \qquad (3\text{-}14)$$

Where X_i is the given feed composition and K_i is the vapor-liquid equilibrium constant for component i. A dual convergence methodology involving the Secant Method and Wegstein's Algorithm is utilized in the computation. The detailed procedure of the solution method is discussed in Appendix D.

To properly use this model during the bubble point temperature calculation, a two-liquid phase condition is always assumed at the beginning. If the value of R approaches either one or zero, then the calculation will use the single liquid phase design equation, Eq. 3-14.

3.1.4 Subcooled Liquid--Two Liquid Phases

If the system temperature is lower than the two liquid phase bubble point temperature, the liquid phase distribution factor must still be determined. The material balance equation, Eq. 3-11, is used, with the liquid phase distribution factor R as the only independent variable. The computational procedure is the same as in the bubble point temperature calculation, except that it is an isothermal evaluation. During the R calculation, if its value approaches zero or one, a single liquid phase will result.

3.1.5 Isothermal Flash

A feed composition, specified by mole fraction Z_i, having a temperature T satisfying the inequality

$$T_{BP} < T < T_{DP} \qquad (3\text{-}15)$$

will separate into a vapor and at least one liquid phase. The relative amounts of material in the different phases can be calculated as follows:

Single liquid phase--For a single liquid phase flash the criteria of an overall material balance between the equilibrium vapor and liquid yields the following equation,

$$F_1 = \sum_i (X_i - y_i) = \sum_i \frac{Z_i(1.0 - K_i)}{W_i} \qquad (3\text{-}16)$$

where

$$W_i = 1.0 + (K_i - 1.0)U \qquad (3\text{-}17)$$

and U = V/F, the molar fraction of the total feed which resides in the vapor phase.

$$X_i = \frac{Z_i}{W_i} \tag{3-18}$$

$$Y_i = K_i \frac{Z_i}{W_i} \tag{3-19}$$

The solution of Eq. 3-16 is described in Appendix D, and involves Newton's method to obtain the distribution factor and the Wegstein algorithm to assist in the phase composition convergence.

Two-Liquid Phases--For a two-liquid phase flash, the criteria of an overall material balance between an equilibrium vapor and two-liquid phase results in two equations,

$$F_1 = \sum_i (X_{1,i} - y_i) = \sum_i \frac{Z_i \ (1.0 - K_{1,i})}{W_i} = 0.0 \tag{3-20}$$

$$F_2 = \sum_i (X_{1,i} - X_{2,i}) = \sum_i \frac{Z_i (1.0 - \frac{K_{1,i}}{K_{2,i}})}{W_i} = 0.0 \tag{3-21}$$

Where

$$W_i = R(1 - U)+(1 - R)(1 - U)\frac{K_{1,i}}{K_{2,i}} + UK_{1,i} \tag{3-22}$$

and

$$X_{1,i} = \frac{Z_i}{W_i} \tag{3-23a}$$

$$X_{2,i} = \frac{Z_i}{W_i} \bullet \frac{K_{1,i}}{K_{2,i}} \tag{3-23b}$$

$$y_i = \frac{Z_i}{W_i} \bullet K_{1,i} \tag{3-23c}$$

The definitions of R and U remain as before. The solution of Eq. 3-20 and Eq. 3-21 is described in Appendix D. In the calculation of the liquid phase distribution factor R, if its value approaches either zero or one, then a single liquid phase is assumed. Also, to calculate the molar vapor fraction of the feed, U, only Eq. 3-20 is required in the calculation. The composition convergence again is enhanced using the Wegstein algorithm.

3.1.6 Adiabatic Flash

When the total enthalpy of the system is specified, the equations associated with the isothermal flash are solved with the enthalpy balance. The general enthalpy balance based on one mole of feed is

$$H_F = UH_V + (1 - U)R\ H_{L1} + (1 - U)\ H_{L2} \qquad (3\text{-}24)$$

where

$$H_V = \sum_i h_{V_i}\ y_i + h_d \qquad (3\text{-}25a)$$

$$H_{L1} = \sum_i h_{L,i}x_{1,i} + h_1^{mix} \qquad (3\text{-}25b)$$

$$H_{L2} = \sum_i h_{L,i}x_{2,i} + h_2^{mix} \qquad (3\text{-}25c)$$

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

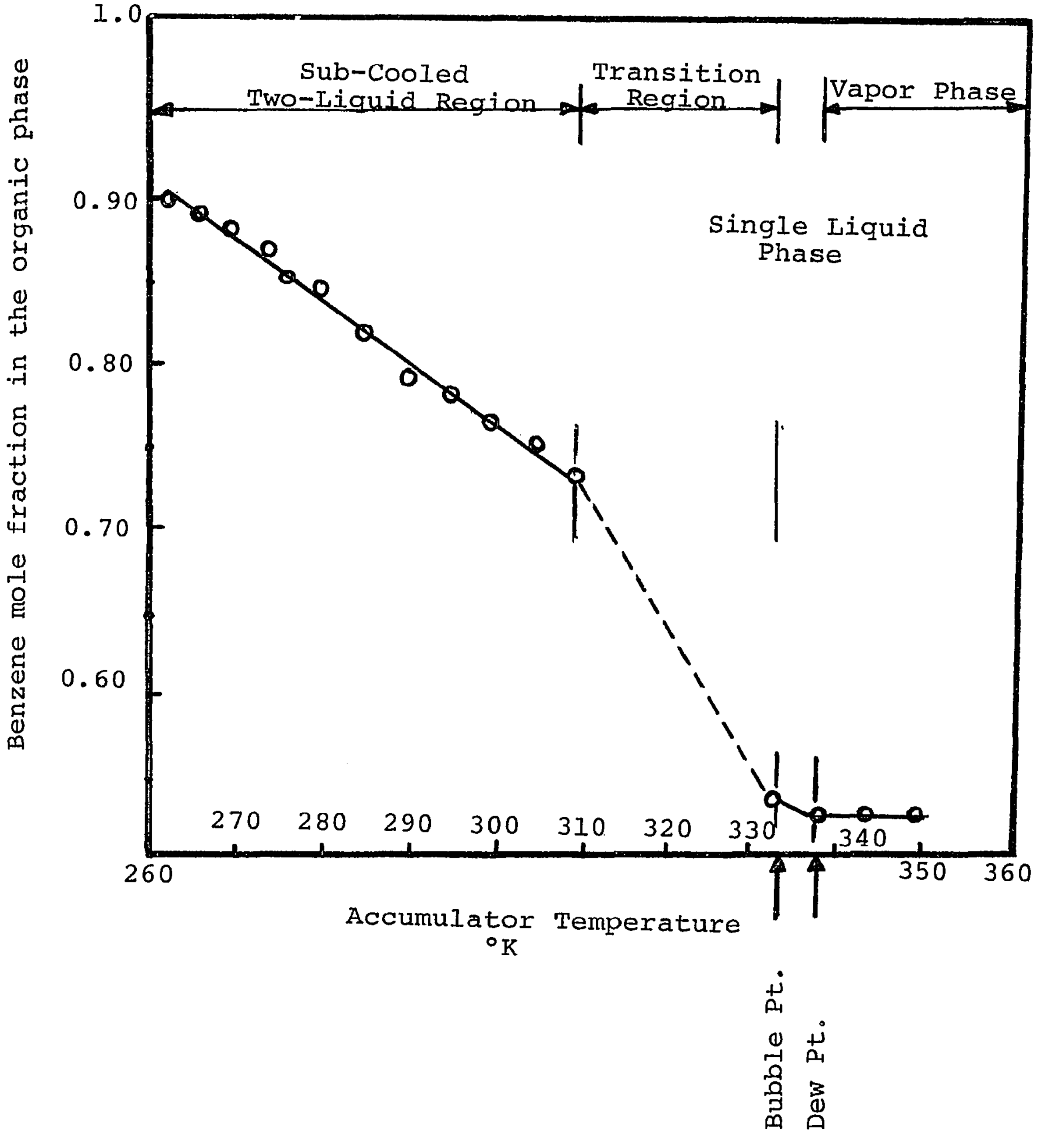
The adiabatic flash solution is achieved by decoupling the enthalpy equation from the equations which define the isothermal flash rather than solving the total set of equations simultaneously. Using temperature as the prime variable, a series of isothermal flash calculations are performed until the enthalpy balance (Eq. 3-24) is satisfied. The Secant Method is used to promote convergence of the overall enthalpy balance. The ideal vapor enthalpy departure is evaluated via the appropriate equation of state (in this study the virial equation of state is used). The heat of mixing is evaluated from the appropriate activity coefficient relationship, i.e. the NRTL or the UNIQUAC equation. The method of solution is described in Appendix D.

3.2 Results and Conclusions

A specific stream, the overhead distillate as generated by the distillation column for the research problem, is used to demonstrate the capabilities of the two-liquid phase flash model. Also, two examples from Roche (1977) were simulated using this model. The results of the above sample runs indicated that this model is a reliable tool for two-liquid phase flash simulation, the computer inputs and outputs are included in Appendix E.

In the context of this dissertation, the focal point is the two-liquid phase separation at the bubble point and at various levels of subcooled liquid. The liquid phase activity coefficients were calculated by the NRTL equation in the above study. The results indicate that at a lower drum (or accumulator) temperature, the benzene (entrainer) concentration level in the light phase is increased. This is a favorable separation in terms of reducing the benzene loss left in the heavy phase to be recovered by further processing. The benzene concentration level in the light phase is plotted vs. the drum temperature over a range of $100^{o}K$, and illustrated in Figure 3.2.

Figure 3.2 Benzene Concentration vs. Accumulator Temperature



The two-liquid phase is stable at a temperature below 315^{o}K, however, a single liquid phase will form between 315^{o}K and 338^{o}K (the dew point temperature). At a drum temperature above the dew point, only the vapor phase exists.

The results of simulating the overhead distillate stream using this two-liquid phase model also compared with the entrainer stream as reported by Chem Share. In the above two cases, the feed conditions and activity coefficient calculation method are identical, however, the resulting liquid phase splitting is different. From the available information, Chem Share seems to use the dew point liquid composition as the entrainer composition in their Gasohol simulation instead of the light phase composition at the reported drum temperature (308^{o}K). The results of the research problem versus Chem Share's is compared and tabulated in Table 3.1.

In conclusion, a reliable two-liquid phase flash model based on Deam (1969) and Roche (1977) has been developed and validated. The desirable subcooling in the overhead distillate drum has been investigated, a drum temperature lower than the bubble point is desirable since it reduces the benzene loss. In the next chapter, this model will be combined with the reboiled absorber/stripping model via a new executive.

TABLE 3.1

Results of Two-Liquid Phase Flash

Research Problem vs. Chem Share's

I. Feed Consitions: Pressure = 760 mmHg
Temperature = 95°F (308°K)

II. Bubble Point Calculated = 337.8°K (148°F)
(for two-liquid phases)

III. Dew Point Calculated = 338.9°K (150°F)

IV. Liquid Phase Distribution factor, R = 0.4265

V. Composition: unit in mol fraction

	Feed Stream	Research Problem Light Phase	Research Problem Dew Point Liquid	Chem Share's Entrainer
Benzene	0.5498	0.7729	0.6710	0.6759
Ethanol	0.3275	0.1855	0.2848	0.2859
Water	0.1267	0.0416	0.0432	0.0382

CHAPTER 4

THE COMPLETE AZEOTROPIC DISTILLATION MODEL

The standalone azeotropic distillation model as described in Chapter 2, and the two-liquid phase flash model which has been discussed in Chapter 3 were combined in this part of the research using an executive program. Also, two distillation columns, one simulating the benzene stripping, the other simulating the ethanol concentrating process (also the water purge) were investigated in this chapter. The complete azeotropic distillation model as illustrated in Figure 4.1 includes the azeotropic distillation column, the two-liquid phase flash decanter, the benzene stripping column, and the ethanol concentration column. This complete mode represents a typical ethanol recovery plant, using benzene as the entrainer.

4.1 Background and Theory

The executive program developed in this chapter performs the following functions:

1. Call the azeotropic distillation program to generate the overhead vapor stream and pass to the two-liquid phase flash model as the feed.
2. Call the two-liquid phase program to generate the two liquid streams.
3. Perform necessary component material balances to calculate the benzene entrainer stream.

4. Test for overall convergence.

4.2 Results

The Combination of the azeotropic distillation model and two-liquid phase flash model was successfully implemented. Sample input and output data are attached in Appendix F for the significant unit operations in the ethanol dehydration process. The scope of this chapter was modified to simulate a typical industrial ethanol purification plant which includes the above mentioned azeotropic column and two-liquid phase separation.

The typical ethanol purification plant as described by Keister (1982), Black (1980), and Van Winkle (1967) is illustrated in Figure 4.1. The simulation of the azeotropic distillation column and accumulator has been accomplished in this chapter via the executive program. The benzene stripping column which serves the purpose of recovering benzene in the feed (heavy phase stream from the accumulator) was simulated as a reboiled absorbed column. The main streams of interest associated with this column are indicated in Figure 4.1. The case input/output data are attached in Appendix F.

The bottom stream from the benzene stripping column is then fed into a conventional distillation column, the ethanol recovery column, to recover the ethanol with small amounts of entrainer from the water (bottoms). The main streams of this column are shown in Figure 4.1, and the sample input/output data are attached in Appendix F.

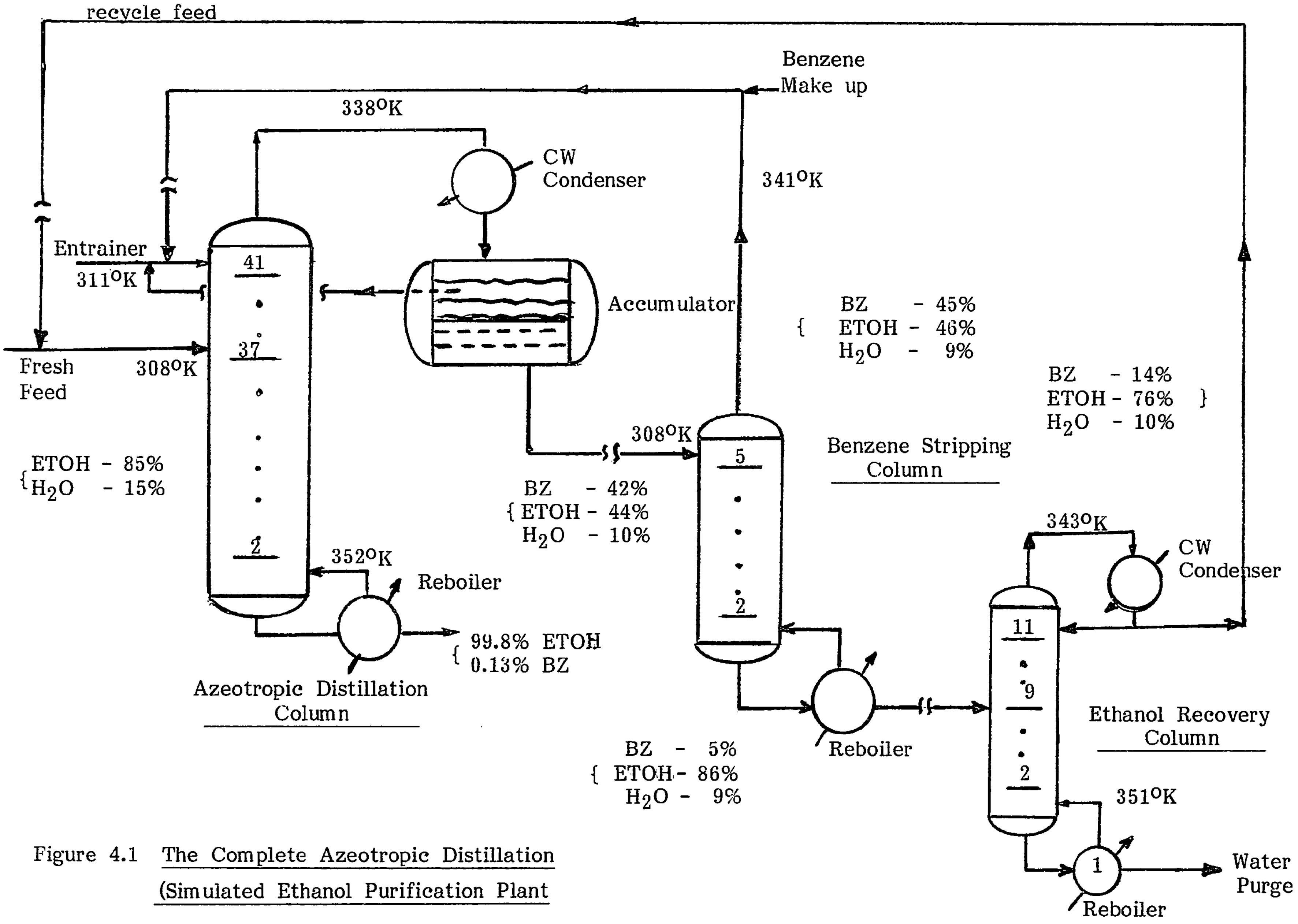


Figure 4.1 The Complete Azeotropic Distillation (Simulated Ethanol Purification Plant

CHAPTER 5

CONCLUSIONS AND RECOMMENDATIONS

5.1 Conclusions

A rigorous multi-stage distillation model based on Naphthali (1972) has been enhanced to handle non ideal systems. Results of an industrial ethanol dehydration column simulated on this model indicate that it yields a better simulation when compared with Chem Share's gasohol simulation results. The in depth studies of the entrainer entry location and rate effects on the azeotropic distillation have determined that the entrainer should enter the column above the feed with at least two theoretical stages separating the feed. Introducing the entrainer below the feed or mixing with the feed will result in poor separation. The optimum entrainer rate was determined via a parametric study.

In the second part of this dissertation, a two-liquid phase flash model based on Roche (1977) and Deam (1967) was used to deal with the two-liquid phase in the distillate accumulator. The temperature effect on the liquid phase splitting was investigated. It is concluded that lower accumulator temperatures are preferred, since it reduces the benzene in the heavy phase (significant water present).

A typical industrial ethanol purification plant was simulated in the last part of the research using the models developed. The azeotropic distillation and two-liquid phase separation were investigated using the combined mode. The benzene stripping column and the ethanol recovery/water purge column were simulated using the stand alone model developed in the first part of this research.

5.2 Recommendations for Future Research

The following areas are recommended for further investigations in the azeotropic distillation research.

5.2.1 Vapor-Liquid Equilibrium (VLE) and Liquid-Liquid Equilibrium (LLE)

At near completion of this research, Keister (1982) presented a similar study on ethanol dehydration simulation to the 1982 AIChE Winter Meeting. According to W. Keister, the Local Effective Molar Fraction (LEMF) method is superior to UNIQUAC and NRTL methods in predicting liquid liquid equilibrium (LLE) in the distillate drum. Future investigators should verify this, as well as the modified UNIQUAC method by Anderson (1978) and UNIFAC method by Fredenslund et al. (1977) in the VLE/LLE package. The modified UNIQUAC method in theory will predict the LLE of a system containing alcohol better than the original UNIQUAC method. The UNIFAC method does not require experimentally determined binary parameters in predicting the VLE, adding this to the existing VLE package should enhance this model's capability.

5.2.2 Two-Liquid Phase Formation in the Column

It has been assumed that two liquid phases do not occur in the column in this research. However, according to Prokopakis et al. (1980), the tendency to form two liquid phases near the feed stage or on the top section of an ethanol dehydration column can not be overlooked. The future investigator should examine the possibility of two liquid phases formation as well as developing a method to predict or avoid it. Ross-Seider (1979), and Boston-Shah (1979) have investigated this problem, but an in depth study of this subject is recommended.

5.2.3 Different Alcohol Dehydration and Entrainer Systems

Using different types of entrainer in the ethanol dehydration process has been reported by Black (1980). The future studies of comparing different entrainer effects on the ethanol dehydration process should be investigated. Also, other alcohol dehydration processes, like isopropanol dehydration, which uses cyclohexane as the entrainer as reported by Prokopakis et al. (1980) should also be investigated for entrainer effect.

5.2.4 Overall Ethanol Purification Process

In Chapter 4 of this dissertation, an investigation to simulate an industrial ethanol purification plant was made. Future studies should concentrate on the following topics:

1. Connect all the major process units together using a flow sheet simulator program (like ASPEN).
2. Determine entry locations for the overhead of the benzene stripping column and the ethanol recovery column.

3. Determine the need for make-up entrainer.
4. Determine the optimum ethanol concentration level in the feed to the azeotropic distillation column, as well as the separation requirements in the subsequent columns.

A schematic is presented in Figure 5.1 to illustrate this future system.

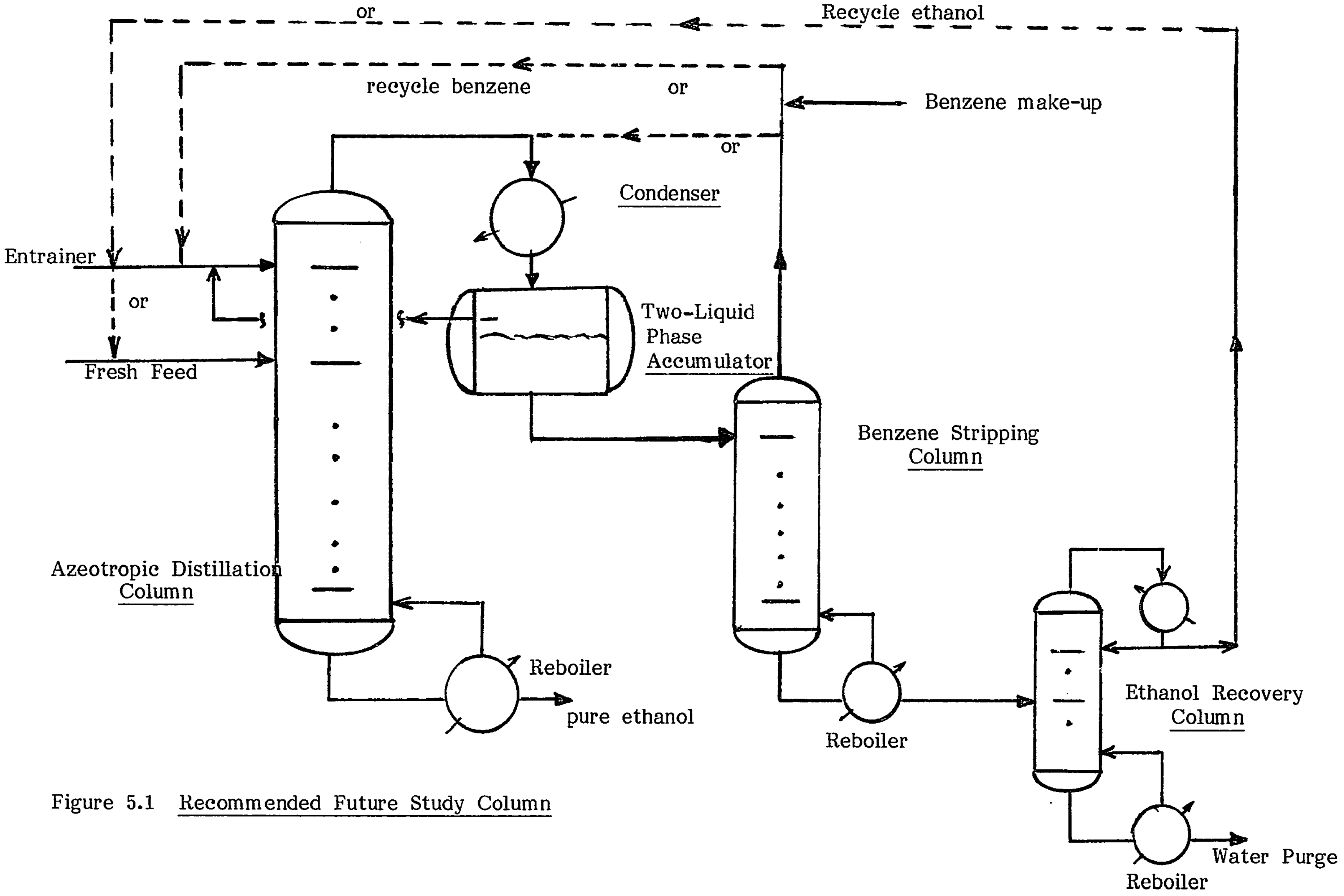


Figure 5.1 Recommended Future Study Column

APPENDIX A

DISTILLATION MODEL SOLUTION ALGORITHM

A.1 Linearization of the Discrepancy Functions

The discrepancy functions (Eq. 2-1 through 2-5) can be linearized using a two term Taylor's expansion about a known set of variables. The variables of interest are the independent variables, l_{ni}, $v_{n,i}$, and T_n. The linearization process generates a new set of 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):

•Original equation

$$F(x_1,x_2,x_3) = 0 \tag{A1-1}$$

•Linearized equation in the restructured mode

$$\frac{\partial F}{\partial X_1}\,\Delta X_1 + \frac{\partial F}{\partial X_2}\,\Delta X_2 + \frac{\partial F}{\partial X_3}\,\Delta X_3 + \ldots . = -F \tag{A1-2}$$

The linearization of each of the discrepancy functions is given in the following summary:

A.1.1 Component Material Balance

$$F_1(n,i) = \left(1 + \frac{S_n{}^L}{L_n}\right) l_{n,i} + \left(1 + \frac{S_n{}^V}{V_n}\right) v_{n,i} - v_{n-1,i} - l_{n-1,i} - f_{n,i} = 0 \tag{2-1}$$

Linearizing the discrepancy equation, Eq. 2-1, one obtains

$$- \Delta v_{n-1,i} + \left(1 + \frac{S_n{}^L}{L_n}\right)\Delta l_{n,i} - \frac{S_n{}^V}{V_n{}^2}\, l_{n,i} \sum_k \Delta\, l_{n,k} + \left(1 + \frac{S_n{}^V}{V_n}\right)\Delta\, v_{n,i} - \frac{S_n{}^V}{V_n{}^2}\, v_{n,i} \sum_k \Delta v_{n,k} - \Delta l_{n+1,i} = -F_1(n,i) \tag{A1-3}$$

A.1.2 Equilibrium Condition

The equilibrium condition is described by the following discrepancy equation:

$$F_2(n,i) = \eta_{n,i} \frac{K_{n,i}V_n}{L_n} l_{n,i} - v_{n,i} + (1 - \eta_{n,i}) \frac{V_n}{V_{n-1}} = 0 \tag{2-2}$$

The above equation can be linearized as follows:

$$\begin{aligned}
&(1 - \eta_n) \frac{V_n}{V_{n-1}} \Delta v_{n-1,i} - (1 - \eta_n) \frac{V_n}{V^2_{n-1}} v_{n-1,i} \sum_k \Delta v_{n-1,k} \\
&+ \eta_n K_{n,i} \frac{V_n}{L_n} \Delta l_{n,i} - \eta_n K_{n,i} \frac{V_n}{L_n{}^2} l_{n,i} \sum_k l_{n,k} \\
&+ \eta_n k_{n,i} \frac{l_{n,i}}{L_n} \sum_k \Delta v_{n,k} + (1 - \eta_n) \frac{v_{n-1,i}}{V_{n-1}} \sum_k \Delta v_{n,k} \\
&+ \eta_n \frac{V_n}{L_n} l_{n,i} \sum_k \frac{\partial K_{n,i}}{\partial l_{n,k}} \Delta l_{n,k} + \eta_n \frac{V_n}{L_n} l_{n,i} \sum_k \frac{\partial K_{n,i}}{\partial v_{n,k}} v_{n,k} \\
&+ \eta_n \frac{V_n}{L_n} l_{n,i} \frac{\partial K_{n,i}}{\partial T_n} \Delta T_n - \Delta v_{n,i} = -F_2(n,i)
\end{aligned} \tag{A1-4}$$

A.1.3 Energy Balance

The discrepancy equation of energy balance is described by the following equation:

$$\begin{aligned}
F_3(n) = (1 + \frac{S_n{}^L}{L_n}) h_n + (1 + \frac{S_n{}^V}{V_n}) H_n - H_{n-1} - h_{n+1} - h_n{}^F - Q_n + \\
h_n{}^{mix} - h^{mix}_{n+1} = 0
\end{aligned} \tag{2-5}$$

Again, the Eq. 2-5 can be linearized as follows:

$$- \sum_k \frac{H_{n-1}}{v_{n-1,k}} \Delta v_{n-1,k} - \frac{\partial H_{n-1}}{\partial T_{n-1}} \Delta T_{n-1} + (1 + \frac{S_n^L}{L_n}) \sum_k \frac{\partial h_n}{\partial l_{n,k}} \Delta l_{n,k}$$

$$+ (1 + \frac{S_n^L}{L_n}) \frac{\partial h_n}{\partial T_n} \Delta T_n + (1 + \frac{S_n^V}{V_n}) \sum_k \frac{\partial H_n}{\partial v_{n,k}} \Delta v_{n,k}$$

$$- \frac{S_n^V}{V_n^2} H_n \sum_k \Delta v_{n,k} + (1 + \frac{S_n^V}{V_n}) \frac{\partial H_n}{\partial T_n} \Delta T_n$$

$$- \sum_k \frac{\partial h_{n+1}}{\partial l_{n+1,k}} \Delta l_{n+1,k} - \frac{\partial h_{n+1}}{\partial T_{n+1}} \Delta T_{n+1}$$

$$+ \sum_k \frac{\partial h_n^{mix}}{\partial l_{n,k}} \Delta l_{n,k} + \frac{\partial h_n^{mix}}{\partial T_n} \Delta T_n$$

$$- \sum_k \frac{\partial h_n^{mix}}{\partial l_{n+1,k}} \Delta l_{n+1,k} - \frac{\partial h_{n+1}^{mix}}{\partial T_n} \Delta T_n = -F_3(n) \tag{A1-5}$$

When the collective set of linearized discrepancy functions are ordered stagewise, the result is a tridiagonal super matrix as shown in Figure A1-1. The solution of the 2c + 1 linearized equations yields the desired corrections which are used to revise the column's flow and temperature maps.

A.2 Solution Algorithm

The linearized set of discrepancy functions arranged stagewise are schematically represented by Figure A1-1. The coefficient matrix is of the order of 5% density, and thus the unique structure is exploited in determination of the flow and temperature map corrections.

The method of solution employed is the Thomas Procedure.

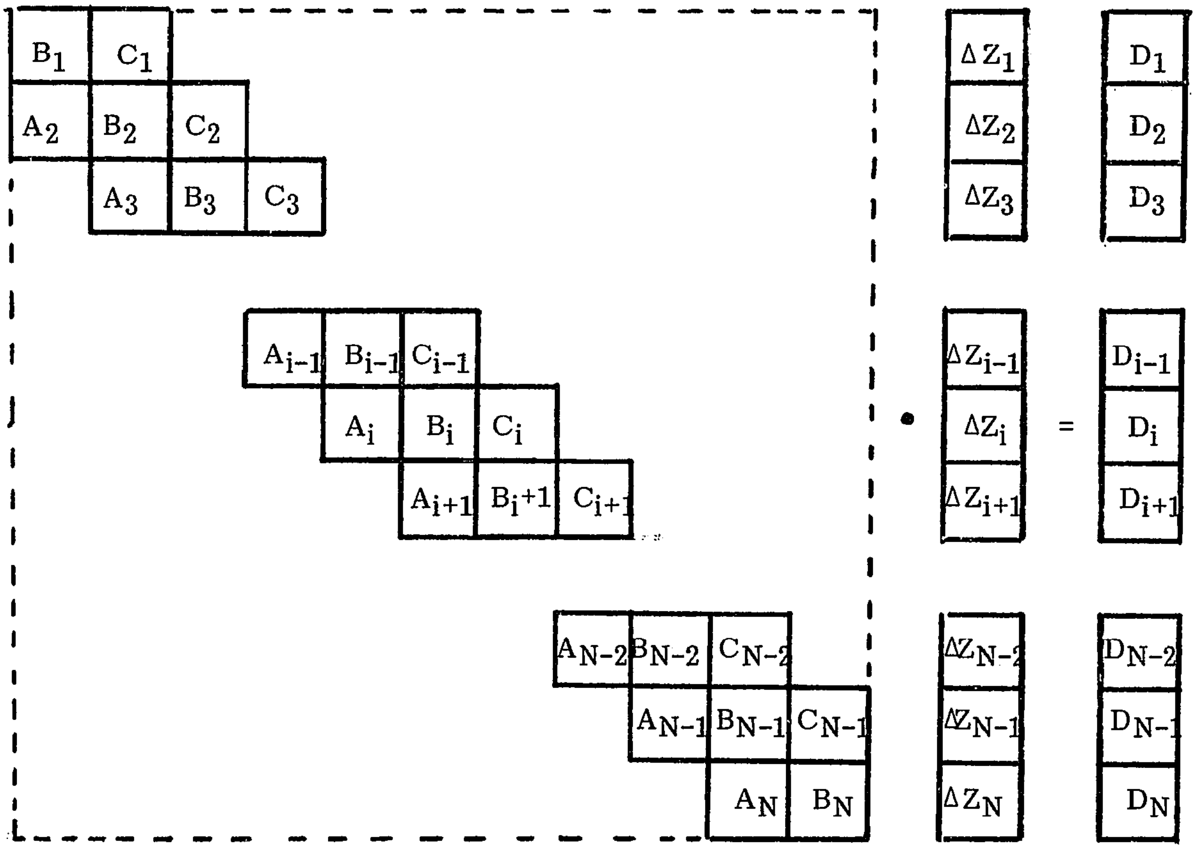


Figure A1-1 Schematic Representation of the Column's Linearized Discrepancy Functions

The Thomas procedure requires that B-matrix and D-matrix for the entire column be generated before the solution methodology be initiated. When this is completed, the inversion procedure is initiated to eliminate the A-matrix, and the C-matrix, starting with stage 2:

- Perform Gaussian elimination on

  $$B^T{}_{m-1} * S^T = A_m{}^T \qquad \text{(A1-6)}$$

  and retain the results in S after transposing.
- Eliminate A_m (by induction) by modifying B_m and D_m (subtract from B_m the product of $S{\bullet}C_{m-1}$ and subtract from D_m the product of $S{\bullet}D_{m-1}$).

The back substitution is initiated with m = N, by performing Gaussian elimination on:

$$B_N * S = D_N$$

The result of this operation is the set of flow and temperature corrections for stage N. The back substitution continues for m = N - 1, N - 2, etc. with the preliminary requirement that the elimination of C_m be accomplished.

The two fold process is thus:

- Eliminate C_m by subtracting from D_m the product of

  $$C_m * D_{m+1}$$

- Perform Graussian elimination on

  $$B_m * S = D_m$$

  to obtain the set of corrections associated with stage m.

It should be noted that C_m is not explicitly defined. Rather, the unique structure of this part of the Jacobian is exploited to minimize the iterative computational effort.

APPENDIX B

THE VLE PREDICTION METHODS

The VLE Package used for this research can be summarized as follows:

B.1 Vapor Phase Component--Fugacity Coefficient Calculation

B.1.1 Ideal Vapor

B.1.2 Redlich-Kwong Equation of State

B.1.3 Virial Equation with Tsonopoulos Correlation

B.2 Liquid Phase Component Activity Coefficient Calculation

B.2.1 Ideal Liquid

B.2.2 Wilson Equation (for single liquid phase only)

B.2.3 NRTL Equation (for two liquid phases)

B.2.4 UNIQUAC Equation (for two liquid phases)

B.3 Vapor Phase Enthalpy Correction

B.3.1 Redlich-Kwong Equation of State

B.3.2 Virial Equation of State

B.4 Liquid Phase Enthalpy of Mixing

B.4.1 Using Wilson Equation

B.4.2 Using NRTL Equation

B.4.3 Using UNIQUAC Equation

B.1 Vapor Phase Component Fugacity Coefficient Calculation

B.1.1 Ideal Vapor

For ideal vapor, the fugacity coefficient of component i is set equal to 1, then the equilibrium constant can be expressed as

$$K_i = \frac{\gamma_i P_i^s}{\pi} \qquad (2\text{-}14)$$

the saturation vapor pressure P_i^s is calculated using Eq. 2-15.

B.1.2 Redlich-Kwong Equation for Real Vapor

The Redlich-Kwong equation of state can be expressed as follows:

$$\ln \phi_i = (Z - 1)\frac{B_i}{B} - \ln(Z - Bp) - \frac{A^2}{B}\left(\frac{2A_i}{A} - \frac{B_i}{B}\right)\ln\left(1 + \frac{Bp}{z}\right)$$

where: (B1-7)

$$A^2{}_i = a\,\frac{T_{ri}{}^{-2.5}}{P_{ci}} \qquad (B1\text{-}8)$$

$$B_i = b/T_{ri}P_{ci} \qquad (B1\text{-}9)$$

$$A = \sum_i y_i A_i \qquad (B1\text{-}10)$$

$$B = \sum_i y_i B_i \qquad (B1\text{-}11)$$

Where the subscript r stands for reduced property and c for the critical point. The compressibility factor Z is obtained by solving the following R-K equation of state, which is a cubic equation of Z.

$$Z^3 - Z^2 + DZ - A^2P^2B = 0 \qquad \text{(B1-12)}$$

where $D = A^2P - BP - B^2P^2$

$$A = \sum_i A_i y_i$$

$$B = \sum_i B_i y_i$$

$$D = D_i$$

$$A_i = a/D$$

$$B_i = b/T$$

Eq. (B1-12) can be further simplified as

$$Z = \frac{1}{1-h} \frac{A^2}{B} \frac{h}{1+h} \qquad \text{(B1-12A)}$$

where $h = \frac{BP}{Z}$

The constants a and b are, respectively, 0.478 and 0.0867, if the first and the second partial derivatives of pressure with respect to volume are set equal to zero at the critical point. If experimental PVT data are available, these constnats may be treated as adjustable parameters to obtain a more accurate representation of the vapor phase.

B.1.3 Virial Equation with Tsonopoulos' Correlation

Tsonopoulos (1972) extended the Pitzer-Curl equation for polar gases. In reduced form, the Pitzer-Curl equation is

$$\frac{B_{ii}P_{ci}}{RT_{ci}} = f_{P_C}{}^{(0)}(T_R) + \omega_i f_{P_C}{}^{(1)}(TR) \qquad \text{(B1-13)}$$

where

$$f_{P_c}^{(0)}(TR) = 0.1445 - \frac{0.330}{T_R} - \frac{0.1385}{T_R^2} - \frac{0.0121}{T_R^3}$$

$$f_{P_c}^{(1)}(TR) = 0.073 + \frac{0.46}{T_R} - \frac{0.50}{T_R^2} - \frac{0.097}{T_R^3} - \frac{0.0073}{T_R^8}$$

P_{c_i} - is the critical pressure

T_{c_i} - is the absolute critical temperature

ω_i - is the acentric factor

Tsonopoulos suggested that a third function in reduced temperature $f^{(2)}(T_R)$ be added to the right hand side of Eq. B1-13 to be used for polar gases.

$$f^{(2)}(T_R) = \frac{a_i}{T_R^6} - \frac{b_i}{T_R^8} \qquad \text{(B1-14)}$$

For nonhydrogen bonded compounds, e.g. ketones, aldehydes, and ethers, "a" is required, and can be correlated as a function of reduced dipole moment, μ_R.

$$\mu_R = \frac{10^5 \mu^2 P_{c_i}}{T_{c_i}^2} \qquad \text{(B1-15)}$$

For hydrogen bonded compounds, e.g. alcohols and water, "b" is also required. A few available values for "a" and "b" along with methods of estimation were provided by Tsonopoulos (1972).

The binary second virial cross coefficient, B_{ij}, can be obtained from the same correlations using Eq. B1-13 by replacing P_{c_i}, T_{c_i}, ω_i, a_i, and b_i with the appropriate $P_{c_{ij}}$, $T_{c_{ij}}$, ω_{ij}, a_{ij} and b_{ij}.

$$\frac{B_{ij} P_{c_{ij}}}{R T_{c_{ij}}} = f_{P_c}^{(0)}(T_R) + \omega_{ij} f_{P_c}^{(1)}(T_R) \qquad \text{(B1-13A)}$$

The mixing rules provided by Tsonopoulos (1972) are:

$$T_{c_{ij}} = (T_{c_i}T_{c_j})^{1/2}(1 - K_{ij}) \tag{B1-16}$$

$$P_{c_{ij}} = \frac{4T_{c_{ij}}(\frac{P_{c_i}v_{c_i}}{T_{c_i}} + \frac{P_{c_j}v_{c_j}}{T_{c_j}})}{(v_{c_i}^{1/3} + v_{c_j}^{1/3})^3} \tag{B1-17}$$

$$\omega_{ij} = 0.5(\omega_i + \omega_j) \tag{B1-18}$$

The value for $T_{c_{ij}}$ requires a "characteristic constant" for each binary, K_{ij}, to account for nonideal mixing in the vapor. The "characteristic constant" for selected compounds were given by Tsonopoulos. For polar/polar binaries, the polar contribution to B_{ij} is calculated by assuming that

$$a_{ij} = 0.5(a_i + a_j) \tag{B1-19}$$

$$b_{ij} = 0.5(b_i + b_j) \tag{B1-20}$$

For polar/nonpolar binaries, B_{ij} is assumed to have no polar term:

$$a_{ij} = 0$$

$$b_{ij} = 0$$

B.2 The Liquid Phase Activity Coefficient Calculations

The activity coefficients, γ_i, can be obtained from G^E, the molar excess Gibbs energy of mixing, by partial differentiation:

$$\left(\frac{\partial n\Delta G^E}{\partial n_i}\right)_{T,p,n_j \neq n_i} = RT \ln \gamma_i$$

There exists a large number of equations for the representation of the molar excess Gibbs energy as a function of concentration at constant temperature. The Wilson, NRTL and UNIQUAC equations are cited here due to their newness and advantages over Margules and VanLaar equations.

For multicomponent systems, the Wilson, NRTL and UNIQUAC require only the binary parameters. This is due to the modern concept of local composition, which has been used in the derivation of these equations, either on the basis of local volume fraction, as with Wilson's equation or of local mole fraction as in the case of NRTL or UNIQUAC.

The Wilson equation is not applicable for a system containing immiscible liquid phases. In this research, the NRTL and UNIQUAC equations are used since the research problem is dealing with heterogeneous azeotropes (two liquid phases). For the completeness of activity coefficient calculation methods survey, the Wilson Equation is also described in this Appendix.

B.2.1 Ideal Liquid

For ideal liquid, the activity coefficient, γ_i, for a given component i is set equal to one in Equation 2-13.

$$\gamma_i = 1.0$$

B.2.2 Wilson Equation

For a solution of m components Wilson's equation is:

$$\frac{g^E}{RT} = - \sum_{i=1}^{m} x_i \ln[\sum_{j=1}^{m} x_j A_{ij}] \qquad \text{(B2-1)}$$

where

$$A_{ij} = \frac{v_j}{v_i} \text{ Exp } - [\frac{(\lambda_{ij} - \lambda_{ii})}{RT}] \qquad (B2-2)$$

$$A_{ji} = \frac{v_i}{v_j} \text{ Exp } - [\frac{(\lambda_{ji} - \lambda_{jj})}{RT}] \qquad (B2-3)$$

and

$$A_{ii} = A_{jj} = 1 \qquad (B2-4)$$

The activity coefficient for any component i is given by:

$$\ln \gamma_i = -\ln[\sum_{j=1}^{m} x_j A_{ij}] + 1 - \sum_{k=1}^{m} - \frac{x_i A_{ki}}{\sum\limits_{j=1}^{m} x_j A_{kj}} \qquad (B2-5)$$

Equation (B2-3) requires only parameters which can be obtained from binary data; for each possible binary pair in the multicomponent solution, two parameters, A_{ij} and A_{ji} are needed.

B.2.3 NRTL (Non Random Two Liquid) Equation

For a solution of m component, Renon's NRTL equation is:

$$\frac{g^E}{RT} = \sum_{i=1}^{m} x_i \frac{\sum\limits_{j=1}^{m} \tau_{ji} G_{ji} x_j}{\sum\limits_{l=1}^{m} G_{li} x_l} \qquad (B2-6)$$

where

$$\tau_{ji} = (\frac{g_{ji} - g_{ii}}{RT}) \text{ and } \tau_{ij} = (\frac{g_{ij} - g_{jj}}{RT}) \qquad (B2-7)$$

$$G_{ji} = \text{Exp}(- \alpha_{ji} \tau_{ji}) \qquad (B2-8)$$

$$\tau_{ii} = \tau_{jj} = 0$$

$$G_{ii} = G_{jj} = 1$$

$\alpha_{ij} = \alpha_{ji}$

The activity coefficient for a component i is given by:

$$\ln\gamma_i = \frac{\sum_{j=1}^{m} \tau_{ji}G_{ji}x_j}{\sum_{l=1}^{m} G_{li}x_l} + \sum_{j=1}^{m} \frac{x_j G_{ij}}{\sum_{l=1}^{m} G_{lj}x_l} \left(\tau_{ij} - \frac{\sum_{n=1}^{m} x_n \; {}_{nj}G_{nj}}{\sum_{l=1}^{m} G_{lj}x_l}\right) \tag{B2-9}$$

For a given binary, three parameters, τ_{ij}, τ_{ji} and α_{ij} are needed to calculate the activity coefficient.

B.2.4 UNIQUAC (Universal Quasi-Chemical) Equation

The activity coefficient for a given i component in the m component solution can be expressed by:

$$\ln\gamma_i = \ln\gamma_i^C + \ln\gamma_i^R \tag{B2-10}$$

where

$$\ln\gamma_i^C = \ln\frac{\phi_i}{x_i} + \frac{z}{2} q_i \ln\frac{\theta_i}{\phi_i} + l_i - \frac{\phi_i}{x_i}\sum_{j=1}^{m} x_j l_j \tag{B2-11}$$

$$\ln\gamma_i^R = q_i\left[1 - \ln\left(\sum_{j=1}^{m} \theta_j\tau_{ji}\right) - \sum_{j=1}^{m} \frac{\theta_j\tau_{ij}}{\sum_{k=1}^{m} \theta_k\tau_{kj}}\right] \tag{B2-12}$$

$$l_i = \frac{z}{2}(r_i - q_i) - (r_i - 1) \tag{B2-13}$$

$$\phi_i = \frac{r_i x_i}{\sum_{k}^{m} r_k x_k} = \text{(area fraction of component)} \tag{B2-14}$$

$$Q_i = \frac{q_i x_i}{\sum_{k}^{m} q_k x_k} = \text{(volume fraction of component)} \tag{B2-15}$$

Notations:

1) A_{ij} and A_{ji} adjustable Wilson's binary parameters.

2) V_i^L, molar volume of pure liquid component.

3) λ_{ij}, an empirically determined interaction energy between components i and j

$$\lambda_{ij} = \lambda_{ji}$$

4) g_{ij}, parameter for interaction between components i and j

$$g_{ij} = g_{ji}$$

5) α_{ij}, nonrandomness parameter for NRTL Equation

$$\alpha_{ij} = \alpha_{ji}$$

6) τ_{ij}, τ_{ji}, adjustable binary parameters in NRTL and UNIQUAC equations.

7) q_i, area parameter of component i.

8) r_i, volume parameter of component i.

9) U_{ij}, parameter of interaction between components i and j,

$$U_{ij} = U_{ji}$$

10) Z, coordination number

11) γ_i^C, combinatorial part of activity coefficient of component i.

12) γ_i^R, residual part of activity coefficient of component i.

and

$$\tau_{ji} = \mathrm{Exp} - \left(\frac{U_{ji} - U_{ii}}{RT}\right) \qquad \text{(B2-16)}$$

B.3 Vapor Phase Enthalpy Correction

The molar enthalpy correction, ΔH, for a vapor at temperature T and pressure π relative to the ideal vapor at the same T and composition is given exactly by

$$\Delta H = \int_{o}^{\pi} [v - T(\frac{\partial v}{\partial T})_{p,y}]dP \tag{B3-1}$$

where v is the vapor phase molar volume.

B.3.1 Redlich-Kwong Equation of State

The vapor enthalpy correction for Redlich-Kwong equation of state is given by Prausnitz et al. (1977) as

$$\Delta H = \frac{bRT}{v-b} - \frac{a}{T^{0.5}(v+b)} - \frac{3a}{2bT^{0.5}} \ln \frac{v+b}{v} \tag{B3-2}$$

B.3.2 Virial Equation of State

The enthalpy correction for the virial equation can be expressed as

$$\Delta H = \pi \sum_{i=1}^{m} \sum_{j=1}^{m} y_i y_j [B_{ij} - T \frac{dB_{ij}}{dT}] \tag{B3-3}$$

B.4 Liquid Phase Enthalpy of Mixing

The liquid enthalpy of mixing can be expressed as:

$$(\frac{\partial \frac{g^E}{T}}{\partial \frac{1}{T}})_{p,x} = h^{mix} \tag{B4-1}$$

or

$$[\frac{\partial(\Sigma x_i \ln {}_{i})}{\partial T}]_{p,x} = - \frac{h^{mix}}{RT^2} \tag{B4-2}$$

B.4.1 Wilson Equation

The enthalpy of mixing calculated from Wilson's equation is

$$h^{mix} = R[\frac{-x_i(x_j \frac{\partial A_{ji}}{\partial(1/T)})}{x_i + x_j A_{ji}} - \frac{x_j(x_i \frac{\partial A_{ij}}{\partial(1/T)})}{x_j + x_i A_{ij}}] \tag{B4-3}$$

where:

$$\frac{\partial A_{ij}}{\partial(1/T)} = -A_{ij}\tau'_{ij} + \frac{A_{ij}}{(V_j/V_i)} \frac{\partial(v_j/V_i)}{\partial(1/T)} \tag{B4-4}$$

$$\tau'_{ij} = \frac{\partial\left[\frac{(\lambda_{ji} - \lambda_{ij})}{RT}\right]}{\partial(1/T)} \qquad \text{(B4-5)}$$

B.4.2 NRTL Equation

The enthalpy of mixing using the NRTL equation can be expressed as

$$\frac{h^{mix}}{R} = x_i x_j \left[\frac{G_{ji}\,\tau'_{ji}}{x_i + x_j G_{ji}} + \tau_{ji}\left(\frac{G^2_{ji} x_j(\alpha_{ji}\tau'_{ji} + \tau_{ji}\alpha'_{ji})}{(x_i + x_j G_{ji})^2} - \frac{G_{ji}(\alpha_{ji}\tau'_{ji} + \tau_{ji}\alpha'_{ji})}{x_i + x_j G_{ji}}\right) + \frac{G_{ij}\,\tau'_{ij}}{x_j + x_i G_{ij}} + T_{ij}\left(\frac{G^2_{ij} x_i(\alpha_{ij}\tau'_{ij} + \tau_{ij}\alpha'_{ij})}{(x_j + x_i G_{ij})^2} - \frac{G_{ij}(\alpha_{ij}\tau'_{ij} + \tau_{ij}\alpha'_{ij})}{x_j + x_i G_{ij}}\right)\right]$$

(B4-1)

where

$$\tau'_{ji} = \frac{\partial\tau_{ji}}{\partial(1/T)} = \frac{A_{ij}}{RT}$$

$$\alpha'_{ij} = \frac{\partial\alpha_{ij}}{\partial(1/T)} = -B'T^2$$

$$(\lambda_{ij} - \lambda_{jj}) = A_{ij} + B_{ij}T$$

$$\alpha_{ij} = A' + B'T$$

$$\tau_{ij} = \frac{A_{ij}}{RT} + \frac{B_{ij}}{R}$$

G_{ji}, $(\lambda_{ij} - \lambda_{jj})$, α_{ij} and τ_{ij} are the same as these defined in Sections B.2.3 and B.2.4.

B.4.3 UNIQUAC Equation

The enthalpy of mixing using the UNIQUAC equation as described by Prausnitz et al. (1980) is

$$h^{mix} = -RT \sum_{i}^{m} \left[\frac{q_i x_i \sum_{j=1}^{m} \theta_j \tau_{ji} \ln \tau_{ji}}{\sum_{j=1}^{m} \theta_j \tau_{ji}} \right] \qquad \text{(B4-3)}$$

In the above equation, if $(U_{ji} - U_{ii})$ is assumed to be temperature dependent, then

$$\tau_{ji} = \mathrm{Exp}\left[- \frac{a_{ji} + b_{ji}/T}{T}\right]$$

and Equation (B4-3) becomes

$$h^{mix} = R \sum_{i=1}^{m} \left\{ \frac{q_i x_i}{\sum_{j=1}^{m} \theta_j \tau'_{ji}} \left[\sum_{j=1}^{m} \theta_j \tau'_{ji} (a_{ji} + 2b_{ji}/T) \right] \right\} \qquad \text{(B4-4)}$$

The parameters are the same as those defined in Section B.2.4.

APPENDIX C

THE RESEARCH PROBLEM--SAMPLE COMPUTER INPUTS AND RESULTS

C.1 A Reboiled Absorber Case Using NRTL Equation for Activity Coefficient Calculation

C.2 A Conventional Distillation Column Case Using the NRTL Equation for Activity Coefficient Calculation

C.3 A Conventional Distillation Column Case Using the UNIQUAC Equation for Activity Coefficient Calculation

C.1 Inputs

```
   0.1     //BAYWAY  JOB  (JA00008-SAI,NJIT,-30,10),'ROCHE-TSAI',
   0.2     //      MSGLEVEL=(1,1),TIME=(2,30)
   0.3     /*PRIORITY -2
?
10055.     //STEP6  EXEC  PGM=BAYWAY2,REGION=230K
10056.     //STEPLIB  DD  DSN='NCE.AJA00.S008.TEST',UNIT=OLS,DISP=SHR
10057.     //FT06F001 DD  SYSOUT=A
10058.     //FT05F001 DD  *
10059.     CHEMSHARE'S ETOH DEHYDRATION --VIRFUG VAPOR--NRTL LIQUID
10060.      3 1 2 2 0 0 1
10061.     ETHANOL 0 46.07     516.2     63.0      167.0     64.0
10062.     0.0878    0.0572    0.248     0.635
10063.     202.06    351.1     0.58                        0.38
10064.     18.9119   -3803.98  -41.68
10065.     WATER   0 18.01     647.3     217.3     56.0      18.84
10066.     0.0279    0.0229    0.229     0.344
10067.     538.7     373.2     1.0                         0.454
10068.     18.3036   -3816.44  -46.13
10069.     BENZENE 0 78.114    562.1     48.3      259.0     92.26
10070.     0.0       0.0       0.544     0.251
10071.     94.118    353.3     0.41                        0.249
10072.     15.9008   -2788.51  -52.36
10073.     0.0       0.20      0.15
10074.     0.20      0.0       0.40
10075.     0.15      0.40      0.0
10076.     -86.763   0.0       1289.908  0.0       282.332   0.0       1096.899
10077.     3820.954  0.0       2213.355  0.0
10078.     0.270     0.295     0.267
10079.      3 042 2 0 020 2 0
10080.     1.0       0.0       0.0
10081.     727.00    0.0       .000005   338.0     352.0     760.0     0.001
10082.     37        310.97    0.0       191.9     66.6      0.0
10083.     41        308.2     0.0       169.2     22.65     400.0
10084.     /*
10085.     //
?
```

C.1. Results

```
*** STAGEWISE SIMULATION PROGRAM ***

CHEMSHARE'S ETOH DEHYDRATION --VIRFUG VAPOR--NRTL LIQUID
NUMBER OF COMPONENTS =  3
VAPOR-LIQUID EQUILIBRIUM DATA CODES:
    LIQUID =    1
    VAPOR =     2
    ENTHALPY = 2

NOTE: ALL FLOWS ARE  PER UNIT TIME, AND ENERGY
      VALUES ARE IN UNITS OF K-BTU PER UNIT TIME.
COMPONENT NO                          1          2          3
NAME                            ETHANOL      WATER    BENZENE
MOLECULAR WEIGHT                   46.1       18.0       78.1
CRITICAL PROPERTIES
TEMPERATURE  (DEG K)              516.2      647.3      562.1
PRESSURE     ( ATM)                63.0      217.3       48.3
VOLUME          (CC/GMOL)         167.0       56.0      259.0
COMPRESSIBILITY                   0.248      0.229      0.544
ACENTRIC FACTOR                   0.635      0.344      0.251
TSONOPOULOS -A-                  0.0878     0.0279     0.0
TSONOPOULOS -B-                  0.0572     0.0229     0.0
AK(1,1)=   0.0
AK(1,2)=   0.200
AK(1,3)=   0.150
AK(2,1)=   0.200
AK(2,2)=   0.0
AK(2,3)=   0.400
AK(3,1)=   0.150
AK(3,2)=   0.400
AK(3,3)=   0.0
VAPOR PRESSURE CONSTANTS
( MMHG AND DEG K)
C(1)                             18.912     18.304     15.901
C(2)                           -3803.98   -3816.44   -2788.51
C(3)                             -41.68     -46.13     -52.36
C(4)                                0.0        0.0        0.0
C(5)                                0.0        0.0        0.0
C(6)                                0.0        0.0        0.0
LIQUID MOLAR VOLUME CONSTANTS
C(1)                             64.000     18.840     92.260
ENTHALPY CONSTANTS (CAL/GM)
LATENT HEAT                       202.1      538.7       94.1
AT DEG K                          351.1      373.2      353.3
LIQUID SP. HEAT CONSTANTS
C(1)                              0.580      1.000      0.410
C(2)                              0.0        0.0        0.0
C(3)                              0.0        0.0        0.0
C(4)                              0.0        0.0        0.0
VAPOR SP. HEAT CONSTANTS
C(1)                              0.380      0.454      0.249
C(2)                              0.0        0.0        0.0
C(3)                              0.0        0.0        0.0
C(4)                              0.0        0.0        0.0
```

```
  NRTL CONSTANTS, CAL/GMOL

        A  12 =   -86.76     B  12 =      0.0           A  21 =  1289.91     B  21 =      0.0
        A  13 =   282.33     B  13 =      0.0           A  31 =  1096.90     B  31 =      0.0
        A  23 =  3820.95     B  23 =      0.0           A  32 =  2213.35     B  32 =      0.0
        ALPHA12 = 0.2700     ALPHA13 = 0.2950     ALPHA23 = 0.2670     ALPHA
CHEMSHARE'S ETOH DEHYDRATION --VIRFUG VAPOR--NRTL LIQUID
DISTILLATION COLUMN; PRODUCT RATES & REFLUX RATIO SPECIFIED
FEED STREAMS:
STAGE                        37.         41.
TEMP                      310.97      308.20
FRACV                     0.0         0.0
H                    -2.8042E 05 -7.9823E 05
COMP 1  ETHANOL          191.900     169.200     361.100
COMP 2  WATER             66.600      22.650      89.250
COMP 3  BENZENE            0.0       400.000     400.000
TOTAL                    258.500     591.850     850.350
NUMBER OF STAGES       42

ESTIMATED OVERHEAD PRODUCT RATE    727.0000
ESTIMATED BOTTOMS PRODUCT RATE     123.3496

PRESSURE AT TOP OF COLUMN         759.99072
CONSTANT DELTA P PER STAGE          0.00100
REFLUX RATIO       0.000005
```

```
      FINAL  COLUMN  PROFILES:
      STAGE     TEMP          PRES          EFF(%)       LIQUID(MOLS)   VAPOR(MOLS)
         1     351.37       760.041        100.00           123.350       742.934
         2     351.15       760.040        100.00           866.284       743.371
         3     350.49       760.038        100.00           866.721       745.182
         4     348.74       760.037        100.00           868.531       752.778
         5     345.47       760.036        100.00           876.127       774.207
         6     342.35       760.035        100.00           897.556       800.991
         7     341.17       760.033        100.00           924.341       814.621
         8     340.94       760.032        100.00           937.970       818.529
         9     340.89       760.031        100.00           941.878       819.462
        10     340.89       760.030        100.00           942.811       819.675
        11     340.88       760.029        100.00           943.024       819.724
        12     340.88       760.027        100.00           943.073       819.735
        13     340.88       760.026        100.00           943.084       819.737
        14     340.88       760.025        100.00           943.086       819.737
        15     340.88       760.024        100.00           943.086       819.736
        16     340.88       760.022        100.00           943.085       819.734
        17     340.88       760.021        100.00           943.083       819.732
        18     340.88       760.020        100.00           943.081       819.727
        19     340.88       760.019        100.00           943.076       819.720
        20     340.88       760.018        100.00           943.070       819.710
        21     340.88       760.016        100.00           943.060       819.696
        22     340.87       760.015        100.00           943.045       819.671
        23     340.87       760.014        100.00           943.021       819.635
        24     340.86       760.013        100.00           942.985       819.580
        25     340.85       760.011        100.00           942.929       819.496
        26     340.84       760.010        100.00           942.845       819.368
        27     340.81       760.009        100.00           942.718       819.177
        28     340.77       760.008        100.00           942.526       818.890
        29     340.72       760.007        100.00           942.239       818.469
        30     340.64       760.005        100.00           941.818       817.864
        31     340.53       760.004        100.00           941.213       817.022
        32     340.37       760.003        100.00           940.371       815.899
        33     340.15       760.002        100.00           939.249       814.492
        34     339.89       760.000        100.00           937.841       812.856
        35     339.57       759.999        100.00           936.205       811.127
        36     339.24       759.998        100.00           934.476       809.481
        37     338.91       759.997        100.00           932.831       788.169
        38     338.90       759.996        100.00           653.018       791.221
        39     338.92       759.994        100.00           656.071       791.480
        40     338.91       759.993        100.00           656.329       791.442
        41     338.89       759.992        100.00           656.291       727.005
        42     338.89       759.991        100.00             0.004       727.001
```

```
      FINAL VAPOR COMPOSITION PROFILE (MOLE%):
      STAGE   ETHANOL       WATER        BENZENE
         1     99.48808     0.00004       0.51191
         2     98.33203     0.00004       1.66794
         3     94.92275     0.00005       5.07721
         4     86.22646     0.00005      13.77351
         5     70.69477     0.00005      29.30522
         6     55.95709     0.00006      44.04287
         7     49.11826     0.00008      50.88168
         8     47.14054     0.00012      52.85934
         9     46.66149     0.00019      53.33833
        10     46.55068     0.00031      53.44902
        11     46.52515     0.00048      53.47440
        12     46.51917     0.00074      53.48011
        13     46.51745     0.00114      53.48141
        14     46.51656     0.00176      53.48168
        15     46.51558     0.00271      53.48170
        16     46.51424     0.00417      53.48162
        17     46.51213     0.00641      53.48147
        18     46.50898     0.00985      53.48119
        19     46.50413     0.01512      53.48077
        20     46.49662     0.02321      53.48017
        21     46.48511     0.03562      53.47927
        22     46.46757     0.05465      53.47781
        23     46.44064     0.08379      53.47559
        24     46.39950     0.12836      53.47216
        25     46.33666     0.19640      53.46695
        26     46.24097     0.29996      53.45910
        27     46.09584     0.45685      53.44730
        28     45.87712     0.69291      53.42998
        29     45.55092     1.04436      53.40473
        30     45.07109     1.55954      53.36937
        31     44.38018     2.29773      53.32209
        32     43.41490     3.32155      53.26357
        33     42.12145     4.67894      53.19964
        34     40.48127     6.37442      53.14432
        35     38.53958     8.34078      53.11963
        36     36.41735    10.43428      53.14838
        37     34.28720    12.47106      53.24174
        38     33.01278    12.14383      54.84340
        39     32.86877    12.12716      55.00408
        40     32.81918    12.16647      55.01435
        41     32.72653    12.27641      54.99706
        42     32.72654    12.27645      54.99701
```

```
2686.      FINAL LIQUID COMPOSITION PROFILE (MOLE%):
2687.      STAGE    ETHANOL        WATER          BENZENE
2688.         1      99.86089       0.00003         0.13909
2689.         2      99.54116       0.00004         0.45882
2690.         3      98.54964       0.00004         1.45035
2691.         4      95.62410       0.00005         4.37590
2692.         5      88.14607       0.00005        11.85392
2693.         6      74.70303       0.00005        25.29696
2694.         7      61.81589       0.00005        38.18405
2695.         8      55.79129       0.00007        44.20865
2696.         9      54.04488       0.00011        45.95501
2697.        10      53.62170       0.00017        46.37814
2698.        11      53.52379       0.00027        46.47595
2699.        12      53.50122       0.00042        46.49835
2700.        13      53.49597       0.00065        46.50340
2701.        14      53.49446       0.00100        46.50455
2702.        15      53.49367       0.00153        46.50480
2703.        16      53.49283       0.00236        46.50480
2704.        17      53.49166       0.00363        46.50471
2705.        18      53.48986       0.00557        46.50457
2706.        19      53.48716       0.00856        46.50429
2707.        20      53.48299       0.01315        46.50388
2708.        21      53.47654       0.02018        46.50329
2709.        22      53.46664       0.03097        46.50239
2710.        23      53.45159       0.04750        46.50093
2711.        24      53.42844       0.07283        46.49872
2712.        25      53.39310       0.11157        46.49533
2713.        26      53.33910       0.17071        46.49020
2714.        27      53.25686       0.26071        46.48243
2715.        28      53.13216       0.39707        46.47077
2716.        29      52.94421       0.60220        46.45359
2717.        30      52.66390       0.90758        46.42853
2718.        31      52.25152       1.35516        46.39332
2719.        32      51.65766       1.99634        46.34599
2720.        33      50.82787       2.88534        46.28680
2721.        34      49.71565       4.06355        46.22082
2722.        35      48.30484       5.53457        46.16060
2723.        36      46.63395       7.23981        46.12624
2724.        37      44.80659       9.05455        46.13885
2725.        38      30.85966       4.85332        64.28702
2726.        39      29.33865       4.49412        66.16724
2727.        40      29.16642       4.47703        66.35657
2728.        41      29.10641       4.52400        66.36962
2729.        42      29.10652       4.52404        66.36944
```

```
2730.      FINAL VAPOR COMPOSITION PROFILE (MOLES):
2731.      STAGE   ETHANOL      WATER        BENZENE
2732.        1       739.131        0.000        3.803
2733.        2       730.972        0.000       12.399
2734.        3       707.347        0.000       37.834
2735.        4       649.094        0.000      103.684
2736.        5       547.324        0.000      226.883
2737.        6       448.211        0.000      352.780
2738.        7       400.127        0.001      414.493
2739.        8       385.859        0.001      432.669
2740.        9       382.373        0.002      437.087
2741.       10       381.564        0.003      438.108
2742.       11       381.378        0.004      438.343
2743.       12       381.334        0.006      438.395
2744.       13       381.321        0.009      438.407
2745.       14       381.313        0.014      438.409
2746.       15       381.305        0.022      438.409
2747.       16       381.293        0.034      438.407
2748.       17       381.275        0.053      438.405
2749.       18       381.247        0.081      438.400
2750.       19       381.204        0.124      438.393
2751.       20       381.138        0.190      438.383
2752.       21       381.036        0.292      438.367
2753.       22       380.881        0.448      438.342
2754.       23       380.644        0.687      438.305
2755.       24       380.281        1.052      438.247
2756.       25       379.727        1.609      438.159
2757.       26       378.884        2.458      438.027
2758.       27       377.606        3.742      437.828
2759.       28       375.683        5.674      437.533
2760.       29       372.820        8.548      437.101
2761.       30       368.620       12.755      436.489
2762.       31       362.596       18.773      435.653
2763.       32       354.222       27.101      434.577
2764.       33       343.076       38.110      433.307
2765.       34       329.054       51.815      431.987
2766.       35       312.605       67.654      430.868
2767.       36       294.792       84.464      430.226
2768.       37       270.241       98.293      419.635
2769.       38       261.204       96.085      433.933
2770.       39       260.150       95.984      435.346
2771.       40       259.745       96.291      435.407
2772.       41       237.923       89.250      399.831
2773.       42       237.922       89.250      399.829
```

```
FINAL LIQUID COMPOSITION PROFILE (MOLES):
STAGE    ETHANOL        WATER         BENZENE
   1       123.178        0.000          0.172
   2       862.309        0.000          3.975
   3       854.150        0.000         12.571
   4       830.525        0.000         38.006
   5       772.271        0.000        103.855
   6       670.502        0.000        227.054
   7       571.389        0.001        352.951
   8       523.305        0.001        414.664
   9       509.037        0.001        432.840
  10       505.551        0.002        437.258
  11       504.742        0.003        438.280
  12       504.556        0.004        438.514
  13       504.512        0.006        438.566
  14       504.499        0.009        438.578
  15       504.491        0.014        438.580
  16       504.483        0.022        438.580
  17       504.471        0.034        438.578
  18       504.453        0.053        438.576
  19       504.425        0.081        438.571
  20       504.382        0.124        438.564
  21       504.316        0.190        438.554
  22       504.214        0.292        438.538
  23       504.060        0.448        438.513
  24       503.822        0.687        438.476
  25       503.459        1.052        438.418
  26       502.905        1.610        438.331
  27       502.062        2.458        438.198
  28       500.784        3.742        437.999
  29       498.861        5.674        437.704
  30       495.998        8.548        437.272
  31       491.798       12.755        436.660
  32       485.774       18.773        435.824
  33       477.400       27.101        434.748
  34       466.254       38.110        433.478
  35       452.232       51.815        432.158
  36       435.783       67.654        431.039
  37       417.970       84.464        430.397
  38       201.519       31.693        419.806
  39       192.482       29.485        434.104
  40       191.428       29.384        435.517
  41       191.023       29.691        435.578
  42         0.001        0.000          0.002
```

```
      STAGE #    1
      TEMP, DEG K   351.372
      PRES, MMHG   760.0408
       #   NAME            K              VP           FUG            GAM
       1   ETHANOL      0.99626         756.57        1.0008         1.0000
       2   WATER          1.1508        330.50       0.97409         2.7169
       3   BENZENE        3.6804        716.99       0.97208         4.0135
      STAGE #    2
      TEMP, DEG K   351.150
      PRES, MMHG   760.0396
       #   NAME            K              VP           FUG            GAM
       1   ETHANOL      0.98785         749.92        1.0012         1.0000
       2   WATER          1.1460        327.50       0.97430         2.7298
       3   BENZENE        3.6353        712.03       0.97293         3.9883
      STAGE #    3
      TEMP, DEG K   350.486
      PRES, MMHG   760.0383
       #   NAME            K              VP           FUG            GAM
       1   ETHANOL      0.96319         730.37        1.0021         1.0002
       2   WATER          1.1324        318.68       0.97490         2.7701
       3   BENZENE        3.5007        697.39       0.97544         3.9112
      STAGE #    4
      TEMP, DEG K   348.743
      PRES, MMHG   760.0371
       #   NAME            K              VP           FUG            GAM
       1   ETHANOL      0.90172         681.04        1.0042         1.0021
       2   WATER          1.1020        296.48       0.97616         2.8940
       3   BENZENE        3.1476        660.06       0.98173         3.6918
      STAGE #    5
      TEMP, DEG K   345.466
      PRES, MMHG   760.0359
       #   NAME            K              VP           FUG            GAM
       1   ETHANOL      0.80201         595.85        1.0069         1.0160
       2   WATER          1.0791        258.24       0.97741         3.2494
       3   BENZENE        2.4722        594.16       0.99257         3.1861
      STAGE #    6
      TEMP, DEG K   342.345
      PRES, MMHG   760.0347
       #   NAME            K              VP           FUG            GAM
       1   ETHANOL      0.74906         523.23        1.0076         1.0799
       2   WATER          1.1879        225.79       0.97724         4.0918
       3   BENZENE        1.7410        536.34        1.0021         2.4620
      STAGE #    7
```

```
2860.      STAGE #    7
2861.      TEMP, DEG K   341.165
2862.      PRES, MMHG   760.0334
2863.       #  NAME             K              VP             FUG            GAM
2864.       1  ETHANOL       0.79459         497.78         1.0068         1.2050
2865.       2  WATER          1.4652         214.44        0.97665         5.3171
2866.       3  BENZENE        1.3325         515.67         1.0060         1.9523
2867.      STAGE #    8
2868.      TEMP, DEG K   340.936
2869.      PRES, MMHG   760.0322
2870.       #  NAME             K              VP             FUG            GAM
2871.       1  ETHANOL       0.84494         492.96         1.0063         1.2945
2872.       2  WATER          1.6709         212.30        0.97641         6.1264
2873.       3  BENZENE        1.1957         511.73         1.0070         1.7636
2874.      STAGE #    9
2875.      TEMP, DEG K   340.894
2876.      PRES, MMHG   760.0310
2877.       #  NAME             K              VP             FUG            GAM
2878.       1  ETHANOL       0.86338         492.09         1.0062         1.3253
2879.       2  WATER          1.7425         211.91        0.97634         6.4011
2880.       3  BENZENE        1.1607         511.01         1.0072         1.7140
2881.      STAGE #   10
2882.      TEMP, DEG K   340.885
2883.      PRES, MMHG   760.0298
2884.       #  NAME             K              VP             FUG            GAM
2885.       1  ETHANOL       0.86813         491.90         1.0062         1.3331
2886.       2  WATER          1.7608         211.83        0.97633         6.4709
2887.       3  BENZENE        1.1525         510.86         1.0072         1.7023
2888.      STAGE #   11
2889.      TEMP, DEG K   340.883
2890.      PRES, MMHG   760.0286
2891.       #  NAME             K              VP             FUG            GAM
2892.       1  ETHANOL       0.86924         491.86         1.0062         1.3349
2893.       2  WATER          1.7650         211.81        0.97633         6.4871
2894.       3  BENZENE        1.1506         510.83         1.0072         1.6996
2895.      STAGE #   12
2896.      TEMP, DEG K   340.883
2897.      PRES, MMHG   760.0273
2898.       #  NAME             K              VP             FUG            GAM
2899.       1  ETHANOL       0.86949         491.85         1.0062         1.3353
2900.       2  WATER          1.7660         211.80        0.97633         6.4909

2901.       3  BENZENE        1.1501         510.82         1.0072         1.6990
```

```
3056.      STAGE #   35
3057.      TEMP, DEG K    339.574
3058.      PRES, MMHG   759.9993
3059.       #  NAME              K              VP              FUG             GAM
3060.       1  ETHANOL        0.79784         465.14           1.0065          1.2952
3061.       2  WATER           1.5070         199.92          0.98483          5.8172
3062.       3  BENZENE         1.1508         488.82           1.0091          1.7730
3063.      STAGE #   36
3064.      TEMP, DEG K    339.240
3065.      PRES, MMHG   759.9980
3066.       #  NAME              K              VP              FUG             GAM
3067.       1  ETHANOL        0.78091         458.50           1.0064          1.2862
3068.       2  WATER           1.4412         196.97          0.98689          5.6347
3069.       3  BENZENE         1.1522         483.31           1.0095          1.7948
3070.      STAGE #   37
3071.      TEMP, DEG K    338.910
3072.      PRES, MMHG   759.9968
3073.       #  NAME              K              VP              FUG             GAM
3074.       1  ETHANOL        0.76522         452.04           1.0062          1.2786
3075.       2  WATER           1.3773         194.10          0.98887          5.4534
3076.       3  BENZENE         1.1539         477.93           1.0099          1.8170
3077.      STAGE #   38
3078.      TEMP, DEG K    338.902
3079.      PRES, MMHG   759.9956
3080.       #  NAME              K              VP              FUG             GAM
3081.       1  ETHANOL         1.0698         451.89           1.0055          1.7892
3082.       2  WATER           2.5022         194.04          0.98829          9.9165
3083.       3  BENZENE        0.85310         477.81           1.0104          1.3429
3084.      STAGE #   39
3085.      TEMP, DEG K    338.917
3086.      PRES, MMHG   759.9944
3087.       #  NAME              K              VP              FUG             GAM
3088.       1  ETHANOL         1.1203         452.18           1.0055          1.8728
3089.       2  WATER           2.6984         194.16          0.98824          10.688
3090.       3  BENZENE        0.83129         478.04           1.0105          1.3079
3091.      STAGE #   40
3092.      TEMP, DEG K    338.912
3093.      PRES, MMHG   759.9932
3094.       #  NAME              K              VP              FUG             GAM
3095.       1  ETHANOL         1.1252         452.08           1.0054          1.8814
3096.       2  WATER           2.7175         194.12          0.98828          10.765
3097.       3  BENZENE        0.82907         477.96           1.0105          1.3046
3098.      STAGE #   41
3099.      TEMP, DEG K    338.894
3100.      PRES, MMHG   759.9919
3101.       #  NAME              K              VP              FUG             GAM
3102.       1  ETHANOL         1.1244         451.74           1.0054          1.8814
3103.       2  WATER           2.7136         193.97          0.98839          10.757
3104.       3  BENZENE        0.82864         477.68           1.0105          1.3047
3105.      STAGE #   42
3106.      TEMP, DEG K    338.894
3107.      PRES, MMHG   759.9907
3108.       #  NAME              K              VP              FUG             GAM
3109.       1  ETHANOL         1.1244         451.74           1.0054          1.8814
3110.       2  WATER           2.7136         193.97          0.98839          10.757
3111.       3  BENZENE        0.82865         477.68           1.0105          1.3047
```

C.2 Inputs

```
   0.1    //BAYWAY  JOB  (JA00008-SAI,NJIT,-30,10),'ROCHE-TSAI',
   0.2    //      MSGLEVEL=(1,1),TIME=(2,30)
   0.3    /*PRIORITY -2
?
10025.    //STEP5  EXEC   PGM=BAYWAY2,REGION=230K
10026.    //STEPLIB  DD  DSN='NCE.AJA00.S008.TEST',UNIT=OLS,DISP=SHR
10027.    //FT06F001 DD  SYSOUT=A
10028.    //FT05F001 DD  *
10029.    CHEMSHARE'S ETOH DEHYDRATIO -VIR VAP-NRTL LIQ--REBOILED ABSOB
10030.     3 1 2 2 1 0 1
10031.    ETHANOL 0 46.07     516.2     63.0      167.0     64.0
10032.    0.0878    0.0572    0.248     0.635
10033.    202.06    351.1     0.58                          0.38
10034.    18.9119   -3803.98  -41.68
10035.    WATER   0 18.01     647.3     217.3     56.0      18.84
10036.    0.0279    0.0229    0.229     0.344
10037.    538.7     373.2     1.0                           0.454
10038.    18.3036   -3816.44  -46.13
10039.    BENZENE 0 78.114    562.1     48.3      259.0     92.26
10040.    0.0       0.0       0.544     0.251
10041.    94.118    353.3     0.41                          0.249
10042.    15.9008   -2788.51  -52.36
10043.    0.0       0.20      0.15
10044.    0.20      0.0       0.40
10045.    0.15      0.40      0.0
10046.    -86.763   0.0       1289.908  0.0       282.332   0.0       1096.899
10047.    3820.954  0.0       2213.355  0.0
10048.    0.270     0.295     0.267
10049.     5 041  2  0 020  2  0
10050.    1.0       0.0       0.0
10051.    727.00    0.0       6.015     338.0     352.0     760.0     0.001
10052.    37        310.97    0.0       191.9     66.6      0.0
10053.    41        308.2     0.0       169.2     22.65     400.0
10054.    /*
?
```

C.2 Results

```
*** STAGEWISE SIMULATION PROGRAM ***

CHEMSHARE'S ETOH DEHYDRATIO -VIR VAP-NRTL LIQ--REBOILED ABSOB
NUMBER OF COMPONENTS =  3
VAPOR-LIQUID EQUILIBRIUM DATA CODES:
    LIQUID =    1
    VAPOR =     2
    ENTHALPY = 2

NOTE: ALL FLOWS ARE  PER UNIT TIME, AND ENERGY
      VALUES ARE IN UNITS OF K-BTU PER UNIT TIME.
COMPONENT NO                           1         2         3
NAME                             ETHANOL     WATER   BENZENE
MOLECULAR WEIGHT                    46.1      18.0      78.1
CRITICAL PROPERTIES
TEMPERATURE  (DEG K)               516.2     647.3     562.1
PRESSURE      ( ATM)                63.0     217.3      48.3
VOLUME         (CC/GMOL)           167.0      56.0     259.0
COMPRESSIBILITY                    0.248     0.229     0.544
ACENTRIC FACTOR                    0.635     0.344     0.251
TSONOPOULOS -A-                   0.0878    0.0279    0.0
TSONOPOULOS -B-                   0.0572    0.0229    0.0
AK(1,1)=   0.0
AK(1,2)=   0.200
AK(1,3)=   0.150
AK(2,1)=   0.200
AK(2,2)=   0.0
AK(2,3)=   0.400
AK(3,1)=   0.150
AK(3,2)=   0.400
AK(3,3)=   0.0
VAPOR PRESSURE CONSTANTS
( MMHG AND DEG K)
C(1)                              18.912    18.304    15.901
C(2)                            -3803.98  -3816.44  -2788.51
C(3)                              -41.68    -46.13    -52.36
C(4)                                0.0       0.0       0.0
C(5)                                0.0       0.0       0.0
C(6)                                0.0       0.0       0.0
LIQUID MOLAR VOLUME CONSTANTS
C(1)                              64.000    18.840    92.260
ENTHALPY CONSTANTS (CAL/GM)
LATENT HEAT                        202.1     538.7      94.1
AT DEG K                           351.1     373.2     353.3
LIQUID SP. HEAT CONSTANTS
C(1)                               0.580     1.000     0.410
C(2)                               0.0       0.0       0.0
C(3)                               0.0       0.0       0.0
C(4)                               0.0       0.0       0.0
VAPOR SP. HEAT CONSTANTS
C(1)                               0.380     0.454     0.249
C(2)                               0.0       0.0       0.0
C(3)                               0.0       0.0       0.0
C(4)                               0.0       0.0       0.0
  NRTL CONSTANTS, CAL/GMOL
UNIQUAC PARAMETERS,CAL/G MOL
```

```
  NRTL CONSTANTS, CAL/GMOL

        A  12 =   -86.76     B  12 =      0.0          A  21 =  1289.91     B  21 =      0.0
        A  13 =   282.33     B  13 =      0.0          A  31 =  1096.90     B  31 =      0.0
        A  23 =  3820.95     B  23 =      0.0          A  32 =  2213.35     B  32 =      0.0
        ALPHA12 = 0.2700     ALPHA13 = 0.2950     ALPHA23 = 0.2670     ALPHA
CHEMSHARE'S ETOH DEHYDRATIO -VIR VAP-NRTL LIQ--REBOILED ABSOB
 REBOILED  ABSORBER
FEED STREAMS:
STAGE                        37.         41.
TEMP                      310.97      308.20
FRACV                     0.0         0.0
H                     -2.8042E 05 -7.9823E 05
COMP 1  ETHANOL          191.900     169.200     361.100
COMP 2  WATER             66.600      22.650      89.250
COMP 3  BENZENE            0.0       400.000     400.000
TOTAL                    258.500     591.850     850.350
NUMBER OF STAGES        41

ESTIMATED OVERHEAD PRODUCT RATE    727.0000
ESTIMATED BOTTOMS PRODUCT RATE     123.3496

PRESSURE AT TOP OF COLUMN         759.99097
CONSTANT DELTA P PER STAGE          0.00100
BOILUP RATIO        6.014999
```

```
INITIAL COLUMN PROFILES:
STAGE     TEMP          PRES        LIQUID(MOLS)    VAPOR(MOLS)
   1     352.00       760.040         123.350         727.251
   2     351.65       760.039         850.601         727.251
   3     351.30       760.037         850.601         727.251
   4     350.95       760.036         850.601         727.251
   5     350.60       760.035         850.601         727.251
   6     350.25       760.034         850.601         727.251
   7     349.90       760.032         850.601         727.251
   8     349.55       760.031         850.601         727.251
   9     349.20       760.030         850.601         727.251
  10     348.85       760.029         850.601         727.251
  11     348.50       760.028         850.601         727.251
  12     348.15       760.026         850.601         727.251
  13     347.80       760.025         850.601         727.251
  14     347.45       760.024         850.601         727.251
  15     347.10       760.023         850.601         727.251
  16     346.75       760.021         850.601         727.251
  17     346.40       760.020         850.601         727.251
  18     346.05       760.019         850.601         727.251
  19     345.70       760.018         850.601         727.251
  20     345.35       760.017         850.601         727.251
  21     345.00       760.015         850.601         727.251
  22     344.65       760.014         850.601         727.251
  23     344.30       760.013         850.601         727.251
  24     343.95       760.012         850.601         727.251
  25     343.60       760.010         850.601         727.251
  26     343.25       760.009         850.601         727.251
  27     342.90       760.008         850.601         727.251
  28     342.55       760.007         850.601         727.251
  29     342.20       760.006         850.601         727.251
  30     341.85       760.004         850.601         727.251
  31     341.50       760.003         850.601         727.251
  32     341.15       760.002         850.601         727.251
  33     340.80       760.001         850.601         727.251
  34     340.45       760.000         850.601         727.251
  35     340.10       759.998         850.601         727.251
  36     339.75       759.997         850.601         727.251
  37     339.40       759.996         850.601         727.251
  38     339.05       759.995         592.101         727.251
  39     338.70       759.993         592.101         727.251
  40     338.35       759.992         592.101         727.251
  41     338.00       759.991         592.101         727.000
```

```
1969.    FINAL COLUMN PROFILES:
1970.    STAGE    TEMP        PRES        EFF(%)      LIQUID(MOLS)    VAPOR(MOLS)
1971.      1     351.38     760.040      100.00        123.351        741.948
1972.      2     351.17     760.039      100.00        865.298        742.353
1973.      3     350.54     760.037      100.00        865.703        744.018
1974.      4     348.88     760.036      100.00        867.368        751.055
1975.      5     345.67     760.035      100.00        874.406        771.619
1976.      6     342.47     760.034      100.00        894.970        798.696
1977.      7     341.19     760.032      100.00        922.047        813.115
1978.      8     340.94     760.031      100.00        936.465        817.336
1979.      9     340.90     760.030      100.00        940.687        818.347
1980.     10     340.89     760.029      100.00        941.698        818.580
1981.     11     340.88     760.028      100.00        941.930        818.633
1982.     12     340.88     760.026      100.00        941.983        818.645
1983.     13     340.88     760.025      100.00        941.996        818.647
1984.     14     340.88     760.024      100.00        941.998        818.647
1985.     15     340.88     760.023      100.00        941.998        818.646
1986.     16     340.88     760.021      100.00        941.996        818.644
1987.     17     340.88     760.020      100.00        941.994        818.641
1988.     18     340.88     760.019      100.00        941.992        818.637
1989.     19     340.88     760.018      100.00        941.988        818.630
1990.     20     340.88     760.017      100.00        941.981        818.620
1991.     21     340.88     760.015      100.00        941.971        818.605
1992.     22     340.87     760.014      100.00        941.955        818.581
1993.     23     340.87     760.013      100.00        941.932        818.544
1994.     24     340.86     760.012      100.00        941.895        818.489
1995.     25     340.85     760.010      100.00        941.839        818.404
1996.     26     340.84     760.009      100.00        941.754        818.276
1997.     27     340.81     760.008      100.00        941.626        818.082
1998.     28     340.77     760.007      100.00        941.433        817.794
1999.     29     340.72     760.006      100.00        941.145        817.372
2000.     30     340.64     760.004      100.00        940.722        816.764
2001.     31     340.52     760.003      100.00        940.115        815.920
2002.     32     340.36     760.002      100.00        939.271        814.797
2003.     33     340.15     760.001      100.00        938.147        813.389
2004.     34     339.88     760.000      100.00        936.740        811.756
2005.     35     339.57     759.998      100.00        935.107        810.032
2006.     36     339.24     759.997      100.00        933.383        808.395
2007.     37     338.91     759.996      100.00        931.746        787.088
2008.     38     338.90     759.995      100.00        651.938        790.137
2009.     39     338.92     759.993      100.00        654.988        790.397
2010.     40     338.91     759.992      100.00        655.247        790.364
2011.     41     338.89     759.991      100.00        655.214        727.000
```

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2012.     FINAL VAPOR COMPOSITION PROFILE (MOLE%):
2013.     STAGE   ETHANOL      WATER        BENZENE
2014.        1     99.51968      0.00004       0.48029
2015.        2     98.43357      0.00004       1.56640
2016.        3     95.21686      0.00005       4.78313
2017.        4     86.91057      0.00005      13.08941
2018.        5     71.66200      0.00005      28.33799
2019.        6     56.58866      0.00006      43.41130
2020.        7     49.33349      0.00008      50.66644
2021.        8     47.19740      0.00013      52.80247
2022.        9     46.67717      0.00020      53.32265
2023.       10     46.55664      0.00031      53.44306
2024.       11     46.52892      0.00048      53.47060
2025.       12     46.52235      0.00075      53.47690
2026.       13     46.52052      0.00116      53.47834
2027.       14     46.51964      0.00179      53.47859
2028.       15     46.51862      0.00275      53.47863
2029.       16     46.51721      0.00423      53.47857
2030.       17     46.51511      0.00650      53.47841
2031.       18     46.51191      0.00998      53.47813
2032.       19     46.50694      0.01531      53.47775
2033.       20     46.49943      0.02350      53.47710
2034.       21     46.48779      0.03605      53.47618
2035.       22     46.47005      0.05527      53.47468
2036.       23     46.44288      0.08470      53.47244
2037.       24     46.40131      0.12970      53.46899
2038.       25     46.33787      0.19835      53.46377
2039.       26     46.24136      0.30278      53.45585
2040.       27     46.09514      0.46090      53.44396
2041.       28     45.87480      0.69864      53.42656
2042.       29     45.54641      1.05236      53.40124
2043.       30     45.06384      1.57044      53.36573
2044.       31     44.36955      2.31208      53.31839
2045.       32     43.40048      3.33958      53.25994
2046.       33     42.10356      4.70018      53.19626
2047.       34     40.46110      6.39740      53.14152
2048.       35     38.51941      8.36302      53.11756
2049.       36     36.39984     10.45293      53.14722
2050.       37     34.27486     12.48391      53.24123
2051.       38     33.00119     12.15590      54.84293
2052.       39     32.85823     12.13803      55.00374
2053.       40     32.81119     12.17429      55.01451
2054.       41     32.72498     12.27647      54.99855
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FINAL LIQUID COMPOSITION PROFILE (MOLE%):
STAGE   ETHANOL        WATER         BENZENE
   1     99.86953       0.00003       0.13045
   2     99.56955       0.00004       0.43042
   3     98.63818       0.00004       1.36180
   4     95.87853       0.00005       4.12146
   5     88.73867       0.00005      11.26131
   6     75.54976       0.00005      24.45023
   7     62.37875       0.00006      37.62119
   8     55.99010       0.00008      44.00985
   9     54.10424       0.00011      45.89565
  10     53.64473       0.00018      46.35510
  11     53.53826       0.00027      46.46147
  12     53.51378       0.00043      46.48580
  13     53.50800       0.00066      46.49135
  14     53.50637       0.00101      46.49261
  15     53.50560       0.00156      46.49284
  16     53.50474       0.00240      46.49287
  17     53.50353       0.00368      46.49282
  18     53.50171       0.00565      46.49264
  19     53.49897       0.00867      46.49237
  20     53.49470       0.01331      46.49200
  21     53.48823       0.02043      46.49134
  22     53.47825       0.03133      46.49044
  23     53.46300       0.04804      46.48896
  24     53.43965       0.07361      46.48673
  25     53.40396       0.11271      46.48333
  26     53.34946       0.17237      46.47816
  27     53.26656       0.26312      46.47033
  28     53.14092       0.40052      46.45857
  29     52.95162       0.60708      46.44130
  30     52.66948       0.91437      46.41616
  31     52.25481       1.36439      46.38081
  32     51.65817       2.00845      46.33338
  33     50.82526       2.90048      46.27426
  34     49.71026       4.08126      46.20848
  35     48.29775       5.55352      46.14875
  36     46.62713       7.25781      46.11506
  37     44.80242       9.06910      46.12848
  38     30.84084       4.85619      64.30297
  39     29.32033       4.49602      66.18366
  40     29.14935       4.47749      66.37317
  41     29.09241       4.52085      66.38676
?
```

```
2098.     FINAL VAPOR COMPOSITION PROFILE (MOLES):
2099.     STAGE   ETHANOL      WATER        BENZENE
2100.        1     738.384        0.000          3.564
2101.        2     730.724        0.000         11.628
2102.        3     708.430        0.000         35.587
2103.        4     652.747        0.000         98.309
2104.        5     552.958        0.000        218.661
2105.        6     451.971        0.000        346.724
2106.        7     401.138        0.001        411.976
2107.        8     385.761        0.001        431.574
2108.        9     381.981        0.002        436.364
2109.       10     381.103        0.003        437.474
2110.       11     380.901        0.004        437.728
2111.       12     380.853        0.006        437.786
2112.       13     380.839        0.009        437.799
2113.       14     380.832        0.015        437.801
2114.       15     380.823        0.023        437.801
2115.       16     380.810        0.035        437.799
2116.       17     380.792        0.053        437.796
2117.       18     380.764        0.082        437.792
2118.       19     380.720        0.125        437.785
2119.       20     380.654        0.192        437.774
2120.       21     380.551        0.295        437.759
2121.       22     380.395        0.452        437.734
2122.       23     380.156        0.693        437.696
2123.       24     379.790        1.062        437.638
2124.       25     379.231        1.623        437.550
2125.       26     378.382        2.478        437.416
2126.       27     377.096        3.771        437.216
2127.       28     375.162        5.713        436.919
2128.       29     372.283        8.602        436.487
2129.       30     368.065       12.827        435.872
2130.       31     362.020       18.865        435.035
2131.       32     353.626       27.211        433.960
2132.       33     342.466       38.231        432.693
2133.       34     328.446       51.931        431.380
2134.       35     312.020       67.743        430.270
2135.       36     294.255       84.501        429.640
2136.       37     269.773       98.259        419.055
2137.       38     260.755       96.048        433.334
2138.       39     259.710       95.939        434.748
2139.       40     259.328       96.221        434.815
2140.       41     237.911       89.250        399.839
?
```

```
 2141.      FINAL LIQUID COMPOSITION PROFILE (MOLES):
 2142.      STAGE   ETHANOL        WATER         BENZENE
 2143.        1      123.190         0.000          0.161
 2144.        2      861.574         0.000          3.724
 2145.        3      853.914         0.000         11.789
 2146.        4      831.620         0.000         35.748
 2147.        5      775.937         0.000         98.470
 2148.        6      676.147         0.000        218.822
 2149.        7      575.161         0.001        346.885
 2150.        8      524.328         0.001        412.137
 2151.        9      508.951         0.001        431.734
 2152.       10      505.171         0.002        436.525
 2153.       11      504.293         0.003        437.635
 2154.       12      504.091         0.004        437.888
 2155.       13      504.043         0.006        437.947
 2156.       14      504.029         0.010        437.959
 2157.       15      504.021         0.015        437.961
 2158.       16      504.013         0.023        437.961
 2159.       17      504.000         0.035        437.960
 2160.       18      503.982         0.053        437.957
 2161.       19      503.954         0.082        437.952
 2162.       20      503.910         0.125        437.946
 2163.       21      503.844         0.192        437.935
 2164.       22      503.741         0.295        437.919
 2165.       23      503.585         0.452        437.894
 2166.       24      503.345         0.693        437.856
 2167.       25      502.979         1.062        437.798
 2168.       26      502.421         1.623        437.710
 2169.       27      501.572         2.478        437.577
 2170.       28      500.286         3.771        437.376
 2171.       29      498.352         5.714        437.080
 2172.       30      495.474         8.602        436.647
 2173.       31      491.255        12.827        436.033
 2174.       32      485.210        18.865        435.196
 2175.       33      476.816        27.211        434.121
 2176.       34      465.656        38.231        432.853
 2177.       35      451.636        51.931        431.540
 2178.       36      435.210        67.743        430.430
 2179.       37      417.445        84.501        429.800
 2180.       38      201.063        31.659        419.216
 2181.       39      192.045        29.448        433.495
 2182.       40      191.000        29.339        434.908
?
 2183.       41      190.618        29.621        434.976
?
```

```
STAGE #     1
TEMP, DEG K   351.378
PRES, MMHG   760.0398
 #  NAME              K               VP              FUG             GAM
 1  ETHANOL        0.99649          756.75          1.0008          1.0000
 2  WATER           1.1510          330.58         0.97408          2.7166
 3  BENZENE         3.6817          717.12         0.97205          4.0142
STAGE #     2
TEMP, DEG K   351.169
PRES, MMHG   760.0386
 #  NAME              K               VP              FUG             GAM
 1  ETHANOL        0.98859          750.50          1.0011          1.0000
 2  WATER           1.1464          327.76         0.97428          2.7286
 3  BENZENE         3.6392          712.46         0.97286          3.9906
STAGE #     3
TEMP, DEG K   350.544
PRES, MMHG   760.0374
 #  NAME              K               VP              FUG             GAM
 1  ETHANOL        0.96531          732.05          1.0020          1.0002
 2  WATER           1.1335          319.44         0.97485          2.7665
 3  BENZENE         3.5124          698.65         0.97522          3.9180
STAGE #     4
TEMP, DEG K   348.883
PRES, MMHG   760.0361
 #  NAME              K               VP              FUG             GAM
 1  ETHANOL        0.90646          684.89          1.0040          1.0019
 2  WATER           1.1041          298.21         0.97608          2.8829
 3  BENZENE         3.1759          662.99         0.98124          3.7104
STAGE #     5
TEMP, DEG K   345.675
PRES, MMHG   760.0349
 #  NAME              K               VP              FUG             GAM
 1  ETHANOL        0.80756          600.99          1.0067          1.0144
 2  WATER           1.0785          260.55         0.97737          3.2189
 3  BENZENE         2.5164          598.19         0.99191          3.2233
STAGE #     6
TEMP, DEG K   342.471
PRES, MMHG   760.0337
 #  NAME              K               VP              FUG             GAM
 1  ETHANOL        0.74902          525.99          1.0076          1.0742
 2  WATER           1.1759          227.02         0.97728          4.0284
 3  BENZENE         1.7755          538.57          1.0017          2.5013
STAGE #     7
TEMP, DEG K   341.194
PRES, MMHG   760.0325
 #  NAME              K               VP              FUG             GAM
 1  ETHANOL        0.79087          498.40          1.0069          1.1978
 2  WATER           1.4488          214.72         0.97667          5.2509
 3  BENZENE         1.3467          516.17          1.0059          1.9714
STAGE #     8
TEMP, DEG K   340.941
PRES, MMHG   760.0313
 #  NAME              K               VP              FUG             GAM
 1  ETHANOL        0.84295          493.07          1.0064          1.2911
 2  WATER           1.6631          212.34         0.97641          6.0964
 3  BENZENE         1.1998          511.82          1.0069          1.7694
STAGE #     9
```

```
2422.     STAGE #   35
2423.     TEMP, DEG K   339.571
2424.     PRES, MMHG   759.9983
2425.      #  NAME            K               VP              FUG             GAM
2426.      1  ETHANOL       0.79754         465.07          1.0065          1.2949
2427.      2  WATER          1.5059         199.89         0.98485          5.8136
2428.      3  BENZENE        1.1510         488.76          1.0091          1.7736
2429.     STAGE #   36
2430.     TEMP, DEG K   339.237
2431.     PRES, MMHG   759.9971
2432.      #  NAME            K               VP              FUG             GAM
2433.      1  ETHANOL       0.78066         458.45          1.0064          1.2860
2434.      2  WATER          1.4402         196.95         0.98691          5.6314
2435.      3  BENZENE        1.1525         483.26          1.0095          1.7954
2436.     STAGE #   37
2437.     TEMP, DEG K   338.908
2438.     PRES, MMHG   759.9958
2439.      #  NAME            K               VP              FUG             GAM
2440.      1  ETHANOL       0.76502         452.01          1.0062          1.2784
2441.      2  WATER          1.3765         194.09         0.98888          5.4507
2442.      3  BENZENE        1.1542         477.90          1.0099          1.8175
2443.     STAGE #   38
2444.     TEMP, DEG K   338.900
2445.     PRES, MMHG   759.9946
2446.      #  NAME            K               VP              FUG             GAM
2447.      1  ETHANOL        1.0700         451.85          1.0055          1.7898
2448.      2  WATER          2.5032         194.02         0.98830          9.9211
2449.      3  BENZENE       0.85288         477.77          1.0104          1.3427
2450.     STAGE #   39
2451.     TEMP, DEG K   338.915
2452.     PRES, MMHG   759.9934
2453.      #  NAME            K               VP              FUG             GAM
2454.      1  ETHANOL        1.1207         452.14          1.0055          1.8735
2455.      2  WATER          2.6997         194.15         0.98825          10.694
2456.      3  BENZENE       0.83107         478.02          1.0105          1.3076
2457.     STAGE #   40
2458.     TEMP, DEG K   338.911
2459.     PRES, MMHG   759.9922
2460.      #  NAME            K               VP              FUG             GAM
2461.      1  ETHANOL        1.1256         452.06          1.0054          1.8821
2462.      2  WATER          2.7190         194.11         0.98828          10.772
2463.      3  BENZENE       0.82886         477.95          1.0105          1.3043
2464.     STAGE #   41
2465.     TEMP, DEG K   338.894
2466.     PRES, MMHG   759.9910
2467.      #  NAME            K               VP              FUG             GAM
2468.      1  ETHANOL        1.1249         451.74          1.0054          1.8822
2469.      2  WATER          2.7155         193.97         0.98839          10.765
2470.      3  BENZENE       0.82846         477.68          1.0105          1.3044
?
```

C.3 Inputs

```
    0.1    //CHEMSHRE  JOB  (JA00008-SAI,NJIT,-30,10),'ROCHE-TSAI',
    0.2    //     MSGLEVEL=(1,1),TIME=(3,00)
    0.3    /*PRIORITY +2
11145.     //CHEMS  EXEC  PGM=BAYWAY,REGION=200K
11150.     //STEPLIB  DD  DSN='NCE.AJA00.S008.TEST',UNIT=OLS,DISP=SHR
11151.     //FT06F001 DD  SYSOUT=A
11152.     //FT05F001 DD  *
11153.     CHEMSHARE'S ETOH  DEHYDRATION-VIR VAPOR-UNIQUAC-WITH PRESS DROP
11154.      3 3 2 2 0 0 1
11155.     ETHANOL 0 46.07     516.2     63.0      167.0     64.0
11155.1    0.0878    0.0572    0.248     0.635
11155.2    2.1055    1.9720
11157.     202.06    351.1     0.58                          0.38
11158.     18.9119   -3803.98  -41.68
11159.      WATER  0 18.01     647.3     217.3     56.0      18.84
11160.     0.0279    0.0229    0.229     0.344
11160.1    0.9200    1.4000
11161.     538.7     373.2     1.0                           0.454
11162.     18.3036   -3816.44  -46.13
11163.     BENZENE 0 78.114    562.1     48.3      259.0     92.26
11164.     0.0       0.0       0.544     0.251
11164.01   3.1878    2.4000
11164.1    94.118    353.3     0.41                          0.249
11165.     15.9008   -2788.51  -52.36
11165.1    0.0       0.20      0.15
11165.2    0.20      0.0       0.40
11165.3    0.15      0.40      0.0
11166.     110.010   0.0       200.054   0.0       -156.567  0.0       850.609
11167.     428.452   0.0       1072.790  0.0
11168.      3 041 2 0 050 2 0
11169.     1.0       0.0       0.0
11170.     726.50    0.0       0.00001   338.0     352.0     760.0     45.0
11171.     37        310.97    0.0       191.9     66.6      0.0
11172.     40        308.2     0.0       169.2     22.65     400.0
11175.     /*
?
```

C.3 Results

```
CHEMSHARE'S ETOH  DEHYDRATION-VIR VAPOR-UNIQUAC-WITH PRESS DROP
NUMBER OF COMPONENTS =  3
VAPOR-LIQUID EQUILIBRIUM DATA CODES:
    LIQUID =    3
    VAPOR =     2
    ENTHALPY = 2

NOTE: ALL FLOWS ARE  PER UNIT TIME, AND ENERGY
      VALUES ARE IN UNITS OF K-BTU PER UNIT TIME.
COMPONENT NO                          1         2         3
NAME                             ETHANOL     WATER   BENZENE
MOLECULAR WEIGHT                    46.1      18.0      78.1
CRITICAL PROPERTIES
TEMPERATURE  (DEG K)               516.2     647.3     562.1
PRESSURE      ( ATM)                63.0     217.3      48.3
VOLUME          (CC/GMOL)          167.0      56.0     259.0
 UNIQUAC COMPONT R(I)              2.1055    0.9200    3.1878
 UNIQUAC COMPONT Q(I)              1.9720    1.4000    2.4000
COMPRESSIBILITY                    0.248     0.229     0.544
ACENTRIC FACTOR                    0.635     0.344     0.251
TSONOPOULOS -A-                   0.0878    0.0279    0.0
TSONOPOULOS -B-                   0.0572    0.0229    0.0
AK(1,1)=   0.0
AK(1,2)=   0.200
AK(1,3)=   0.150
AK(2,1)=   0.200
AK(2,2)=   0.0
AK(2,3)=   0.400
AK(3,1)=   0.150
AK(3,2)=   0.400
AK(3,3)=   0.0
VAPOR PRESSURE CONSTANTS
( MMHG AND DEG K)
C(1)                              18.912    18.304    15.901
C(2)                            -3803.98  -3816.44  -2788.51
C(3)                              -41.68    -46.13    -52.36
C(4)                                0.0       0.0       0.0
C(5)                                0.0       0.0       0.0
C(6)                                0.0       0.0       0.0
LIQUID MOLAR VOLUME CONSTANTS
C(1)                              64.000    18.840    92.260
ENTHALPY CONSTANTS (CAL/GM)
LATENT HEAT                        202.1     538.7      94.1
AT DEG K                           351.1     373.2     353.3
LIQUID SP. HEAT CONSTANTS
C(1)                               0.580     1.000     0.410
C(2)                               0.0       0.0       0.0
C(3)                               0.0       0.0       0.0
C(4)                               0.0       0.0       0.0
VAPOR SP. HEAT CONSTANTS
C(1)                               0.380     0.454     0.249
C(2)                               0.0       0.0       0.0
C(3)                               0.0       0.0       0.0
C(4)                               0.0       0.0       0.0
```

```
UNIQUAC PARAMETERS,CAL/G MOL
       A  12 =   110.01    B  12 =     0.0          A  21 =   200.05     B  21 =     0.0
       A  13 =  -156.57    B  13 =     0.0          A  31 =   850.61     B  31 =     0.0
       A  23 =   428.45    B  23 =     0.0          A  32 =  1072.79     B  32 =     0.0
CHEMSHARE'S ETOH  DEHYDRATION-VIR VAPOR-UNIQUAC-WITH PRESS DROP
DISTILLATION COLUMN; PRODUCT RATES & REFLUX RATIO SPECIFIED
FEED STREAMS:
STAGE                        37.        40.
TEMP                      310.97     308.20
FRACV                      0.0        0.0
H                     -2.8042E 05 -7.9823E 05
COMP 1  ETHANOL           191.900    169.200    361.100
COMP 2   WATER             66.600     22.650     89.250
COMP 3  BENZENE             0.0      400.000    400.000
TOTAL                     258.500    591.850    850.350
NUMBER OF STAGES        41

ESTIMATED OVERHEAD PRODUCT RATE    726.5000
ESTIMATED BOTTOMS PRODUCT RATE     123.8496

PRESSURE AT TOP OF COLUMN         760.00000
CONSTANT DELTA P PER STAGE         45.00000
REFLUX RATIO       0.000010
```

```
      ITERATION # =    1
      SUM DT**2 =      0.0
      SUM (DF/F)**2 =  25832.5
                41 0.0              1     2  157.29              3     2  6.2428
      ITERATION # =    2
      SUM DT**2 =        5807.61
      SUM (DF/F)**2 =  15502.5
                 1  24.935          1     2  124.05              1     2  2.4719
      ITERATION # =    3
      SUM DT**2 =        3262.81
      SUM (DF/F)**2 = 0.161315E 07
                 1  22.074          1     2  1269.6              1     2  19.646
      ITERATION # =    4
      SUM DT**2 =        987.885
      SUM (DF/F)**2 =  55108.4
                 1  20.112          4     2  105.67              1     2  99.790
      ITERATION # =    5
      SUM DT**2 =        159.510
      SUM (DF/F)**2 =  30528.0
                27  3.5894         30     2  71.750             27     2  47.668
      ITERATION # =    6
      SUM DT**2 =        49.8170
      SUM (DF/F)**2 =  17994.6
                 4  3.5137         16     2  49.866             16     2  65.588
      ITERATION # =    7
      SUM DT**2 =        21.5095
      SUM (DF/F)**2 =  50.9166
                 6  3.2831          6     2  3.8350              5     2  3.6582
      ITERATION # =    8
      SUM DT**2 =        8.64310
      SUM (DF/F)**2 =  1.74704
                 7  2.1977          8     3 0.63446              7     3 0.63476
      ITERATION # =    9
      SUM DT**2 =      0.721670
      SUM (DF/F)**2 = 0.383326E-01
                 8 0.63337          9     3 0.96522E-01          8     3 0.96553E-0
      ITERATION # =  10
      SUM DT**2 =      0.182898E-02
      SUM (DF/F)**2 = 0.165059E-02
                 9 0.29642E-01      1     3 0.11050E-01          1     3 0.11039E-0
      ITERATION # =  11
      SUM DT**2 =      0.112582E-02
      SUM (DF/F)**2 = 0.104351E-02
                 8 0.20203E-01      1     3 0.87315E-02          1     3 0.87170E-0
      ITERATION # =  12
      SUM DT**2 =      0.761609E-05
      SUM (DF/F)**2 = 0.528009E-07
                 8 0.15828E-02      4     3 0.66723E-04          3     3 0,66613E-0
      REBOILER DUTY    =  7.042080E 06
```

```
REBOILER DUTY     =  7.042080E 06
CONDENSER DUTY    =  2.001900E 04
PRODUCT STREAMS:
STAGE                              1.           41.
TEMP                          385.38        339.09
FRACV                         0.0           1.0000
H                         1.1345E 05    5.8300E 06
COMP 1  ETHANOL              123.788       237.312
COMP 2   WATER                 0.001        89.249
COMP 3  BENZENE                0.061       399.939
TOTAL                        123.850       726.501
```

```
166.      FINAL COLUMN PROFILES:
167.      STAGE     TEMP       PRES          EFF(%)       LIQUID(MOLS)    VAPOR(MOLS)
168.        1     385.38     2560.000       100.00          123.850         781.710
169.        2     384.79     2515.000       100.00          905.560         781.197
170.        3     384.15     2470.000       100.00          905.046         780.870
171.        4     383.38     2425.000       100.00          904.720         781.001
172.        5     382.37     2380.000       100.00          904.851         782.253
173.        6     380.90     2335.000       100.00          906.103         786.189
174.        7     378.76     2290.000       100.00          910.039         795.485
175.        8     376.13     2245.000       100.00          919.335         811.159
176.        9     373.79     2200.000       100.00          935.009         827.830
177.       10     372.25     2155.000       100.00          951.679         838.814
178.       11     371.25     2110.000       100.00          962.664         843.774
179.       12     370.46     2065.000       100.00          967.624         845.399
180.       13     369.72     2020.000       100.00          969.248         845.593
181.       14     369.00     1975.000       100.00          969.442         845.226
182.       15     368.26     1930.000       100.00          969.076         844.644
183.       16     367.52     1885.000       100.00          968.493         843.973
184.       17     366.76     1840.000       100.00          967.822         843.256
185.       18     365.99     1795.000       100.00          967.105         842.513
186.       19     365.20     1750.000       100.00          966.362         841.745
187.       20     364.39     1705.000       100.00          965.594         840.953
188.       21     363.56     1660.000       100.00          964.802         840.132
189.       22     362.71     1615.000       100.00          963.981         839.278
190.       23     361.84     1570.000       100.00          963.127         838.387
191.       24     360.95     1525.000       100.00          962.236         837.447
192.       25     360.03     1480.000       100.00          961.296         836.446
193.       26     359.08     1435.000       100.00          960.296         835.367
194.       27     358.09     1390.000       100.00          959.217         834.185
195.       28     357.07     1345.000       100.00          958.034         832.870
196.       29     355.99     1300.000       100.00          956.719         831.382
197.       30     354.86     1255.000       100.00          955.232         829.673
198.       31     353.67     1210.000       100.00          953.522         827.693
199.       32     352.40     1165.000       100.00          951.542         825.399
200.       33     351.05     1120.000       100.00          949.249         822.777
201.       34     349.61     1075.000       100.00          946.626         819.863
202.       35     348.08     1030.000       100.00          943.712         816.752
203.       36     346.48      985.000       100.00          940.602         813.591
204.       37     344.83      940.000       100.00          937.440         787.305
205.       38     343.46      895.000       100.00          652.655         791.227
206.       39     342.09      850.000       100.00          656.576         791.430
207.       40     340.66      805.000       100.00          656.779         726.508
208.       41     339.09      760.000       100.00            0.007         726.501
```

```
209.      FINAL  VAPOR  COMPOSITION  PROFILE  (MOLE%):
210.      STAGE    ETHANOL          WATER          BENZENE
211.         1      99.86929        0.00062          0.13010
212.         2      99.68407        0.00070          0.31525
213.         3      99.26102        0.00077          0.73825
214.         4      98.30552        0.00084          1.69368
215.         5      96.21408        0.00091          3.78504
216.         6      91.96247        0.00097          8.03659
217.         7      84.55057        0.00103         15.44843
218.         8      74.68391        0.00113         25.31500
219.         9      65.60950        0.00132         34.38920
220.        10      59.84085        0.00170         40.15745
221.        11      56.99171        0.00233         43.00597
222.        12      55.70491        0.00329         44.29179
223.        13      55.08259        0.00470         44.91273
224.        14      54.71482        0.00672         45.27847
225.        15      54.43802        0.00959         45.55241
226.        16      54.19054        0.01367         45.79580
227.        17      53.94911        0.01949         46.03140
228.        18      53.70462        0.02779         46.26762
229.        19      53.45297        0.03964         46.50741
230.        20      53.19155        0.05659         46.75186
231.        21      52.91756        0.08089         47.00156
232.        22      52.62752        0.11573         47.25676
233.        23      52.31689        0.16576         47.51735
234.        24      51.97922        0.23763         47.78315
235.        25      51.60530        0.34084         48.05387
236.        26      51.18252        0.48887         48.32862
237.        27      50.69342        0.70061         48.60598
238.        28      50.11356        1.00200         48.88446
239.        29      49.41057        1.42763         49.16182
240.        30      48.54383        2.02144         49.43473
241.        31      47.46495        2.83509         49.69996
242.        32      46.12267        3.92155         49.95578
243.        33      44.47471        5.32150         50.20381
244.        34      42.50569        7.04216         50.45215
245.        35      40.24881        9.03501         50.71620
246.        36      37.79687       11.18638         51.01677
247.        37      35.29266       13.33579         51.37157
248.        38      33.24677       12.81634         53.93689
249.        39      32.79996       12.60751         54.59253
250.        40      32.66510       12.28474         55.05014
251.        41      32.66511       12.28481         55.05007
```

```
       FINAL LIQUID COMPOSITION PROFILE (MOLE%):
       STAGE   ETHANOL         WATER        BENZENE
          1     99.95022        0.00055        0.04924
          2     99.88037        0.00061        0.11904
          3     99.72048        0.00068        0.27885
          4     99.35535        0.00074        0.64393
          5     98.53062        0.00080        1.46860
          6     96.72476        0.00086        3.27441
          7     93.04956        0.00091        6.94957
          8     86.62514        0.00097       13.37391
          9     78.03063        0.00105       21.96833
         10     70.07853        0.00122       29.92026
         11     65.00105        0.00155       34.99740
         12     62.49012        0.00210       37.50777
         13     61.35857        0.00294       38.63851
         14     60.81460        0.00417       39.18124
         15     60.49599        0.00593       39.49808
         16     60.25806        0.00843       39.73352
         17     60.04629        0.01199       39.94173
         18     59.84013        0.01706       40.14282
         19     59.63149        0.02429       40.34423
         20     59.41682        0.03462       40.54855
         21     59.19386        0.04940       40.75673
         22     58.96019        0.07056       40.96925
         23     58.71282        0.10092       41.18627
         24     58.44779        0.14450       41.40771
         25     58.15963        0.20709       41.63330
         26     57.84036        0.29695       41.86269
         27     57.47918        0.42582       42.09500
         28     57.06109        0.61011       42.32880
         29     56.56503        0.87236       42.56261
         30     55.96324        1.24260       42.79416
         31     55.22082        1.75895       43.02022
         32     54.29627        2.46615       43.23759
         33     53.14563        3.40997       43.44441
         34     51.73271        4.62535       43.64194
         35     50.04452        6.11805       43.83745
         36     48.10973        7.84544       44.04485
         37     46.00824        9.70857       44.28320
         38     32.13780        5.88275       61.97945
         39     29.69117        5.30129       65.00756
         40     29.15386        5.05197       65.79419
         41     31.60366        5.56455       62.83181
```

```
FINAL VAPOR COMPOSITION PROFILE (MOLES):
STAGE    ETHANOL        WATER        BENZENE
   1      780.688        0.005          1.017
   2      778.729        0.005          2.463
   3      775.100        0.006          5.765
   4      767.768        0.007         13.228
   5      752.638        0.007         29.609
   6      722.999        0.008         63.183
   7      672.587        0.008        122.890
   8      605.805        0.009        205.345
   9      543.135        0.011        284.684
  10      501.954        0.014        336.846
  11      480.881        0.020        362.873
  12      470.929        0.028        374.442
  13      465.774        0.040        379.779
  14      462.464        0.057        382.706
  15      459.807        0.081        384.756
  16      457.354        0.115        386.504
  17      454.929        0.164        388.163
  18      452.468        0.234        389.811
  19      449.938        0.334        391.474
  20      447.316        0.476        393.161
  21      444.577        0.680        394.875
  22      441.691        0.971        396.616
  23      438.618        1.390        398.379
  24      435.298        1.990        400.158
  25      431.651        2.851        401.945
  26      427.562        4.084        403.721
  27      422.877        5.844        405.464
  28      417.381        8.345        407.144
  29      410.791       11.869        408.723
  30      402.755       16.771        410.147
  31      392.864       23.466        411.363
  32      380.696       32.368        412.335
  33      365.928       43.784        413.065
  34      348.489       57.736        413.639
  35      328.733       73.794        414.226
  36      307.512       91.011        415.068
  37      277.861      104.993        404.451
  38      263.057      101.406        426.763
  39      259.589       99.780        432.062
  40      237.315       89.250        399.944
  41      237.312       89.249        399.939
```

```
FINAL LIQUID COMPOSITION PROFILE (MOLES):
STAGE    ETHANOL         WATER         BENZENE
   1       123.788         0.001          0.061
   2       904.476         0.006          1.078
   3       902.516         0.006          2.524
   4       898.887         0.007          5.826
   5       891.555         0.007         13.289
   6       876.426         0.008         29.670
   7       846.787         0.008         63.244
   8       796.375         0.009        122.951
   9       729.593         0.010        205.406
  10       666.923         0.012        284.745
  11       625.741         0.015        336.907
  12       604.669         0.020        362.934
  13       594.717         0.029        374.503
  14       589.562         0.040        379.839
  15       586.252         0.057        382.766
  16       583.595         0.082        384.816
  17       581.141         0.116        386.565
  18       578.717         0.165        388.223
  19       576.256         0.235        389.871
  20       573.725         0.334        391.534
  21       571.104         0.477        393.222
  22       568.365         0.680        394.936
  23       565.479         0.972        396.676
  24       562.406         1.390        398.440
  25       559.086         1.991        400.219
  26       555.438         2.852        402.006
  27       551.350         4.085        403.782
  28       546.665         5.845        405.524
  29       541.169         8.346        407.205
  30       534.579        11.870        408.783
  31       526.543        16.772        410.208
  32       516.652        23.467        411.424
  33       504.484        32.369        412.396
  34       489.716        43.785        413.126
  35       472.276        57.737        413.699
  36       452.521        73.794        414.287
  37       431.300        91.012        415.129
  38       209.749        38.394        404.512
  39       194.945        34.807        426.824
  40       191.476        33.180        432.122
  41         0.002         0.000          0.005
STAGE #     1
```

```
STAGE #    1
TEMP, DEG K   385.380
PRES, MMHG  2560.0000
 #  NAME              K                VP             FUG            GAM
 1  ETHANOL      0.99919           2550.8          1.0028        0.99999
 2   WATER        1.1350           1157.4         0.95681         2.6237
 3  BENZENE       2.6421           1858.2         0.96580         3.7688
STAGE #    2
TEMP, DEG K   384.793
PRES, MMHG  2515.0000
 #  NAME              K                VP             FUG            GAM
 1  ETHANOL      0.99804           2503.0          1.0029        0.99999
 2   WATER        1.1353           1135.1         0.95718         2.6281
 3  BENZENE       2.6484           1831.0         0.96609         3.7654
STAGE #    3
TEMP, DEG K   384.148
PRES, MMHG  2470.0000
 #  NAME              K                VP             FUG            GAM
 1  ETHANOL      0.99538           2451.2          1.0030         1.0000
 2   WATER        1.1353           1110.9         0.95761         2.6360
 3  BENZENE       2.6474           1801.4         0.96673         3.7550
STAGE #    4
TEMP, DEG K   383.384
PRES, MMHG  2425.0000
 #  NAME              K                VP             FUG            GAM
 1  ETHANOL      0.98943           2391.1          1.0034         1.0000
 2   WATER        1.1347           1082.9         0.95817         2.6519
 3  BENZENE       2.6302           1766.8         0.96813         3.7290
STAGE #    5
TEMP, DEG K   382.375
PRES, MMHG  2380.0000
 #  NAME              K                VP             FUG            GAM
 1  ETHANOL      0.97649           2313.5          1.0043         1.0002
 2   WATER        1.1327           1046.7         0.95897         2.6857
 3  BENZENE       2.5773           1721.8         0.97114         3.6684
STAGE #    6
TEMP, DEG K   380.903
PRES, MMHG  2335.0000
 #  NAME              K                VP             FUG            GAM
 1  ETHANOL      0.95077           2204.1          1.0061         1.0011
 2   WATER        1.1298           995.75         0.96010         2.7595
 3  BENZENE       2.4544           1657.9         0.97709         3.5379
STAGE #    7
TEMP, DEG K   378.760
PRES, MMHG  2290.0000
 #  NAME              K                VP             FUG            GAM
 1  ETHANOL      0.90865           2052.5          1.0086         1.0052
 2   WATER        1.1327           925.25         0.96133         2.9163
 3  BENZENE       2.2229           1568.0         0.98708         3.2889
STAGE #    8
TEMP, DEG K   376.130
PRES, MMHG  2245.0000
 #  NAME              K                VP             FUG            GAM
 1  ETHANOL      0.86215           1878.2          1.0106         1.0197
 2   WATER        1.1647           844.38         0.96189         3.2193
 3  BENZENE       1.8928           1462.9         0.99963         2.9059
```

```
       STAGE #    34
       TEMP, DEG K    349.608
       PRES, MMHG  1075.0000
         #  NAME              K                  VP               FUG              GAM
         1  ETHANOL       0.82164             705.16           1.0071           1.2437
         2   WATER         1.5225             307.33          0.97993           5.4346
         3  BENZENE        1.1560             678.39           1.0119           1.8103
       STAGE #    35
       TEMP, DEG K    348.082
       PRES, MMHG  1030.0000
         #  NAME              K                  VP               FUG              GAM
         1  ETHANOL       0.80425             663.08           1.0070           1.2406
         2   WATER         1.4768             288.40          0.98265           5.3673
         3  BENZENE        1.1569             646.32           1.0119           1.8221
       STAGE #    36
       TEMP, DEG K    346.484
       PRES, MMHG   985.0000
         #  NAME              K                  VP               FUG              GAM
         1  ETHANOL       0.78563             621.28           1.0068           1.2372
         2   WATER         1.4258             269.64          0.98544           5.2855
         3  BENZENE        1.1583             614.04           1.0118           1.8364
       STAGE #    37
       TEMP, DEG K    344.834
       PRES, MMHG   940.0000
         #  NAME              K                  VP               FUG              GAM
         1  ETHANOL       0.76709             580.49           1.0065           1.2342
         2   WATER         1.3736             251.37          0.98812           5.1984
         3  BENZENE        1.1601             582.06           1.0116           1.8519
       STAGE #    38
       TEMP, DEG K    343.456
       PRES, MMHG   895.0000
         #  NAME              K                  VP               FUG              GAM
         1  ETHANOL        1.0345             548.16           1.0054           1.6799
         2   WATER         2.1786             236.91          0.98756           8.3339
         3  BENZENE       0.87024             556.37           1.0120           1.3833
       STAGE #    39
       TEMP, DEG K    342.091
       PRES, MMHG   850.0000
         #  NAME              K                  VP               FUG              GAM
         1  ETHANOL        1.1047             517.64           1.0052           1.8046
         2   WATER         2.3782             223.29          0.98770           9.1656
         3  BENZENE       0.83978             531.82           1.0115           1.3269
       STAGE #    40
       TEMP, DEG K    340.663
       PRES, MMHG   805.0000
         #  NAME              K                  VP               FUG              GAM
         1  ETHANOL        1.1204             487.28           1.0051           1.8417
         2   WATER         2.4317             209.77          0.98780           9.4469
         3  BENZENE       0.83669             507.07           1.0109           1.3139
       STAGE #    41
       TEMP, DEG K    339.087
       PRES, MMHG   760.0000
         #  NAME              K                  VP               FUG              GAM
         1  ETHANOL        1.0336             455.51           1.0052           1.7156
         2   WATER         2.2077             195.64          0.98833           8.6774
         3  BENZENE       0.87615             480.82           1.0103           1.3708
```

APPENDIX D

THE SOLUTION METHOD OF TWO-LIQUID PHASE FLASH MODEL

D.1 Temperature Determination via the Secant Method for Dew Point, Bubble Point, and the Adiabatic Flash

D.2 Solution Methodology for Single Liquid Phase Isothermal Flash Design Equation

D.3 Wegstein's Algorithm for the Acceleration of Compositional Convergence

D.4 Solution Method of Two-Liquid Phase Systems

D.5 Solution Method of the Two-Liquid Phases Isothermal Flash Design Equation

D.1 Temperature Determination Via the Secant Method for Dew Point, Bubble Point, and the Adiabatic Flash

The Secant method is a variation on Newton's method except that the first derivative of the function is not explicitly evaluated. Expansion of the function, $F(T) = 0.0$, yields

$$F(T) \cong F(T_i) + \frac{F(T_i) - F(T_{i-1})}{T_i - T_{i-1}} (T_{i+1} - T_i) = 0.0 \tag{D1-1}$$

Solving for the value of T_{i+1}, the next estimate of the desired temperature is obtained

$$T_{i+1} = T_i - F(T_i) [\frac{T_i - T_{i-1}}{F(T_i) - F(T_{i-1})} \tag{D1-2}$$

The Secant method is not applicable until two iterations have been completed. For the first iteration, an estimate of the temperature is made, usually the given system temperature. For the second trial, an aribitrary estimate of the temperature is made predicted on the first temperature estimate being either too high or too low

$$T_2 = T_1 \pm 5.0 \tag{D1-3}$$

For the dew point temperature the following relationship is to be solved

$$F(T) = \sum_i \frac{Y_i}{K_i} - 1.0 = 0.0 \tag{D1-4}$$

The estimation of T_2 can be aided by evaluating the data obtained from the first trial. Therefore if

$$F(T_1) > 0.0 \qquad T_2 = T_1 + 5.0 \tag{D1-5A}$$

$$F(T_1) < 0.0 \quad T_2 = T_1 + 5.0 \tag{D1-5B}$$

The bubble point temperature evaluation for the single liquid phase system and the two liquid phase system follow the same procedure except that different functional relationships are used.

Single Liquid Phase

$$F(T) = \sum_i K_i X_i - 1.0 = 0.0 \tag{D1-6}$$

Two Liquid Phases

$$F(T) = \sum_i \frac{Z_i}{W_i}\left(1.0 - \frac{K_{1i}}{K_{2i}}\right) = 0.0 \tag{D1-7}$$

where

$$W_i = R + (1.0 - R)\,\frac{K_{1i}}{K_{2i}} \tag{D1-8}$$

For two liquid phase systems the liquid phase distribution factor, R, is assumed to be constant. In both cases, the estimation of T_2 can be obtained as follows:

$$F(T_1) < 0.0 \quad T_2 = T_1 - 5.0 \tag{D1-9A}$$

$$F(T_1) > 0.0 \quad T_2 = T_1 + 5.0 \tag{D1-9B}$$

For the adiabatic flash calculation an initial temperature is assumed and an isothermal flash is performed including the system enthalpy at the temperature. The enthalpy function used as the design expression is

$$F(T) = H(T) - H_{specified} = 0.0 \tag{D1-10}$$

For the second temperature estimation the following is used:

$$F(T_1) < 0.0 \quad T_2 = T_1 + 10.0 \tag{D1-11A}$$

$$F(T_2) > 0.0 \quad T_2 = T_1 - 10.0 \tag{D1-11B}$$

D.2 Derivation of and the Solution of the Single Liquid Phase Isothermal Flash Design Equation

This appendix covers the derivation of the design equation and its solution.

The relationships governing the two-phase flash are:

Material Balance: $(L + V)Z_i = LX_i + VY_i$ (D2-1A)

Equilibrium Relationship: $Y_i = K_iX_i$ (D2-1B)

Constraints: $X_i = 1.0$ (D2-1C)

$$Y_i = 1.0 \tag{D2-1D}$$

When combined, the desired design equation

$$F = \sum_i (X_i - Y_i) = 0.0 \tag{D2-2}$$

is obtained.

Using the material balance relation and the vapor phase distribution factor, U, the following is obtained:

$$(L + V)Z_i = Lx_i + Vy_i \tag{D2-1A}$$

$$Z_i = \frac{L}{L + V} X_i + \frac{V}{L + V} Y_i \tag{D2-3}$$

$$U = \frac{V}{L + V}, \tag{D2-4A}$$

$$1 - U = \frac{L}{L + V} \tag{D2-4B}$$

$$Z_i = (1 - U)X_i + UY_i \tag{D2-5}$$

Substituting equation (D2-1B)

$$Z_i = [1 + (K_i - 1)U]X_i \qquad \text{(D2-6)}$$

$$W_i = 1 + (K_i - 1)U \qquad \text{(D2-7)}$$

The phase compositions are defined by

$$X_i = \frac{Z_i}{W_i} \qquad \text{(D2-8)}$$

$$Y_i = \frac{Z_i}{W_i} \qquad \text{(D2-9)}$$

The resulting design equation is thus

$$F = \sum_i (X_i - Y_i) = \sum_i \frac{Z_i(1 - K_i)}{W_i} = 0.0 \qquad \text{(D2-10)}$$

The unknown in the design equation (D2-11) is U, the vapor phase distribution factor which has the following range of values

$$0.0 < U < 1.0 \qquad \text{(D2-11)}$$

Solution of the Design Equation

The solution of equation (D2-11) is accomplished by use of Newton's method. Assuming an initial value of U = 0.5 for the vapor phase distribution factor, Newton's method provides the mechanism of evaluating successive values of U. The iterative procedure is repeated until both the function and the correction to the vapor phase distribution factor are essentially zero, that is

$$|F| < \delta_1 = 10^{-5} \qquad \text{(D2-12A)}$$

$$| U| < \delta_2 = 10^{-5} \qquad \text{(D2-12B)}$$

For a given value of $U = U^o$, the next value of U is given by

$$U = U^o + \Delta U \qquad \text{(D2-13A)}$$

$$\Delta U = - \frac{F}{\frac{dF}{du}} \qquad \text{(D2-13B)}$$

where

$$\frac{dF}{du} = -\sum_i \frac{Z_i(1 - K_i)}{W_i{}^2} \bullet \frac{dw_i}{du} = \sum_i \frac{Z_i(1 - K_i)^2}{W_i{}^2} \qquad \text{(D2-14)}$$

evaluated at $U = U^o$.

The initialization of the solution method requires:

- Liquid phase compositions...obtained from the dew point temperature evaluation.
- Vapor phase compositions...obtained from the bubble point temperature evaluation.
- Assume that the flash has $U = 0.5$, as previously mentioned.

With the above initialization data, the equilibrium data can be generated, as well as the function and the associated derivative.

D.3 Acceleration of Compositional Convergence Using the Wegstein Algorithm

In all of the equilibrium calculations encountered in the multicomponent nonideal flash program compositional convergence is essential. Thus, the Wegstein convergence promotion algorithm is used throughout the program. The Wegstein algorithm is, as with the Secant method, a variation of Newton's method except that the function to be solved is:

$$F(Z) = Z \qquad \text{(D3-1)}$$

Expansion of the function into a linearized form yields

$$F(Z) = F(Z_i) + \frac{F(Z_i) - F(Z_{i-1})}{Z_i - Z_{i-1}} (Z_{i+1} - Z_i) = Z_{i+1}) \tag{D3-2}$$

Solving for Z_{i+1}, the next estimate of the component's mole fraction is

$$Z_{i+1} = \frac{f(Z_i) - SZ_i}{1 - S} \tag{D3-3}$$

where

$$S = \frac{F(Z_i) - F(Z_{i-1})}{Z_i - Z_{i-1}} \tag{D3-4}$$

As encountered in the Secant method, the Wegstein algorithm can not be applied until two iterations have passed. For the first iteration, the composition estimation is either based on ideality or a pre-established methodology. The second iteration is initialized via the mode of direct substitution. For the third and subsequent trials the relation described in equation (D3-3) is applied.

D.4 Solution Method of Two Liquid Phase Systems

The solution method of the design equation, Eq. 3-11, is accomplished by use of Newton's method. Assuming an initial value of R = 0.5 for the liquid phase distribution factor, Newton's method provides the means of obtaining successive value of R. The iterative procedure is repeated until both the function and correction to the distribution factor are essentially zero,

$$|\Delta R| < \delta = 10^{-5} \tag{D4-1}$$

For a given value of $R = R^o$, the next value of R is given by

$$R = R^o + \quad R \qquad (D4-2)$$

$$R = - \frac{F}{dF/dR} \qquad (D4-3)$$

where

$$\frac{dF}{dR} = -\sum_i \frac{z_i}{W_i^2} \frac{d \quad i}{dR} = -\sum_i \frac{z_i}{W_i} (1 - \frac{\gamma_{1,i}}{\gamma_{2,i}}) \qquad (D4-4)$$

are evaluated at $R = R^o$. The only requirement is that the liquid phase composition be properly initiated so that the liquid-liquid distribution factor can be properly evaluated.

D.5 Solution Methodology for the Two Liquid Phases Isothermal Flash Design Equation

The design equations as discussed in Chapter 3 are as follow:

$$F_1 = \sum_i (x_{1,i} - y_i) = \sum_i \frac{z_i (1 - K_{1,i})}{\quad_i} = 0.0 \qquad (3-20)$$

and

$$F_2 = \sum_i (x_{1,i} - x_{2,i}) = \sum_i \frac{z_i (1 - \frac{K_{1,i}}{K_{2,i}})}{\quad_i} = 0.0 \qquad (3-21)$$

where

$$W_i = R(1 - U) + (1 - R)(1-U) \frac{K_{1,i}}{K_{2,i}} + U\, K_{1,i} \qquad (3-22)$$

Substituting Eq. 3-22 into Eq. 3-20 and Eq. 3-21, the unknowns in the resulting equations are U and R, the vapor phase and liquid phase distribution factors.

These factors have the following range of values:

$$0.0 < U < 1.0 \qquad \text{(D5-1)}$$

$$0.0 < R < 1.0 \qquad \text{(D5-2)}$$

For a given set of initial values, $U = U^o$ and $R = R^o$, the next set is given by

$$U = U^o + \Delta U \qquad \text{(D5-3)}$$

$$R = R^o + \Delta R \qquad \text{(D5-4)}$$

The values of ΔU and ΔR are obtained by solving simultaneously the following pair of linearized equations:

$$F_1 + \frac{\partial F_1}{\partial U} \Delta U + \frac{\partial F_1}{\partial R} \Delta R = 0 \qquad \text{(D5-5A)}$$

$$F_2 + \frac{\partial F_2}{\partial U} \Delta U + \frac{\partial F_2}{\partial R} \Delta R = 0 \qquad \text{(D5-5B)}$$

in matrix form,

$$\left| \begin{matrix} \frac{\partial F_1}{\partial U} & \frac{\partial F_1}{\partial R} \\ \frac{\partial F_2}{\partial U} & \frac{\partial F_2}{\partial R} \end{matrix} \right| \cdot \left| \begin{matrix} \Delta U \\ \Delta R \end{matrix} \right| = \left| \begin{matrix} -F_1 \\ -F_2 \end{matrix} \right| \qquad \text{(D5-6)}$$

where

$$\frac{\partial F_1}{\partial U} = - \sum_i \frac{Z_i(1 - K_{1,i})}{W_i^2} \frac{\partial W_i}{\partial U} \qquad \text{(D5-7A)}$$

$$\frac{\partial F_1}{\partial R} = - \sum_i \frac{Z_i(1 - K_{1,i})}{W_i^2} \frac{\partial W_i}{\partial R} \qquad \text{(D5-7B)}$$

$$\frac{\partial F_2}{\partial U} = - \sum_i \frac{Z_i(1 - \frac{K_{1,i}}{K_{2,i}})}{W_i^2} \frac{\partial W_i}{\partial U} \tag{D5-7C}$$

$$\frac{\partial F_2}{\partial R} = - \sum_i \frac{Z_i(1 - \frac{K_{1,i}}{K_{2,i}})}{W_i^2} \frac{\partial W_i}{\partial R} \tag{D5-7D}$$

$$\frac{\partial W_i}{\partial U} = R(\frac{K_{1,i}}{K_{2,i}} - 1) - \frac{K_{1,i}}{K_{2,i}} + K_{1,i} \tag{D5-8}$$

$$\frac{\partial W_i}{\partial R} = (1-U)(1 - \frac{K_{1,i}}{K_{2,i}}) \tag{D5-9}$$

The initialization of the solution method requires:

- Liquid phase composition, obtained by an arbitrary positioning of the feed.
- Vapor phase composition, obtained from the bubble point temperature evaluation.
- Assume the isothermal flash has $U = R = 0.5$

Using the above, the vapor liquid equilibrium constant can be generated as well as the functions F_1 and F_2, and the associated derivatives.

APPENDIX E

SAMPLE PROBLEMS OF TWO-LIQUID PHASE FLASH MODEL

E.1 <u>The Research Problem Distillate Flash Example</u>

E.2 a. <u>System--Benzene-Ethyl Acetate-Water</u>

b. <u>System--Benzene-Ethanol-Ethylacetate-Water</u>

E.1 Inputs

```
 1
   1.      //EXXON   JOB  (JA00008-SAI,NJIT,-30,10),'ROCHE-TSAI-CASES',
   1.1     //        MSGLEVEL=(1,1),TIME=(2,30)
   1.2     /*PRIORITY +0
 6000.     //STEP6   EXEC   PGM=EXXON,REGION=100K
 6001.     //STEPLIB   DD   DSN='NCE.AJA00.S008.TEST',UNIT=OLS,DISP=SHR
 6002.     //FT06F001   DD   SYSOUT=A
 6003.     //FT05F001   DD   *
 6004.     CHEMSARE'S BZ-ETOH-WATER*** TWO LIQUID PHASE FLASH- FD @308 DEG K
 6005.      3 1 2 2 0 0 1
 6006.      2         308.      760.
 6007.     31226.5    10968.2   1606.5
 6008.     BENZENE 0 78.114     562.1     48.3      259.0     92.26
 6009.     0.0       0.0        0.544     0.251
 6010.     94.118    353.3      0.41                          0.249
 6011.     15.9008   -2788.51   -52.36
 6012.     ETHANOL 0 46.07      516.2     63.0      167.0     64.0
 6013.     0.0878    0.0572     0.248     0.635
 6014.     202.06    351.1      0.58                          0.38
 6015.     18.9119   -3803.98   -41.68
 6016.     WATER   0 18.01      647.3     217.3     56.0      18.84
 6017.     0.0279    0.0229     0.229     0.344
 6018.     538.7     373.2      1.0                           0.454
 6019.     18.3036   -3816.44   -46.13
 6020.     0.0       0.15       0.40
 6021.     0.15      0.0        0.10
 6022.     0.40      0.10       0.0
 6023.     1096.889  0.0        282.332   0.0       2213.355  0.0       3820.95
 6024.     -86.763   0.0        1289.908  0.0
 6025.     0.295     0.267      0.270
 6026.     /*
 8019.     //
 8020.
 8021.
 8022.
?
```

```
 1 30/81
  30.     COMPONENT NO                         1          2          3
  31.     NAME                           BENZENE    ETHANOL    WATER
  32.     MOLECULAR WEIGHT                  78.1       46.1       18.0
  33.     CRITICAL PROPERTIES
  34.     TEMPERATURE  (DEG K)             562.1      516.2      647.3
  35.     PRESSURE     ( ATM)               48.3       63.0      217.3
  36.     VOLUME          (CC/GMOL)        259.0      167.0       56.0
  37.     COMPRESSIBILITY                  0.544      0.248      0.229
  38.     ACENTRIC FACTOR                  0.251      0.635      0.344
  39.     TSONOPOULOS -A-                0.0        0.0878     0.0279
  40.     TSONOPOULOS -B-                0.0        0.0572     0.0229
  41.     AK(1,1)=   0.0
  42.     AK(1,2)=   0.150
  43.     AK(1,3)=   0.400
  44.     AK(2,1)=   0.150
  45.     AK(2,2)=   0.0
  46.     AK(2,3)=   0.100
  47.     AK(3,1)=   0.400
  48.     AK(3,2)=   0.100
  49.     AK(3,3)=   0.0
  50.     VAPOR PRESSURE CONSTANTS
  51.     ( MMHG AND DEG K)
  52.     C(1)                            15.901     18.912     18.304
  53.     C(2)                          -2788.51   -3803.98   -3816.44
  54.     C(3)                            -52.36     -41.68     -46.13
  55.     C(4)                             0.0        0.0        0.0
  56.     C(5)                             0.0        0.0        0.0
  57.     C(6)                             0.0        0.0        0.0
  58.     LIQUID MOLAR VOLUME CONSTANTS
  59.     C(1)                            92.260     64.000     18.840
  60.     ENTHALPY CONSTANTS (CAL/GM)
  61.     LATENT HEAT                       94.1      202.1      538.7
  62.     AT DEG K                         353.3      351.1      373.2
  63.     LIQUID SP. HEAT CONSTANTS
  64.     C(1)                            0.410      0.580      1.000
  65.     C(2)                            0.0        0.0        0.0
  66.     C(3)                            0.0        0.0        0.0
  67.     C(4)                            0.0        0.0        0.0
  68.     VAPOR SP. HEAT CONSTANTS
  69.     C(1)                            0.249      0.380      0.454
  70.     C(2)                            0.0        0.0        0.0
  71.     C(3)                            0.0        0.0        0.0
  72.     C(4)                            0.0        0.0        0.0
  73.       NRTL CONSTANTS, CAL/GMOL
  74.     UNIQUAC PARAMETERS,CAL/G MOL
  75.             A  12 =  1096.89     B  12 =      0.0          A  21 =    282.33     B  21 =      0.0
  76.             A  13 =  2213.35     B  13 =      0.0          A  31 =   3820.95     B  31 =      0.0
  77.             A  23 =   -86.76     B  23 =      0.0          A  32 =   1289.91     B  32 =      0.0
  78.             ALPHA12 = 0.2950     ALPHA13 = 0.2670     ALPHA23 = 0.2700      ALPHA
  79.     FEED =  43801. LBS   =  727.03 MOLES       PRESS =  760.00 MMHG       TEMP =  308.00 DEG K
  80.                           BENZENE   ETHANOL   WATER
  81.     FEED MOLEFRACTIONS      0.54985   0.32746   0.12269
```

```
 1 82/100
  82.     RESULTS OF DEW POINT CALCULATION
  83.     DEW POINT OF FEED AT 760.00 MMHG IS 338.89 DEG K
  84.                               BENZENE   ETHANOL   WATER
  85.     DEW PT LIQ MOLE FRAC       0.67180   0.28479   0.04341
  86.
  87.     'VLE' DATA FOR VAPOR AND LIQUID PHASE #  1
  88.
  89.                               BENZENE   ETHANOL   WATER
  90.     VAP MOLE FRAC              0.54985   0.32746   0.12269
  91.     LIQ MOLE FRAC              0.67180   0.28479   0.04341
  92.     VALUES OF K=Y/X            0.81846   1.14986   2.82611
  93.     VAPOR PRESSURES            477.577   451.617   193.915
  94.     FUGACITY FACTORS           1.00954   1.00739   0.99498
  95.     ACTIVITY COEFFICIENTS       1.2902    1.9208   11.1321
  96.     ACTIVITY                    0.8667    0.5470    0.4833
  97.
  98.
  99.
 100.
? 1 118/133
 118.     TWOLIQ CALCULATION TERMINATED
 119.     CALCULATION CONTINUING
 120.
 121.
 122.
 123.     TWOLIQ CALCULATION TERMINATED
 124.     CALCULATION CONTINUING
 125.
 126.
 127.
 128.     TWOLIQ CALCULATION TERMINATED
 129.     CALCULATION CONTINUING
 130.
 131.
 132.
 133.     TWO LIQ PHASE REGION, LIQUID PHASE MOLE RATIO    0.423069
?
```

```
1 133/164
133.     TWO LIQ PHASE REGION, LIQUID PHASE MOLE RATIO    0.423069
134.     BUBBLE POINT OF FEED AT 760.00 MMHG IS 337.85 DEG K
135.                              BENZENE   ETHANOL   WATER
136.     BUB PT VAP MOLE FRAC      0.53936   0.27362   0.18701
137.
138.     'VLE' DATA FOR VAPOR AND LIQUID PHASE #  1
139.
140.                              BENZENE   ETHANOL   WATER
141.     VAP MOLE FRAC             0.53936   0.27362   0.18701
142.     LIQ MOLE FRAC             0.64933   0.26810   0.08257
143.     VALUES OF K=Y/X           0.83065   1.02059   2.26494
144.     VAPOR PRESSURES           460.977   431.810   185.127
145.     FUGACITY FACTORS          1.00960   1.00829   0.99997
146.     ACTIVITY COEFFICIENTS      1.3564    1.7815    9.2985
147.     ACTIVITY                   0.8808    0.4776    0.7678
148.
149.     'VLE' DATA FOR VAPOR AND LIQUID PHASE #  2
150.
151.                              BENZENE   ETHANOL   WATER
152.     VAP MOLE FRAC             0.53936   0.27362   0.18701
153.     LIQ MOLE FRAC             0.47689   0.37099   0.15211
154.     VALUES OF K=Y/X           1.13106   0.73750   1.22928
155.     VAPOR PRESSURES           460.977   431.810   185.127
156.     FUGACITY FACTORS          1.00960   1.00829   0.99997
157.     ACTIVITY COEFFICIENTS      1.8470    1.2873    5.0467
158.     ACTIVITY                   0.8808    0.4776    0.7677
159.     FEED AT OR BELOW BUBBLE POINT
160.     TWOLIQ CALCULATION TERMINATED
161.     CALCULATION CONTINUING
162.
163.
164.
?
```

```
1 164/189
164.
165.      TWO LIQ PHASE REGION, LIQUID PHASE MOLE RATIO    0.404562
166.
167.      'VLE' DATA FOR VAPOR AND LIQUID PHASE #  1
168.
169.                                BENZENE   ETHANOL   WATER
170.      VAP MOLE FRAC              0.0       0.0       0.0
171.      LIQ MOLE FRAC              0.77289   0.18548   0.04163
172.      VALUES OF K=Y/X            0.0       0.0       0.0
173.      VAPOR PRESSURES              0.0       0.0       0.0
174.      FUGACITY FACTORS           1.00960   1.00829   0.99997
175.      ACTIVITY COEFFICIENTS       1.1660    2.7285   17.8293
176.      ACTIVITY                    0.9012    0.5061    0.7423
177.
178.      'VLE' DATA FOR VAPOR AND LIQUID PHASE #  2
179.
180.                                BENZENE   ETHANOL   WATER
181.      VAP MOLE FRAC              0.0       0.0       0.0
182.      LIQ MOLE FRAC              0.39830   0.42394   0.17777
183.      VALUES OF K=Y/X            0.0       0.0       0.0
184.      VAPOR PRESSURES              0.0       0.0       0.0
185.      FUGACITY FACTORS           1.00960   1.00829   0.99997
186.      ACTIVITY COEFFICIENTS       2.2628    1.1937    4.1758
187.      ACTIVITY                    0.9013    0.5060    0.7423
188.      IDEAL LIQ ENTHALPY =  -0.138381E 04     DELTA H =   0.250980E 00
189.      IDEAL LIQ ENTHALPY =  -0.127482E 04     DELTA H =   0.173376E 03
?
```

E.2.a Inputs

```
   1.      //EDWARD  JOB  (JA00008-SAI,NJIT,-30,10),'ROCHE-TSAI-CASES',
   1.1     //        MSGLEVEL=(1,1),TIME=(2,30)
   1.2     /*PRIORITY +0
6000.      //STEP4   EXEC   PGM=EDWARD,REGION=100K
6001.      //STEPLIB   DD   DSN='NCE.AJA00.S008.TEST',UNIT=OLS,DISP=SHR
6002.      //FT06F001   DD   SYSOUT=A
6003.      //FT05F001   DD   *
6004.       BZ-ETAC-WTR ***  TWO LIQUID PHASE TEST  ---- TEST CASE #1
6005.      3 2 1 2 0 1 0 0 0 0 176.0     175.0     14.696
6006.       BZ        78.114   1011.8    710.      4.152     1.414     .42748    .08664
6007.      169.8     .45684    .00135    .00000148 .46295  -.00031304.000000961
6008.      5.192     -2179.9                                 365.42
6009.       ETAC    0 88.107   341.28    555.51    4.576     1.565     .42748    .08864
6010.      157.45    0.35                          0.5
6011.      5.30095   -2181.42                                302.17
6012.       WATER    18.016    1165.1    3918.7    .8977     .289      .42748    .08864
6013.      992.6     .94776    .0001795  .000000908 .19203   .00017491 .000000027
6014.       6.23553  -2983.444                               376.636
6015.       201.0    -119.12   1736.38   4001.43   -455.96   2599.45
6016.      0.3       0.2       0.082
6017.      78.114    88.107    18.016
6018.      /*
7000.      //STEP5   EXEC   PGM=EDWARD,REGION=100K
7001.      //STEPLIB   DD   DSN='NCE.AJA00.S008.TEST',UNIT=OLS,DISP=SHR
7002.      //FT06F001   DD   SYSOUT=A
7003.      //FT05F001   DD   *
7004.       BZ- ETOH - ETAC - WTR *** TEST CASE #2
7005.      4 2 1 2 0 1 0 0 0 0 176.0     160.0     14.696
7006.       BZ        78.114   1011.8    710.      4.152     1.414     .42748    .08664
7007.      169.8     .45684    .00135    .00000148 .46295  -.00031304.000000961
7008.      5.192     -2179.9                                 365.42
7009.       ETOH      46.069   923.4     892.05    2.673     0.943     .42748    .08664
7010.      362.0     0.35                          0.5
7011.      6.4982    -2973.06                                384.64
7012.       ETAC    0 88.107   341.28    555.51    4.576     1.565     .42748    .08864
7013.      157.45    0.35                          0.5
7014.      5.30095   -2181.42                                302.17
7015.       WATER    18.016    1165.1    3918.7    .8977     .289      .42748    .08864
7016.      992.6     .94776    .0001795  .000000908 .19203   .00017491 .000000027
7017.       6.23553  -2983.444                               376.636
7018.      1192.8    561.86    201.0     -119.12   1736.38   4001.43   1064.2    -43.04
7019.      323.3     358.73    -455.96   2599.45
7020.      0.47      0.3       0.2       0.3       0.3       0.082
7021.      78.114    46.069    88.107    18.016
7022.      /*
?
```

E.2.b Inputs

```
 BZ-ETAC-WTR ***  TWO LIQUID PHASE TEST  ---- TEST CASE #1
COMPONENT NO                         1          2          3
NAME                                BZ        ETAC       WATER
COMPOSITION TYPE                     1          1          1
MOLECULAR WEIGHT                    78.1       88.1       18.0
CRITICAL PROPERTIES
TEMPERATURE  (DEG R)              1011.8      341.3     1165.1
PRESSURE     (PSIA)                710.0      555.5     3918.7
VOLUME       (CFT/LBMOL)             4.2        4.6        0.9
VAPOR PRESSURE CONSTANTS
(PSIA AND DEG F)
C(1)                              5.1920     5.3009     6.2355
C(2)                             -2179.9    -2181.4    -2983.4
C(3)                                 0.0        0.0        0.0
C(4)                                 0.0        0.0        0.0
C(5)                                 0.0        0.0        0.0
C(6)                               365.4      302.2      376.6
LIQUID MOLAR VOLUME CONSTANTS
C(1)                              1.4140     1.5650     0.2890
C(2)                              0.0        0.0        0.0
C(3)                              0.0        0.0        0.0
ENTHALPY CONSTANTS (BTU/LB)
LATENT HEAT AT  176.0 DEG F        169.8      157.4      992.6
LIQUID SP. HEAT CONSTANTS
C(1)                              0.4568     0.3500     0.9478
C(2)                              0.0013     0.0        0.0002
C(3)                              0.0000     0.0        0.0000
VAPOR SP. HEAT CONSTANTS
C(1)                              0.4629     0.5000     0.1920
C(2)                             -0.0003     0.0        0.0002
C(3)                              0.0000     0.0        0.0000
 RENON CONSTANTS, CAL/GMOL
A12 =    201.     A21 =  -119.         A13 =  1736.     A31 =  4001.          A23 =  -456.     A32 =  2599.
ALPHA12 = 0.3000    ALPHA13 = 0.2000    ALPHA23 = 0.0820    ALPHA
FEED =    184. LBS    =    3.00 MOLES       PRESS =   14.70 PSIA        TEMP =  175.00 DEG F
                             BZ        ETAC       WATER
FEED MOLEFRACTIONS       0.33333   0.33333   0.33333
RESULTS OF DEW POINT CALCULATION
DEW POINT OF FEED AT  14.70 PSIA IS 188.28 DEG F
                             BZ        ETAC       WATER
DEW PT LIQ MOLE FRAC     0.24285   0.69450   0.06265

'VLE' DATA FOR VAPOR AND LIQUID PHASE #  1

                             BZ        ETAC       WATER
VAP MOLE FRAC            0.33333   0.33333   0.33333
LIQ MOLE FRAC            0.24285   0.69450   0.06265
VALUES OF K=Y/X          1.37260   0.47996   5.32015
VAPOR PRESSURES           17.990     7.131     9.002
FUGACITY FACTORS         0.98933   0.99967   1.00249
ACTIVITY COEFFICIENTS     1.1333    0.9894    8.6640
ACTIVITY                  0.2752    0.6872    0.5428
```

```
RESULTS OF BUBBLE POINT CALCULATION
TWO LIQ PHASE REGION, LIQUID PHASE MOLE RATIO    0.718023
BUBBLE POINT OF FEED AT  14.70 PSIA IS 169.44 DEG F
                             BZ        ETAC      WATER
BUB PT VAP MOLE FRAC     0.46580   0.13969   0.39452

'VLE' DATA FOR VAPOR AND LIQUID PHASE #  1

                             BZ        ETAC      WATER
VAP MOLE FRAC            0.46580   0.13969   0.39452
LIQ MOLE FRAC            0.46397   0.45401   0.08202
VALUES OF K=Y/X          1.00395   0.30767   4.81016
VAPOR PRESSURES           13.073     4.737     5.918
FUGACITY FACTORS         1.00069   0.99803   1.00334
ACTIVITY COEFFICIENTS     1.1278    0.9564   11.9059
ACTIVITY                  0.5233    0.4342    0.9765

'VLE' DATA FOR VAPOR AND LIQUID PHASE #  2

                             BZ        ETAC      WATER
VAP MOLE FRAC            0.46580   0.13969   0.39452
LIQ MOLE FRAC            0.00069   0.02603   0.97328
VALUES OF K=Y/X        675.17114   5.36557   0.40535
VAPOR PRESSURES           13.073     4.737     5.918
FUGACITY FACTORS         1.00069   0.99803   1.00334
ACTIVITY COEFFICIENTS   758.4580   16.6786    1.0033
ACTIVITY                  0.5232    0.4342    0.9765
RESULTS OF ISOTHERMAL FLASH CALCULATION


    LIQUID HAS GONE TO A ONE PHASE SYSTEM


SYSTEM IS IN THE V/L PHASE REGION AT 175.00 DEG F AND  14.70 PSIA.    VAPOR/FEED MOLE RATIO = 0.667825

'VLE' DATA FOR VAPOR AND LIQUID PHASE #  1

                             BZ        ETAC      WATER
VAP MOLE FRAC            0.35124   0.20779   0.44098
LIQ MOLE FRAC            0.29734   0.58574   0.11692
VALUES OF K=Y/X          1.18125   0.35474   3.77173
VAPOR PRESSURES           14.397     5.363     6.717
FUGACITY FACTORS         0.99669   0.99948   1.00355
ACTIVITY COEFFICIENTS     1.2098    0.9727    8.2230
ACTIVITY                  0.3597    0.5697    0.9614
IDEAL LIQ ENTHALPY =  -0.373583E 02     DELTA H =   0.0
IDEAL VAP ENTHALPY =   0.154041E 05     DELTA H =  -0.345228E 02
ENTHALPY OF VAPOR PHASE/LBMOL OF FEED  =  10287.26 BTU
ENTHALPY OF LIQUID PHASE/LBMOL OF FEED =    -12.41 BTU
ENTHALPY OF SYSTEM WITH REFERENCE TO PURE LIQUID AT 176.00 DEG F   10274.85 BTU/LBMOL
```

```
163.     BZ- ETOH - ETAC - WTR *** TEST CASE #2
164.    COMPONENT NO                          1         2         3         4
165.    NAME                                 BZ       ETOH      ETAC      WATER
166.    COMPOSITION TYPE                      1         1         1         1
167.    MOLECULAR WEIGHT                     78.1      46.1      88.1      18.0
168.    CRITICAL PROPERTIES
169.    TEMPERATURE  (DEG R)               1011.8     923.4     341.3    1165.1
170.    PRESSURE     (PSIA)                 710.0     892.0     555.5    3918.7
171.    VOLUME       (CFT/LBMOL)              4.2       2.7       4.6       0.9
172.    VAPOR PRESSURE CONSTANTS
173.    (PSIA AND DEG F)
174.    C(1)                               5.1920    6.4982    5.3009    6.2355
175.    C(2)                              -2179.9   -2973.1   -2181.4   -2983.4
176.    C(3)                                  0.0       0.0       0.0       0.0
177.    C(4)                                  0.0       0.0       0.0       0.0
178.    C(5)                                  0.0       0.0       0.0       0.0
179.    C(6)                                365.4     384.6     302.2     376.6
180.    LIQUID MOLAR VOLUME CONSTANTS
181.    C(1)                               1.4140    0.9430    1.5650    0.2890
182.    C(2)                               0.0       0.0       0.0       0.0
183.    C(3)                               0.0       0.0       0.0       0.0
184.    ENTHALPY CONSTANTS (BTU/LB)
185.    LATENT HEAT AT  176.0 DEG F         169.8     362.0     157.4     992.6
186.    LIQUID SP. HEAT CONSTANTS
187.    C(1)                               0.4568    0.3500    0.3500    0.9478
188.    C(2)                               0.0013    0.0       0.0       0.0002
189.    C(3)                               0.0000    0.0       0.0       0.0000
190.    VAPOR SP. HEAT CONSTANTS
191.    C(1)                               0.4629    0.5000    0.5000    0.1920
192.    C(2)                              -0.0003    0.0       0.0       0.0002
193.    C(3)                               0.0000    0.0       0.0       0.0000
194.     RENON CONSTANTS, CAL/GMOL
195.    A12 =  1193.     A21 =   562.          A13 =   201.     A31 =  -119.          A14 =  1736.     A41 =  4001.
196.    A23 =  1064.     A32 =   -43.          A24 =   323.     A42 =   359.          A34 =  -456.     A43 =  2599.
197.    ALPHA12 = 0.4700     ALPHA13 = 0.3000     ALPHA14 = 0.2000     ALPHA23 = 0.3000     ALPHA24 = 0.3000     ALPHA34 = 0.0820
198.    FEED =     230. LBS    =     4.00 MOLES         PRESS =     14.70 PSIA         TEMP =  160.00 DEG F
199.                                    BZ        ETOH      ETAC      WATER
200.    FEED MOLEFRACTIONS        0.25000   0.25000   0.25000   0.25000
201.    RESULTS OF DEW POINT CALCULATION
202.    DEW POINT OF FEED AT  14.70 PSIA IS 178.83 DEG F
203.                                    BZ        ETOH      ETAC      WATER
204.    DEW PT LIQ MOLE FRAC      0.19634   0.10190   0.63309   0.06867
205.
206.    'VLE' DATA FOR VAPOR AND LIQUID PHASE #  1
207.
208.                                    BZ        ETOH      ETAC      WATER
209.    VAP MOLE FRAC             0.25000   0.25000   0.25000   0.25000
210.    LIQ MOLE FRAC             0.19634   0.10190   0.63309   0.06867
211.    VALUES OF K=Y/X           1.27332   2.45328   0.39489   3.64068
212.    VAPOR PRESSURES            15.370    16.667     5.831     7.319
213.    FUGACITY FACTORS          0.99509   0.99697   0.99910   1.00310
214.    ACTIVITY COEFFICIENTS      1.2235    2.1697    0.9961    7.2873
215.    ACTIVITY                   0.2402    0.2211    0.6306    0.5004
216.
  ?
```

```
217.
218.
219.
220.     RESULTS OF BUBBLE POINT CALCULATION
221.     TWO LIQ PHASE REGION, LIQUID PHASE MOLE RATIO    0.739141
222.     BUBBLE POINT OF FEED AT  14.70 PSIA IS 159.48 DEG F
223.                                   BZ         ETOH       ETAC       WATER
224.     BUB PT VAP MOLE FRAC      0.36602    0.31140    0.08105    0.24153
225.
226.     'VLE' DATA FOR VAPOR AND LIQUID PHASE #  1
227.
228.                                   BZ         ETOH       ETAC       WATER
229.     VAP MOLE FRAC             0.36602    0.31140    0.08105    0.24153
230.     LIQ MOLE FRAC             0.33484    0.23401    0.32336    0.10779
231.     VALUES OF K=Y/X           1.09309    1.33071    0.25066    2.24087
232.     VAPOR PRESSURES            10.940     10.820      3.764      4.684
233.     FUGACITY FACTORS          1.00613    1.00508    0.99674    1.00338
234.     ACTIVITY COEFFICIENTS      1.4594     1.7982     0.9818     7.0069
235.     ACTIVITY                   0.4887     0.4208     0.3175     0.7552
236.
237.     'VLE' DATA FOR VAPOR AND LIQUID PHASE #  2
238.
239.                                   BZ         ETOH       ETAC       WATER
240.     VAP MOLE FRAC             0.36602    0.31140    0.08105    0.24153
241.     LIQ MOLE FRAC             0.00959    0.29531    0.04213    0.65297
242.     VALUES OF K=Y/X          38.15723    1.05449    1.92375    0.36990
243.     VAPOR PRESSURES            10.940     10.820      3.764      4.684
244.     FUGACITY FACTORS          1.00613    1.00508    0.99674    1.00338
245.     ACTIVITY COEFFICIENTS     50.9438     1.4250     7.5348     1.1566
246.     ACTIVITY                   0.4887     0.4208     0.3175     0.7553
247.     RESULTS OF ISOTHERMAL FLASH CALCULATION
?
```

```
SYSTEM IS IN THE V/L PHASE REGION AT 160.00 DEG F AND  14.70 PSIA.    VAPOR/FEED MOLE RATIO = 0.056955
TWO LIQ PHASE REGION, LIQUID PHASE MOLE RATIO    0.745013

'VLE' DATA FOR VAPOR AND LIQUID PHASE #  1

                             BZ        ETOH       ETAC       WATER
VAP MOLE FRAC              0.35853   0.31080    0.08521    0.24546
LIQ MOLE FRAC              0.32364   0.23156    0.33399    0.11080
VALUES OF K=Y/X            1.10781   1.34217    0.25513    2.21525
VAPOR PRESSURES             11.044    10.951      3.811      4.742
FUGACITY FACTORS           1.00582   1.00488    0.99687    1.00342
ACTIVITY COEFFICIENTS       1.4656    1.7925     0.9870     6.8413
ACTIVITY                    0.4743    0.4151     0.3297     0.7581

'VLE' DATA FOR VAPOR AND LIQUID PHASE #  2

                             BZ        ETOH       ETAC       WATER
VAP MOLE FRAC              0.35853   0.31080    0.08521    0.24546
LIQ MOLE FRAC              0.00913   0.28947    0.04362    0.65778
VALUES OF K=Y/X           39.25723   1.07366    1.95357    0.37317
VAPOR PRESSURES             11.044    10.951      3.811      4.742
FUGACITY FACTORS           1.00582   1.00488    0.99687    1.00342
ACTIVITY COEFFICIENTS      51.9362    1.4339     7.5577     1.1525
ACTIVITY                    0.4743    0.4151     0.3297     0.7581
IDEAL LIQ ENTHALPY =  -0.550023E 03     DELTA H =   0.0
IDEAL LIQ ENTHALPY =  -0.294764E 03     DELTA H =   0.0
IDEAL VAP ENTHALPY =   0.151238E 05     DELTA H =  -0.511989E 02
ENTHALPY OF VAPOR PHASE/LBMOL OF FEED  =    861.37 BTU
ENTHALPY OF LIQUID PHASE/LBMOL OF FEED =   -386.44 BTU
ENTHALPY OF LIQUID PHASE/LBMOL OF FEED =    -70.88 BTU
ENTHALPY OF SYSTEM WITH REFERENCE TO PURE LIQUID AT 176.00 DEG F     404.06 BTU/LBMOL
```

APPENDIX F

RESEARCH PROBLEM COMPUTER INPUTS AND RESULTS USING THE COMPLETE MODEL

F.1 The Combined Model

F.2 The Benzxene Stripping Column

F.3 The Ethanol Recovery/Water Purge Column

F.1 Inputs

```
//FINAL2  JOB  (JA00008,NJIT,15000,30,0),'RCOHE-TSAI-FINAL2',
//         REGION=280K,TIME=(4,30)
//*PASSWORD SAI
//*MAIN  CLASS=+2,REPORT=YES,FAILURE=RESTART
//*FORMAT PR,DDNAME=,DEST=RMT20,COPIES=1
//STEP5  EXEC  PGM=FINAL2,REGION=280K
//STEPLIB  DD  DSN='NCE.AJA00.S008.TEST',UNIT=OLS,DISP=SHR
//FT06F001 DD  SYSOUT=A
//FT05F001 DD  *
COMPLETE AZEOTROPIC DISTILLATION MODEL-ETOH DEHYDRATION-REB ABS
 3 1 2 2 0 0 1
 2        308.0       760.0
0.77289   0.18548     0.04163
0.39830   0.42394     0.17777
BENZENE 0 78.114    562.1     48.3      259.0     92.26
0.0       0.0       0.544     0.251
94.118    353.3     0.41                          0.249
15.9008   -2788.51  -52.36
ETHANOL 0 46.07     516.2     63.0      167.0     64.0
0.0878    0.0572    0.248     0.635
202.06    351.1     0.58                          0.38
18.9119   -3803.98  -41.68
WATER   0 18.01     647.3     217.3     56.0      18.84
0.0279    0.0229    0.229     0.344
538.7     373.2     1.0                           0.454
18.3036   -3816.44  -46.13
0.0       0.15      0.40
0.15      0.0       0.20
0.40      0.20      0.0
1096.889  0.0       282.332   0.0       2213.335  0.0       3820.95
-86.763   0.0       1289.908  0.0
0.295     0.267     0.270
 5 041 2 0 020 2 0
1.0       0.0       0.0
727.00    0.0       6.015     338.0     352.0     760.0     0.001
41        308.2     0.0       400.0     169.2     22.65
37        310.97    0.0       0.0       191.9     66.6
/*
//
?
```

F.1 Results

```
COMPLETE AZEOTROPIC DISTILLATION MODEL-ETOH DEHYDRATION-REB ABS
 REBOILED  ABSORBER
FEED STREAMS:
STAGE                        41.         37.
TEMP                      308.20      310.97
FRACV                     0.0         0.0
H                    -7.9823E 05 -2.8042E 05
COMP 1  BENZENE          400.000       0.0         400.000
COMP 2  ETHANOL          169.200     191.900     361.100
COMP 3  WATER             22.650      66.600      89.250
TOTAL                    591.850     258.500     850.350
NUMBER OF STAGES       41

ESTIMATED OVERHEAD PRODUCT RATE    727.0000
ESTIMATED BOTTOMS PRODUCT RATE     123.3496

PRESSURE AT TOP OF COLUMN         759.99097
CONSTANT DELTA P PER STAGE          0.00100
BOILUP RATIO       6.014999
  TRIAL # =     1

*************************************************************************


ITERATION # =    1
SUM DT**2 =     0.0
SUM (DF/F)**2 =  81754.1
       41 0.0                26    3  46.322            25    3  56.931
ITERATION # =    2
SUM DT**2 =      793.034
SUM (DF/F)**2 =  134860.
        4  8.6276            24    3  62.298            23    3  82.182
ITERATION # =    3
SUM DT**2 =      41.5678
SUM (DF/F)**2 =  9769.94
        1  3.1751             1    3  57.191             2    3  29.796
ITERATION # =    4
SUM DT**2 =      25.0274
SUM (DF/F)**2 =  8429.71
        2  4.1163             1    1  15.082             1    3  89.586
ITERATION # =    5
SUM DT**2 =      33.3969
SUM (DF/F)**2 =  71.1272
        3  4.8819             3    1  5.1586             2    1  5.2222
ITERATION # =    6
SUM DT**2 =      24.1685
SUM (DF/F)**2 =  6.29141
        4  4.3304             5    1  1.3458             4    1  1.3477
ITERATION # =    7
SUM DT**2 =      5.21764
SUM (DF/F)**2 = 0.308386
```

```
201.     FINAL COLUMN PROFILES:
202.     STAGE    TEMP        PRES          EFF(%)      LIQUID(MOLS)   VAPOR(MOLS)
203.        1    351.38      760.040       100.00        123.351       741.948
204.        2    351.17      760.039       100.00        865.298       742.352
205.        3    350.54      760.037       100.00        865.703       744.017
206.        4    348.88      760.036       100.00        867.368       751.055
207.        5    345.68      760.035       100.00        874.406       771.617
208.        6    342.47      760.034       100.00        894.968       798.694
209.        7    341.19      760.032       100.00        922.045       813.114
210.        8    340.94      760.031       100.00        936.465       817.336
211.        9    340.90      760.030       100.00        940.686       818.347
212.       10    340.89      760.029       100.00        941.697       818.580
213.       11    340.88      760.028       100.00        941.930       818.633
214.       12    340.88      760.026       100.00        941.983       818.645
215.       13    340.88      760.025       100.00        941.995       818.647
216.       14    340.88      760.024       100.00        941.998       818.647
217.       15    340.88      760.023       100.00        941.998       818.646
218.       16    340.88      760.021       100.00        941.996       818.644
219.       17    340.88      760.020       100.00        941.994       818.642
220.       18    340.88      760.019       100.00        941.992       818.637
221.       19    340.88      760.018       100.00        941.988       818.630
222.       20    340.88      760.017       100.00        941.981       818.620
223.       21    340.88      760.015       100.00        941.971       818.604
224.       22    340.87      760.014       100.00        941.955       818.581
225.       23    340.87      760.013       100.00        941.931       818.544
226.       24    340.86      760.012       100.00        941.895       818.489
227.       25    340.85      760.010       100.00        941.839       818.404
228.       26    340.84      760.009       100.00        941.754       818.276
229.       27    340.81      760.008       100.00        941.626       818.082
230.       28    340.77      760.007       100.00        941.433       817.794
231.       29    340.72      760.006       100.00        941.145       817.372
232.       30    340.64      760.004       100.00        940.722       816.764
233.       31    340.52      760.003       100.00        940.115       815.920
234.       32    340.36      760.002       100.00        939.271       814.796
235.       33    340.15      760.001       100.00        938.147       813.389
236.       34    339.88      760.000       100.00        936.740       811.756
237.       35    339.57      759.998       100.00        935.107       810.033
238.       36    339.24      759.997       100.00        933.383       808.395
239.       37    338.91      759.996       100.00        931.746       787.088
240.       38    338.90      759.995       100.00        651.938       790.137
241.       39    338.92      759.993       100.00        654.988       790.397
242.       40    338.91      759.992       100.00        655.247       790.365
243.       41    338.89      759.991       100.00        655.215       727.000
```

```
244.      FINAL VAPOR COMPOSITION PROFILE (MOLE%):
245.      STAGE   BENZENE        ETHANOL        WATER
246.        1       0.48026       99.51971        0.00004
247.        2       1.56628       98.43370        0.00004
248.        3       4.78276       95.21722        0.00005
249.        4      13.08850       86.91148        0.00005
250.        5      28.33657       71.66340        0.00005
251.        6      43.41020       56.58976        0.00006
252.        7      50.66597       49.33396        0.00008
253.        8      52.80228       47.19760        0.00013
254.        9      53.32252       46.67729        0.00020
255.       10      53.44294       46.55676        0.00031
256.       11      53.47053       46.52899        0.00048
257.       12      53.47678       46.52247        0.00075
258.       13      53.47822       46.52064        0.00116
259.       14      53.47850       46.51973        0.00179
260.       15      53.47854       46.51871        0.00275
261.       16      53.47846       46.51733        0.00423
262.       17      53.47830       46.51522        0.00650
263.       18      53.47801       46.51203        0.00998
264.       19      53.47760       46.50709        0.01531
265.       20      53.47702       46.49950        0.02350
266.       21      53.47604       46.48792        0.03605
267.       22      53.47453       46.47020        0.05527
268.       23      53.47229       46.44303        0.08470
269.       24      53.46887       46.40143        0.12970
270.       25      53.46362       46.33802        0.19835
271.       26      53.45573       46.24148        0.30279
272.       27      53.44390       46.09520        0.46091
273.       28      53.42646       45.87491        0.69866
274.       29      53.40113       45.54649        1.05238
275.       30      53.36561       45.06393        1.57047
276.       31      53.31833       44.36955        2.31211
277.       32      53.25983       43.40056        3.33963
278.       33      53.19610       42.10366        4.70024
279.       34      53.14136       40.46119        6.39746
280.       35      53.11745       38.51946        8.36307
281.       36      53.14713       36.39991       10.45297
282.       37      53.24111       34.27495       12.48394
283.       38      54.84291       33.00118       12.15591
284.       39      55.00373       32.85826       12.13803
285.       40      55.01451       32.81120       12.17428
286.       41      54.99857       32.72499       12.27648
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287.     FINAL LIQUID COMPOSITION PROFILE (MOLE%):
288.     STAGE   BENZENE       ETHANOL      WATER
289.        1     0.13045      99.86953      0.00003
290.        2     0.43039      99.56958      0.00004
291.        3     1.36170      98.63829      0.00004
292.        4     4.12114      95.87884      0.00005
293.        5    11.26053      88.73945      0.00005
294.        6    24.44898      75.55099      0.00005
295.        7    37.62022      62.37972      0.00006
296.        8    44.00944      55.99051      0.00008
297.        9    45.89547      54.10442      0.00011
298.       10    46.35499      53.64485      0.00018
299.       11    46.46136      53.53838      0.00027
300.       12    46.48572      53.51385      0.00043
301.       13    46.49126      53.50809      0.00066
302.       14    46.49252      53.50647      0.00101
303.       15    46.49276      53.50568      0.00156
304.       16    46.49278      53.50483      0.00240
305.       17    46.49271      53.50363      0.00368
306.       18    46.49253      53.50181      0.00565
307.       19    46.49227      53.49907      0.00867
308.       20    46.49188      53.49482      0.01331
309.       21    46.49126      53.48831      0.02043
310.       22    46.49032      53.47837      0.03133
311.       23    46.48883      53.46313      0.04804
312.       24    46.48660      53.43978      0.07362
313.       25    46.48323      53.40406      0.11272
314.       26    46.47805      53.34958      0.17238
315.       27    46.47023      53.26665      0.26313
316.       28    46.45851      53.14097      0.40053
317.       29    46.44120      52.95170      0.60709
318.       30    46.41607      52.66953      0.91439
319.       31    46.38072      52.25488      1.36441
320.       32    46.33337      51.65815      2.00848
321.       33    46.27416      50.82532      2.90053
322.       34    46.20834      49.71035      4.08131
323.       35    46.14863      48.29781      5.55357
324.       36    46.11498      46.62715      7.25786
325.       37    46.12839      44.80247      9.06914
326.       38    64.30287      30.84096      4.85623
327.       39    66.18366      29.32035      4.49602
328.       40    66.37316      29.14938      4.47750
329.       41    66.38677      29.09241      4.52086
?
```

```
          FINAL VAPOR COMPOSITION PROFILE (MOLES):
          STAGE   BENZENE       ETHANOL       WATER
             1         3.563       738.384         0.000
             2        11.627       730.725         0.000
             3        35.585       708.433         0.000
             4        98.302       652.753         0.000
             5       218.650       552.967         0.000
             6       346.715       451.979         0.000
             7       411.972       401.141         0.001
             8       431.572       385.763         0.001
             9       436.363       381.982         0.002
            10       437.473       381.104         0.003
            11       437.727       380.902         0.004
            12       437.785       380.854         0.006
            13       437.798       380.840         0.009
            14       437.800       380.832         0.015
            15       437.800       380.823         0.023
            16       437.798       380.811         0.035
            17       437.796       380.793         0.053
            18       437.791       380.765         0.082
            19       437.784       380.721         0.125
            20       437.774       380.654         0.192
            21       437.757       380.552         0.295
            22       437.732       380.396         0.452
            23       437.694       380.157         0.693
            24       437.637       379.791         1.062
            25       437.548       379.232         1.623
            26       437.415       378.383         2.478
            27       437.215       377.097         3.771
            28       436.918       375.162         5.714
            29       436.486       372.284         8.602
            30       435.871       368.066        12.827
            31       435.035       362.020        18.865
            32       433.959       353.626        27.211
            33       432.691       342.467        38.231
            34       431.378       328.446        51.932
            35       430.269       312.020        67.744
            36       429.639       294.255        84.501
            37       419.054       269.774        98.260
            38       433.334       260.755        96.048
            39       434.748       259.711        95.939
            40       434.815       259.328        96.221
            41       399.839       237.911        89.250
?
```

```
373.      FINAL LIQUID COMPOSITION PROFILE (MOLES):
374.      STAGE   BENZENE       ETHANOL       WATER
375.        1          0.161       123.190          0.000
376.        2          3.724       861.574          0.000
377.        3         11.788       853.915          0.000
378.        4         35.745       831.623          0.000
379.        5         98.463       775.943          0.000
380.        6        218.811       676.157          0.000
381.        7        346.875       575.169          0.001
382.        8        412.133       524.331          0.001
383.        9        431.732       508.953          0.001
384.       10        436.524       505.172          0.002
385.       11        437.634       504.294          0.003
386.       12        437.888       504.092          0.004
387.       13        437.946       504.044          0.006
388.       14        437.958       504.030          0.010
389.       15        437.961       504.022          0.015
390.       16        437.960       504.013          0.023
391.       17        437.959       504.001          0.035
392.       18        437.956       503.983          0.053
393.       19        437.951       503.955          0.082
394.       20        437.945       503.911          0.125
395.       21        437.934       503.844          0.192
396.       22        437.918       503.742          0.295
397.       23        437.893       503.586          0.453
398.       24        437.855       503.346          0.693
399.       25        437.797       502.980          1.062
400.       26        437.709       502.422          1.623
401.       27        437.576       501.573          2.478
402.       28        437.376       500.287          3.771
403.       29        437.079       498.352          5.714
404.       30        436.646       495.474          8.602
405.       31        436.032       491.256         12.827
406.       32        435.196       485.210         18.865
407.       33        434.120       476.816         27.211
408.       34        432.852       465.656         38.231
409.       35        431.539       451.636         51.932
410.       36        430.429       435.210         67.744
411.       37        429.799       417.445         84.501
412.       38        419.215       201.064         31.660
413.       39        433.495       192.045         29.448
414.       40        434.908       191.000         29.339
?
```

```
  583.     ******** TWO-LIQUID FLASH PROGRAM *****
?
  584.
  585.
  586.
  587.     FD MOL =726.9995 MOLES        PRESS =   760.00 MMHG        TEMP
  588.                                BENZENE   ETHANOL   WATER
  589.     FEED MOLEFRACTIONS          0.54999   0.32725   0.12276
?



  591.     DEW POINT OF FEED AT 760.00 MMHG IS 338.89 DEG K
?



  592.                                BENZENE   ETHANOL   WATER
  593.     DEW PT LIQ MOLE FRAC        0.66365   0.29109   0.04525
  594.
?



  595.     'VLE' DATA FOR VAPOR AND LIQUID PHASE #  1
  596.
  597.                                BENZENE   ETHANOL   WATER
  598.     VAP MOLE FRAC               0.54999   0.32725   0.12276
  599.     LIQ MOLE FRAC               0.66365   0.29109   0.04525
  600.     VALUES OF K=Y/X             0.82872   1.12420   2.71290
  601.     VAPOR PRESSURES             477.685   451.746   193.972
  602.     FUGACITY FACTORS            1.01047   1.00544   0.98839
  603.     ACTIVITY COEFFICIENTS        1.3048    1.8811   10.7543
  604.     ACTIVITY                     0.8660    0.5476    0.4867
?




  625.     BUBBLE POINT OF FEED AT 760.00 MMHG IS 337.88 DEG K
?
  624.     TWO LIQ PHASE REGION, LIQUID PHASE MOLE RATIO    0.423302
?

  626.                                BENZENE   ETHANOL   WATER
  627.     BUB PT VAP MOLE FRAC        0.54064   0.27305   0.18630
  628.
?
```

```
  650.    FEED AT OR BELOW BUBBLE POINT
  651.
  652.    'VLE' DATA FOR VAPOR AND LIQUID PHASE #  1
  653.
  654.                            BENZENE   ETHANOL   WATER
  655.    VAP MOLE FRAC            0.54064   0.27305   0.18630
  656.    LIQ MOLE FRAC            0.77247   0.18574   0.04178
  657.    VALUES OF K=Y/X          0.83009   1.02347   2.27463
  658.    VAPOR PRESSURES          461.493   432.423   185.399
  659.    FUGACITY FACTORS         1.01084   1.00496   0.99462
  660.    ACTIVITY COEFFICIENTS     1.1667    2.7235   17.7750
  661.    ACTIVITY                  0.9013    0.5059    0.7427
  662.
  663.    'VLE' DATA FOR VAPOR AND LIQUID PHASE #  2
  664.
  665.                            BENZENE   ETHANOL   WATER
  666.    VAP MOLE FRAC            0.54064   0.27305   0.18630
  667.    LIQ MOLE FRAC            0.39766   0.42413   0.17821
  668.    VALUES OF K=Y/X          1.13670   0.73476   1.21964
  669.    VAPOR PRESSURES          461.493   432.423   185.399
  670.    FUGACITY FACTORS         1.01084   1.00496   0.99462
  671.    ACTIVITY COEFFICIENTS     2.2664    1.1928    4.1678
  672.    ACTIVITY                  0.9013    0.5059    0.7427
  673.    IDEAL LIQ ENTHALPY =  -0.138368E 04     DELTA H =   0.0
  674.    IDEAL LIQ ENTHALPY =  -0.127464E 04     DELTA H =   0.173270E 03
  675.    ENTHALPY OF SYSTEM WITH REFERENCE TO PURE LIQUID AT   0.0  DEG K   -1318.96 BTU/LBMOL
?



  676.    CONV CHECK FOR WTR       76.9016        66.6000        22.6500        12.3459
  677.    CONV CHECK FOR BEZN       171.760       0.0             400.000       0.0
  678.    CONV CHECK FOR ETOH      306.213        191.900        169.200        54.8823
?
  679.      TRIAL # =     2
?
  680.
?
  681.    ********************************************************************************************
?
```

F.2 Inputs

```
   1.      //FINAL2  JOB  (JA00008,NJIT,15000,30,0),'RCOHE-TSAI-FINAL2',
   1.01    //        REGION=280K,TIME=(0,30)
   1.02    //*PASSWORD SAI
   1.03    //*MAIN  CLASS=+2,REPORT=YES,FAILURE=RESTART
   1.04    //*FORMAT PR,DDNAME=,DEST=RMT20,COPIES=1
 7003.     //STEP5  EXEC  PGM=BAYWAY2,REGION=280K
 7004.     //STEPLIB  DD  DSN='NCE.AJA00.S008.TEST',UNIT=OLS,DISP=SHR
 7005.     //FT06F001 DD  SYSOUT=A
 7006.     //FT05F001 DD  *
 7007.     COMPLETE AZEOTRPIC DIST. MODEL--BENZENE STRIPPING COLUMN-REB.ABS
 7008.      3 1 2 2 0 0 1
 7012.     BENZENE 0 78.114    562.1     48.3      259.0     92.26
 7013.     0.0       0.0       0.544     0.251
 7014.     94.118    353.3     0.41                          0.249
 7015.     15.9008   -2788.51  -52.36
 7016.     ETHANOL 0 46.07     516.2     63.0      167.0     64.0
 7017.     0.0878    0.0572    0.248     0.635
 7018.     202.06    351.1     0.58                          0.38
 7019.     18.9119   -3803.98  -41.68
 7020.     WATER   0 18.01     647.3     217.3     56.0      18.84
 7021.     0.0279    0.0229    0.229     0.344
 7022.     538.7     373.2     1.0                           0.454
 7023.     18.3036   -3816.44  -46.13
 7024.     0.0       0.15      0.40
 7025.     0.15      0.0       0.20
 7026.     0.40      0.20      0.0
 7027.     1096.889  0.0       282.332   0.0       2213.335  0.0       3820.95
 7028.     -86.763   0.0       1289.908  0.0
 7029.     0.295     0.267     0.270
 7030.      5 0 5 1 0 020 2 0
 7031.     1.0       0.0       0.0
 7032.     413.0     0.0        1.0      339.0     354.0     760.0     0.001
 7034.      5        308.0     0.0       184.5     206.9     39.6
 7035.     /*
 7036.     //
?
'RUN.STRIPPING' (RE)CATALOGED AND RESAVED ON WYL106
?
3443 IS YOUR JOB NUMBER  04/03/82 Saturday   9:26:33 p.m.
?
```

F.2 Results

```
COMPLETE AZEOTRPIC DIST. MODEL--BENZENE STRIPPING COLUMN-REB.ABS
NUMBER OF COMPONENTS =  3
VAPOR-LIQUID EQUILIBRIUM DATA CODES:
    LIQUID =   1
    VAPOR =    2
    ENTHALPY = 2

NOTE: ALL FLOWS ARE  PER UNIT TIME, AND ENERGY
      VALUES ARE IN UNITS OF K-BTU PER UNIT TIME.
COMPONENT NO                       1         2         3
NAME                         BENZENE   ETHANOL   WATER
MOLECULAR WEIGHT                 78.1      46.1      18.0
CRITICAL PROPERTIES
TEMPERATURE  (DEG K)            562.1     516.2     647.3
PRESSURE     ( ATM)              48.3      63.0     217.3
VOLUME         (CC/GMOL)        259.0     167.0      56.0
COMPRESSIBILITY                 0.544     0.248     0.229
ACENTRIC FACTOR                 0.251     0.635     0.344
TSONOPOULOS -A-                0.0       0.0878    0.0279
TSONOPOULOS -B-                0.0       0.0572    0.0229
AK(1,1)=   0.0
AK(1,2)=   0.150
AK(1,3)=   0.400
AK(2,1)=   0.150
AK(2,2)=   0.0
AK(2,3)=   0.200
AK(3,1)=   0.400
AK(3,2)=   0.200
AK(3,3)=   0.0
VAPOR PRESSURE CONSTANTS
( MMHG AND DEG K)
C(1)                           15.901    18.912    18.304
C(2)                         -2788.51  -3803.98  -3816.44
C(3)                           -52.36    -41.68    -46.13
C(4)                             0.0       0.0       0.0
C(5)                             0.0       0.0       0.0
C(6)                             0.0       0.0       0.0
LIQUID MOLAR VOLUME CONSTANTS
C(1)                           92.260    64.000    18.840
ENTHALPY CONSTANTS (CAL/GM)
LATENT HEAT                      94.1     202.1     538.7
AT DEG K                        353.3     351.1     373.2
LIQUID SP. HEAT CONSTANTS
C(1)                            0.410     0.580     1.000
C(2)                            0.0       0.0       0.0
C(3)                            0.0       0.0       0.0
C(4)                            0.0       0.0       0.0
VAPOR SP. HEAT CONSTANTS
C(1)                            0.249     0.380     0.454
C(2)                            0.0       0.0       0.0
C(3)                            0.0       0.0       0.0
C(4)                            0.0       0.0       0.0
  NRTL CONSTANTS, CAL/GMOL
```

```
 126.      COMPLETE AZEOTRPIC DIST. MODEL--BENZENE STRIPPING COLUMN-REB.ABS
 127.       REBOILED  ABSORBER
 128.      FEED STREAMS:
 129.      STAGE                          5.
 130.      TEMP                       308.00
 131.      FRACV                      0.0
 132.      H                     -5.5245E 05
 133.      COMP 1  BENZENE           184.500     184.500
 134.      COMP 2  ETHANOL           206.900     206.900
 135.      COMP 3  WATER              39.600      39.600
 136.      TOTAL                     431.000     431.000
 137.      NUMBER OF STAGES        5
 138.
 139.      ESTIMATED OVERHEAD PRODUCT RATE    413.0000
 140.      ESTIMATED BOTTOMS PRODUCT RATE      17.9998
 141.
 142.      PRESSURE AT TOP OF COLUMN         759.99902
 143.      CONSTANT DELTA P PER STAGE          0.00100
 144.      BOILUP RATIO       1.000000
?
```

```
 181.      REBOILER DUTY    =  1.671029E 05
 182.      CONDENSER DUTY   = -3.243844E 06
 183.      PRODUCT STREAMS:
 184.      STAGE                          1.          5.
 185.      TEMP                       348.48      341.15
 186.      FRACV                      0.0         1.0000
 187.      H                     -1.9991E 03  3.4129E 06
 188.      COMP 1  BENZENE             0.652     183.848
 189.      COMP 2  ETHANOL            15.528     191.372
 190.      COMP 3  WATER               1.820      37.780
 191.      TOTAL                      18.000     413.000
?
```

```
      FINAL COLUMN PROFILES:
      STAGE    TEMP        PRES        EFF(%)      LIQUID(MOLS)   VAPOR(MOLS)
        1     348.48      760.004      100.00         18.000         18.000
        2     345.71      760.003      100.00         36.000         18.307
        3     343.24      760.001      100.00         36.307         18.651
        4     341.80      760.000      100.00         36.651         18.872
        5     341.15      759.999      100.00         36.872        413.000
      FINAL VAPOR COMPOSITION PROFILE (MOLE%):
      STAGE    BENZENE       ETHANOL       WATER
        1       13.25762      76.96699      9.77547
        2       25.57612      65.21938      9.20457
        3       35.98048      55.15580      8.86385
        4       41.90915      49.17363      8.91733
        5       44.51516      46.33718      9.14771
      FINAL LIQUID COMPOSITION PROFILE (MOLE%):
      STAGE    BENZENE       ETHANOL       WATER
        1        3.62488      86.26432     10.11089
        2        8.44121      81.61567      9.94318
        3       14.69342      75.65270      9.65390
        4       20.09009      70.43363      9.47630
        5       23.21991      67.28013      9.50000
      FINAL VAPOR COMPOSITION PROFILE (MOLES):
      STAGE    BENZENE       ETHANOL       WATER
        1          2.386        13.854        1.760
        2          4.682        11.940        1.685
        3          6.711        10.287        1.653
        4          7.909         9.280        1.683
        5        183.848       191.372       37.780
      FINAL LIQUID COMPOSITION PROFILE (MOLES):
      STAGE    BENZENE       ETHANOL       WATER
        1          0.652        15.528        1.820
        2          3.039        29.381        3.580
        3          5.335        27.468        3.505
        4          7.363        25.815        3.473
        5          8.562        24.808        3.503
?
```

```
 228.      TEMP, DEG K   348.476
 229.      PRES, MMHG   760.0039
 230.       #  NAME              K               VP              FUG              GAM
 231.       1  BENZENE      3.6574           654.49          0.98302           4.3204
 232.       2  ETHANOL     0.89222           673.74           1.0039           1.0026
 233.       3  WATER       0.96682           293.19          0.98492           2.5445
 234.      STAGE #     2
 235.      TEMP, DEG K   345.714
 236.      PRES, MMHG   760.0027
 237.       #  NAME              K               VP              FUG              GAM
 238.       1  BENZENE      3.0299           598.96          0.99165           3.8769
 239.       2  ETHANOL     0.79910           601.97           1.0062           1.0027
 240.       3  WATER       0.92571           260.98          0.98587           2.7344
 241.      STAGE #     3
 242.      TEMP, DEG K   343.243
 243.      PRES, MMHG   760.0015
 244.       #  NAME              K               VP              FUG              GAM
 245.       1  BENZENE      2.4487           552.49          0.99872           3.3728
 246.       2  ETHANOL     0.72906           543.30           1.0074           1.0124
 247.       3  WATER       0.91815           234.75          0.98611           3.0144
 248.      STAGE #     4
 249.      TEMP, DEG K   341.795
 250.      PRES, MMHG   760.0002
 251.       #  NAME              K               VP              FUG              GAM
 252.       1  BENZENE      2.0861           526.62           1.0026           3.0026
 253.       2  ETHANOL     0.69815           511.23           1.0076           1.0300
 254.       3  WATER       0.94101           220.44          0.98617           3.2898
 255.      STAGE #     5
 256.      TEMP, DEG K   341.148
 257.      PRES, MMHG   759.9990
 258.       #  NAME              K               VP              FUG              GAM
 259.       1  BENZENE      1.9171           515.37           1.0043           2.8148
 260.       2  ETHANOL     0.68872           497.42           1.0076           1.0444
 261.       3  WATER       0.96291           214.28          0.98632           3.4626
?
```

F.3 Inputs

```
   1.     //FINAL2  JOB  (JA00008,NJIT,15000,30,0),'RCDHE-TSAI-FINAL2',
   1.01   //       REGION=280K,TIME=(0,30)
   1.02   //*PASSWORD SAI
   1.03   //*MAIN  CLASS=+2,REPORT=YES,FAILURE=RESTART
   1.04   //*FORMAT PR,DDNAME=,DEST=RMT20,COPIES=1
7003.     //STEP5  EXEC  PGM=BAYWAY2,REGION=280K
7004.     //STEPLIB  DD  DSN='NCE.AJA00.S008.TEST',UNIT=OLS,DISP=SHR
7005.     //FT06F001 DD  SYSOUT=A
7006.     //FT05F001 DD  *
7007.     COMPLETE AZEOTROPIC DISTILLATION---- ETOH RECOVERY COLUMN
7008.      3 1 2 2 0 0 1
7012.     BENZENE 0 78.114    562.1     48.3      259.0     92.26
7013.     0.0       0.0       0.544     0.251
7014.     94.118    353.3     0.41                          0.249
7015.     15.9008   -2788.51  -52.36
7016.     ETHANOL 0 46.07     516.2     63.0      167.0     64.0
7017.     0.0878    0.0572    0.248     0.635
7018.     202.06    351.1     0.58                          0.38
7019.     18.9119   -3803.98  -41.68
7020.     WATER   0 18.01     647.3     217.3     56.0      18.84
7021.     0.0279    0.0229    0.229     0.344
7022.     538.7     373.2     1.0                           0.454
7023.     18.3036   -3816.44  -46.13
7024.     0.0       0.15      0.40
7025.     0.15      0.0       0.20
7026.     0.40      0.20      0.0
7027.     1096.889  0.0       282.332   0.0       2213.335  0.0       3820.95
7028.     -86.763   0.0       1289.908  0.0
7029.     0.295     0.267     0.270
7030.      3 011 1 0 020 2 1
7031.     1.0       0.0       0.0
7032.     16.230    0.0       4.0       351.0     373.0     760.0     0.001
7034.      9        351.0     0.0       2.386     13.854    1.760
7035.     /*
7036.     //
?
```

F.3 Results

```
  124.     COMPLETE AZEOTROPIC DISTILLATION---- ETOH RECOVERY COLUMN
  125.     DISTILLATION COLUMN; PRODUCT RATES & REFLUX RATIO SPECIFIED
  126.     FEED STREAMS:
  127.     STAGE                         9.
  128.     TEMP                     351.00
  129.     FRACV                    0.0
  130.     H                     -9.1638E 02
  131.     COMP 1  BENZENE           2.386        2.386
  132.     COMP 2  ETHANOL          13.854       13.854
  133.     COMP 3  WATER             1.760        1.760
  134.     TOTAL                    18.000       18.000
  135.     NUMBER OF STAGES       11
  136.
  137.     ESTIMATED OVERHEAD PRODUCT RATE      16.2300
  138.     ESTIMATED BOTTOMS PRODUCT RATE        1.7700
  139.
  140.     PRESSURE AT TOP OF COLUMN          759.99756
  141.     CONSTANT DELTA P PER STAGE           0.00100
  142.     REFLUX RATIO       4.000000
?


  171.     REBOILER DUTY    =  7.470238E 05
  172.     CONDENSER DUTY   =  7.503814E 05
  173.     PRODUCT STREAMS:
  174.     STAGE                         1.          11.
  175.     TEMP                     351.26       343.20
  176.     FRACV                    0.0          0.0
  177.     H                     -4.9485E 01  1.3762E 05
  178.     COMP 1  BENZENE           0.000        2.386
  179.     COMP 2  ETHANOL           1.627       12.227
  180.     COMP 3  WATER             0.143        1.617
  181.     TOTAL                     1.770       16.230
?
```

```
182.      FINAL COLUMN PROFILES:
183.      STAGE     TEMP         PRES          EFF(%)       LIQUID(MOLS)    VAPOR(MOLS)
184.         1     351.26      760.010        100.00            1.770          79.816
185.         2     351.25      760.009        100.00           81.586          79.796
186.         3     351.25      760.007        100.00           81.566          79.778
187.         4     351.24      760.006        100.00           81.548          79.761
188.         5     351.24      760.005        100.00           81.531          79.746
189.         6     351.22      760.004        100.00           81.516          79.732
190.         7     351.16      760.002        100.00           81.502          79.723
191.         8     350.92      760.001        100.00           81.493          79.733
192.         9     349.96      760.000        100.00           81.503          80.370
193.        10     348.16      759.999        100.00           64.140          81.150
194.        11     343.20      759.998        100.00           64.920           0.0
195.      FINAL VAPOR COMPOSITION PROFILE (MOLE%):
196.      STAGE    BENZENE       ETHANOL       WATER
197.         1       0.00008      91.53092       8.46901
198.         2       0.00032      91.14850       8.85119
199.         3       0.00130      90.79516       9.20357
200.         4       0.00536      90.46901       9.52563
201.         5       0.02221      90.16066       9.81714
202.         6       0.09242      89.83108      10.07650
203.         7       0.38480      89.32071      10.29451
204.         8       1.58694      87.98400      10.42907
205.         9       6.22384      83.45498      10.32118
206.        10      14.70113      75.33339       9.96550
207.        11       0.0           0.0           0.0
208.      FINAL LIQUID COMPOSITION PROFILE (MOLE%):
209.      STAGE    BENZENE       ETHANOL       WATER
210.         1       0.00002      91.94177       8.05826
211.         2       0.00008      91.53984       8.46010
212.         3       0.00031      91.16572       8.83399
213.         4       0.00127      90.82003       9.17870
214.         5       0.00524      90.50099       9.49378
215.         6       0.02173      90.19933       9.77895
216.         7       0.09041      89.87693      10.03266
217.         8       0.37645      89.37765      10.24592
218.         9       1.55248      88.06999      10.37756
219.        10       4.07876      85.51009      10.41119
220.        11      14.70113      75.33339       9.96550
?
```

```
FINAL VAPOR COMPOSITION PROFILE (MOLES):
STAGE   BENZENE       ETHANOL       WATER
  1        0.000        73.057          6.760
  2        0.000        72.733          7.063
  3        0.001        72.434          7.342
  4        0.004        72.159          7.598
  5        0.018        71.899          7.829
  6        0.074        71.624          8.034
  7        0.307        71.209          8.207
  8        1.265        70.152          8.315
  9        5.002        67.073          8.295
 10       11.930        61.133          8.087
 11        0.0           0.0            0.0
FINAL LIQUID COMPOSITION PROFILE (MOLES):
STAGE   BENZENE       ETHANOL       WATER
  1        0.000         1.627          0.143
  2        0.000        74.684          6.902
  3        0.000        74.360          7.206
  4        0.001        74.062          7.485
  5        0.004        73.786          7.740
  6        0.018        73.527          7.971
  7        0.074        73.252          8.177
  8        0.307        72.836          8.350
  9        1.265        71.780          8.458
 10        2.616        54.847          6.678
 11        9.544        48.906          6.470
```

```
STAGE #    1
TEMP, DEG K   351.258
PRES, MMHG   760.0098
 #  NAME             K              VP            FUG           GAM
 1  BENZENE       4.1447          714.43        0.97322        4.5304
 2  ETHANOL      0.99553          753.14         1.0007        1.0039
 3  WATER         1.0510          328.95        0.98144        2.4741
STAGE #    2
TEMP, DEG K   351.253
PRES, MMHG   760.0085
 #  NAME             K              VP            FUG           GAM
 1  BENZENE       4.1702          714.32        0.97327        4.5588
 2  ETHANOL      0.99572          752.99         1.0006        1.0044
 3  WATER         1.0462          328.88        0.98177        2.4626
STAGE #    3
TEMP, DEG K   351.248
PRES, MMHG   760.0073
 #  NAME             K              VP            FUG           GAM
 1  BENZENE       4.1942          714.22        0.97331        4.5855
 2  ETHANOL      0.99593          752.85         1.0006        1.0048
 3  WATER         1.0418          328.82        0.98206        2.4520
STAGE #    4
TEMP, DEG K   351.244
PRES, MMHG   760.0061
 #  NAME             K              VP            FUG           GAM
 1  BENZENE       4.2165          714.12        0.97336        4.6103
 2  ETHANOL      0.99613          752.72         1.0006        1.0052
 3  WATER         1.0378          328.76        0.98233        2.4422
STAGE #    5
TEMP, DEG K   351.238
PRES, MMHG   760.0049
 #  NAME             K              VP            FUG           GAM
 1  BENZENE       4.2366          713.98        0.97340        4.6329
 2  ETHANOL      0.99624          752.53         1.0006        1.0055
 3  WATER         1.0341          328.68        0.98258        2.4335
```

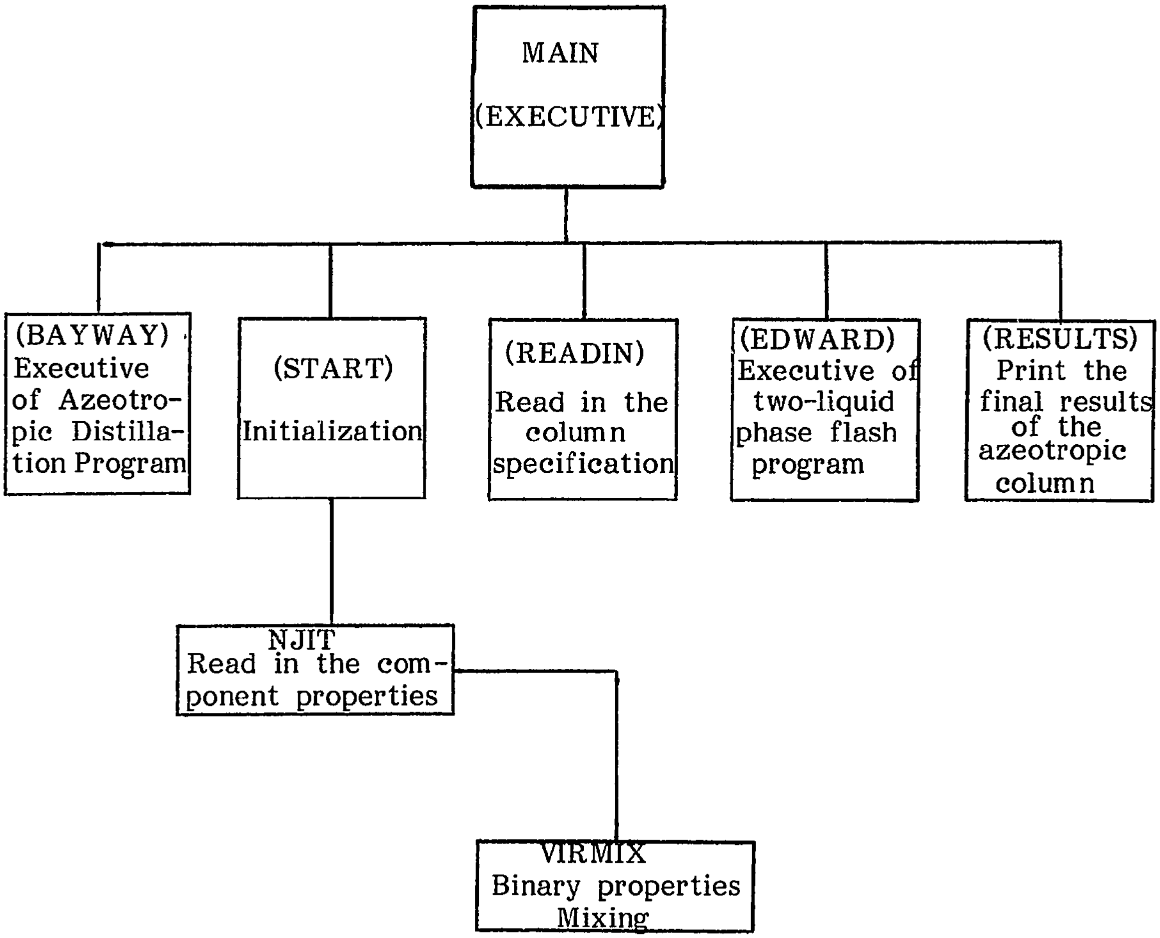
```
281.      3  WATER          1.0341        328.68       0.98258       2.4335
282.     STAGE #    6
283.     TEMP, DEG K   351.221
284.     PRES, MMHG   760.0037
285.      #  NAME              K             VP           FUG           GAM
286.      1  BENZENE        4.2524        713.62       0.97349       4.6522
287.      2  ETHANOL       0.99592        752.05        1.0006       1.0059
288.      3  WATER          1.0304        328.46       0.98281       2.4260
289.     STAGE #    7
290.     TEMP, DEG K   351.160
291.     PRES, MMHG   760.0024
292.      #  NAME              K             VP           FUG           GAM
293.      1  BENZENE        4.2562        712.26       0.97373       4.6640
294.      2  ETHANOL       0.99380        750.23        1.0006       1.0061
295.      3  WATER          1.0261        327.64       0.98305       2.4212
296.     STAGE #    8
297.     TEMP, DEG K   350.917
298.     PRES, MMHG   760.0012
299.      #  NAME              K             VP           FUG           GAM
300.      1  BENZENE        4.2156        706.86       0.97463       4.6505
301.      2  ETHANOL       0.98441        743.00        1.0010       1.0060
302.      3  WATER          1.0179        324.38       0.98341       2.4251
303.     STAGE #    9
304.     TEMP, DEG K   349.965
305.     PRES, MMHG   760.0000
306.      #  NAME              K             VP           FUG           GAM
307.      1  BENZENE        4.0090        686.05       0.97800       4.5410
308.      2  ETHANOL       0.94759        715.30        1.0022       1.0046
309.      3  WATER         0.99456        311.90       0.98422       2.4623
310.     STAGE #   10
311.     TEMP, DEG K   348.156
312.     PRES, MMHG   759.9988
313.      #  NAME              K             VP           FUG           GAM
314.      1  BENZENE        3.6043        647.86       0.98407       4.2966
315.      2  ETHANOL       0.88099        665.08        1.0042       1.0025
316.      3  WATER         0.95719        289.30       0.98530       2.5521
317.     STAGE #   11
318.     TEMP, DEG K   343.201
319.     PRES, MMHG   759.9976
320.      #  NAME              K             VP           FUG           GAM
321.      1  BENZENE        2.4545        551.72       0.99882       3.3851
322.      2  ETHANOL       0.72763        542.35        1.0074       1.0122
323.      3  WATER         0.91318        234.32       0.98634       3.0029
?
```

APPENDIX G

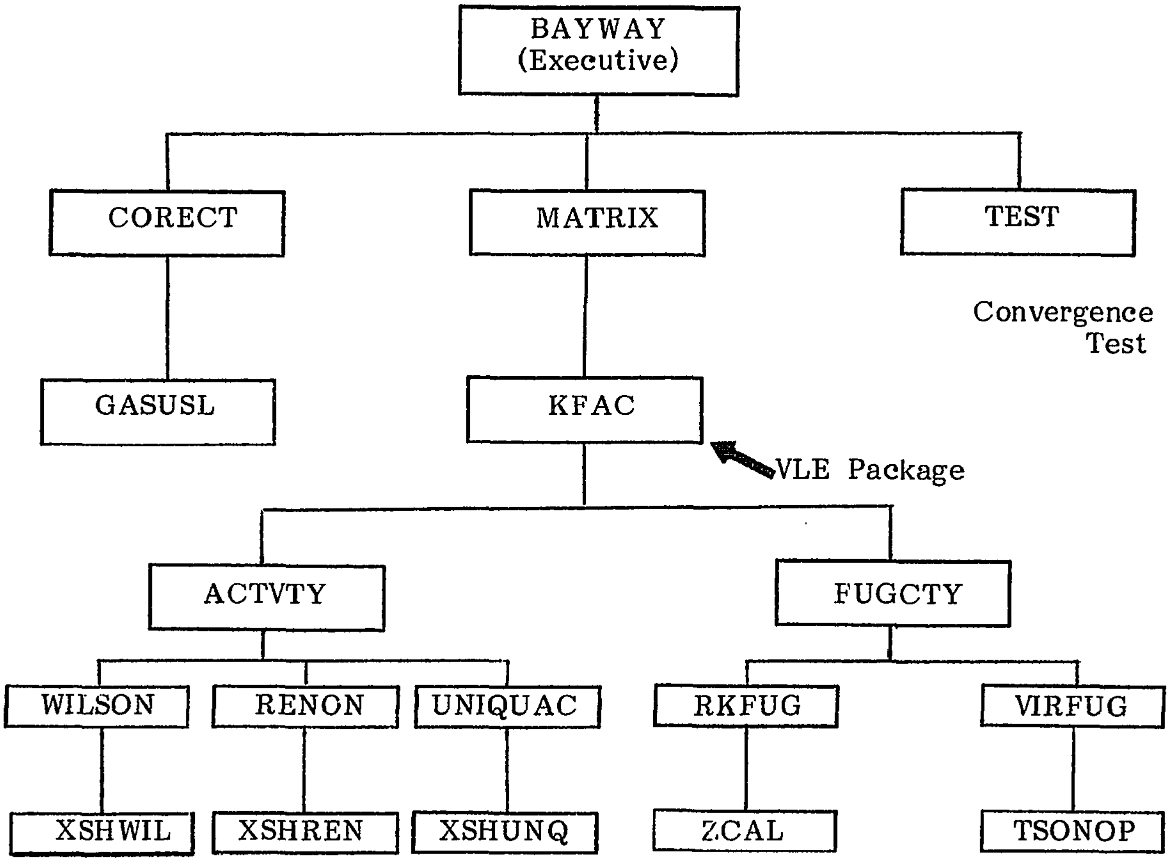
COMPUTER PROGRAMS

Structure of Computer Programs

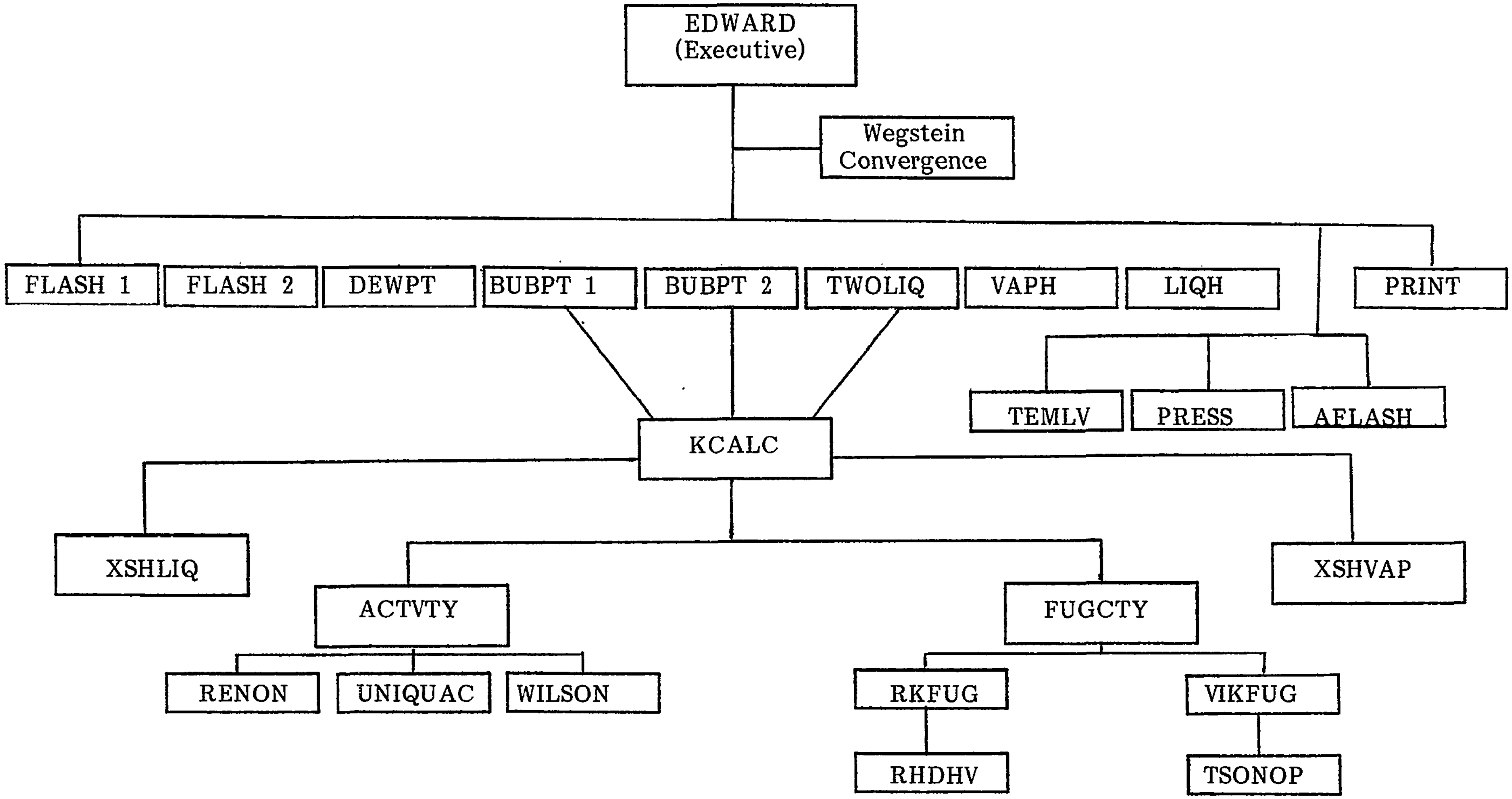
1. The Complete Azeotropic Distillation Program



2. The Azeotropic Distillation Program



3. The Two-Liquid Phase Flash Program



```
C
C     ****************************************************************
C
C     THIS IS THE EXECUTIVE PROGRAM WHICH LINKS THE AZEOTROPIC
C     DISTILLATION MODEL (BAYWAY) WITH THE TWO-LIQUID PHASE
C     FLASH MODEL(EDWARD).
C
C     OLD MAIN IN EDWAARD BECOMES SUBROUTINE EDWARD
C     THE MAIN IN BAYWAY IS REPLACED BY SUBROUTIINES BAYWAY,START,TEST
C
C     MARCH 10,1982------ EDWARD C ROCHE,JR. / CHARLES M. TSAI
C     ****************************************************************
C
      IMPLICIT REAL     (M)
      INTEGER           COMPNT
      REAL              LIQUID
C
      COMMON /B2L/      FD(11),Z(10),EK(10,2),PF,TF,HI,XSAVE(10,2)
      COMMON /CONTRL/   TDUM,P,NOBUB,NODEW,ISO,NLIQ
      COMMON /LIQUID/    X(10,2),GAM(10,2),DHL(2),HIDLL(2),HREALL(2),
     +                   FRACL
      COMMON  /CTRL/    NCR, NPRT, NSTART, TITLE(20)
      COMMON  /NJIT0/   NC, NCM1, IDLL, IDLV, IDH, LDBUG, ISW,
     *                  NAME(2,10), L(10), NDIM, COMPNT(10)
      COMMON  /NJIT1/   CPL(10,4), CPV(10,4), ENP(10,10), ANT(6,10),
     *                  W(10)
      COMMON  /NJIT2/   C(180), ALPHA(45), VC(10), VOL(10), TC(10),
     *                  PC(10), OA(10), OB(10), AA(10,10), G(10,10),
     *                  THETA(10), THS(10), HFAC(10), HHFA(10), HM(10),
     *                  Q(10),R(10),XL(10),PHI(10),DUMMY(10)
      COMMON  /NJIT3/   TTC(10,10),PPC(10,10),VVC(10,10),ZZC(10,10),
     *                  AK(10,10), AVALUE(10,10), BVALUE(10,10),
     *                  BCROSS(10,10), OMEGA(10), DIPOLE(10), B(10,10)
      COMMON  /INR0/    NST, NSTM1, NK1, NK2, NK11, NK21, NCASE, KUNITS,
     *                  NFEED, LF(9), IOCODE, ITR, ITRMAX,ICODE,KOUNT
      COMMON  /INR1/    FSTR(9,11), FKV(9), HF(9), FLMAX(10), FVMAX(10),
     *                  DEST,DESTV,DESTL, BTMS, RFLX,BOTL, PP(50), T(50),
     *                  MU(50), SL(50), SV(50), FL(50), FLL(50,10),
     *                  FV(50), FVV(50,10), ZCONVT, ZCONVF
      COMMON  /INR2/    DFK(10,21), HL(50), HLL(50,10), CL(50), HHE(50),
     *                  DEXH(50,11), HV(50), HVV(50,10), CV(50)
      COMMON  /INR3/    AMAT(21,21), BMAT(50,21,21), D(50,21)
      COMMON  /INR4/    VAPOR, LIQUID, FEED(11)
      COMMON  /KNST/    XFKNST(10)
C
      DATA              SMALL /0.00005/
      KOUNT=0
C
      NCR=5
      NPRT=6
C
       CALL START
C
C
   25 CALL READIN
C
```

```
              C
              C
              C      TOCODE IS THE OVERALL CONVERGENCE COUNTER
              C
0024                 IF (ICODE.EQ.1) GO TO 170
              C
              C      KOUNT IS THE CONVERGENCE COUNTER FOR TWO LIQUID PHASES
              C      SEPARATION ROUTINE, THE MAX ITERATION NO IS SET AT 20
              C
0025              30 KOUNT=KOUNT+1
0026                 WRITE(6,31) KOUNT
0027              31 FORMAT ('1  TRIAL # = ',I5//1X,100('*')//)
              C
              C      CALL THE AZEOTROPIC DISTILLATION COLUMN SIMULATION PROGRAM
              C
0028                 CALL BAYWAY
              C
              C
              C      SAVE THE COLUMN SIMULATION RESULTS ,OVERHEAD DISTILLATE
              C      RATES INTO THE FEED STREAM OF THE TWO-LIQ PHASES SEPARATION
              C      ROUTINE
              C
              C
0029                 FD(NC+1)=0
0030                 DO 120 I=1,NC
0031                 FD(I)=FVV(NST,I)
0032             120 FD(NC+1) = FD(NC+1) + FD(I)
              C
              C      SAVE THE ENTRAINER FEED TO THE COLUMN FOR EACH COMPONENT
              C
              C
0033                 BSAVE=FSTR(1,1)
0034                 ESAVE=FSTR(1,2)
0035                 WSAVE=FSTR(1,3)
              C
              C      CALL THE TWO-LIQUID SEPARATION PROGRAM FOR PHASE SPLITTING
              C
              C
0036                 CALL EDWARD
              C
              C
              C      BEFORE CALLING SUB RESULT CHECK THE COMPOSITION IN XSAVE
              C      VS. TWOLIQ'S  FOR THE FOLLOWINGS
              C      1A. WATER BALANCE.... WATER RATE IN THE DRUM STREAM(AQUEOUS)
              C                            + WATER IN ETOH PRODUCT(BOTMS) MUST EQ.
              C                            TO WATER RATE IN THE COLUMN FEED
              C
              C      1B....... WATER IN ORGANIC PHASE FROM DRUM = WATER IN ENTRAINER
              C
              C       NET WATER BALANCE CHECK
0037                  WOUT=FLL(1,3) + X(3,2)*(1-FRACL)*FD(NC+1)
0038                  WIN= FSTR(2,3)
              C
              C      CHECK WATER IN THE  ENTRAINER
              C       WSAVE= WATER IN ENTRAINER
0039                  WCALC= X(3,1)*FRACL*FD(NC+1)
```

```
C
      WRITE(6,130) WOUT,WIN,WSAVE,WCALC
C     2  ETOH BALANCE ... ETOH IN BOTMS + ETOH IN PURGE(AQEOUS)
C                         MUST BE CHECKED AGAINST ETOH IN THE
C                         FRESH FEED
C     2B........ETOH IN ORGANIC PHASE FROM DRUM =WATER IN ENTRAINER
C
C
C     NET ETOH BALANCE
C
      EOUT=FLL(1,2)+X(2,2)*(1-FRACL)*FD(NC+1)
      EIN=FSTR(2,2)
C
C     CHECK ETOH IN THE ENTRAINER
C
C     ESAVE = ETOH IN THE ENTRAINER
      ECALC = X(2,1)*FRACL*FD(NC+1)
C     3  BENZENE BALANCE... BZ IN FEED #1(FROM COLUMN) MUST BE CHECKED
C                         WITH BZ IN BOTMS(SMALL AMT) ,PURGE, THE SUM
C                         BOTM BZ AND PURGE BZ IS THE REQUIRED MAKE UP
C
C     NET BENZENE BALANCE
C
      BOUT= FLL(1,1) + X(1,2)*(1-FRACL)*FD(NC+1)
      BIN = 0.0
      WRITE(6,132) BOUT,BIN,BSAVE,BCALC
C
C
C     CHECK BENZENE IN THE ENTRAINER---BSAVE
C
      BCALC= X(1,1)*FRACL*FD(NC+1) + BOUT
C
C     UPDATE THE ENTRAINER FEED RATE VIA DIRECT SUBSTITUTION
C
      FSTR(1,1) = BCALC
      FSTR(1,2) = ECALC
      FSTR(1,3) = WCALC
C
C     BY-PASS THE  MAX ITER TENTATIVELY AND PRINT THE CONV CHECKS
C
      WRITE(6,131) EOUT,EIN,ESAVE,ECALC
C       CALL RESULT
C
C
  130 FORMAT(' CONV CHECK FOR WTR ',2X,4G15.6)
  131 FORMAT(' CONV CHECK FOR ETOH',2X,4G15.6)
  132 FORMAT(' CONV CHECK FOR BEZN ',2X,4G15.6)
      IF(KOUNT.LE.5) GO TO 30
C 160 CALL RESULT
C
  170 CALL EXIT
      STOP
      END
```

```
0001                   SUBROUTINE BAYWAY
              C        PROGRAM       MAIN:BAYWAY AS MEMBER OF NCE.AJA00.S008.TEST
              C                      REBOILER DUTY CALCULATION MODIFIED 3-28-81
              C                            WITH 'SMALL' IN KFAC CHANGED TO 0.0
              C                            AS OF APRIL 5,1981(NO UNIQUAC MODIFICATION)
              C                            REBOILED ABSORBER OPTION IMPLEMENTED NCASE=5
              C
              C        READIN MODIFIED ON DEC. 17,1981
              C
              C        MAIN PROGRAM MODIFIED TO MAIN PLUS START,TEST SUBROUTINES
              C        ON DEC. 19,1981
              C
0002                   IMPLICIT REAL      (M)
0003                   INTEGER            COMPNT
0004                   REAL               LIQUID
              C
0005                   COMMON /B2L/       FD(11),Z(10),FK(10,2),PF,TF,HI,XSAVE(10,2)
0006                   COMMON  /CTRL/     NCR, NPRT, NSTART, TITLE(20)
0007                   COMMON  /NJIT0/    NC, NCM1, IDLL, IDLV, IDH, LDBUG, ISW,
                     *                    NAME(2,10), L(10), NDIM, COMPNT(10)
0008                   COMMON  /NJIT1/    CPL(10,4), CPV(10,4), ENP(10,10), ANT(6,10),
                     *                    W(10)
0009                   COMMON  /NJIT2/    C(180), ALPHA(45), VC(10), VOL(10), TC(10),
                     *                    PC(10), UA(10), OB(10), AA(10,10), G(10,10),
                     *                    THETA(10), THS(10), HFAC(10), HHFA(10), HM(10),
                     *                    Q(10),R(10),XL(10),PHI(10),DUMMY(10)
0010                   COMMON  /NJIT3/    TTC(10,10),PPC(10,10),VVC(10,10),ZZC(10,10),
                     *                    AK(10,10), AVALUE(10,10), BVALUE(10,10),
                     *                    BCROSS(10,10), OMEGA(10), DIPOLE(10), B(10,10)
0011                   COMMON  /INR0/     NST, NSTM1, NK1, NK2, NK11, NK21, NCASE, KUNITS,
                     *                    NFEED, LF(9), IDCODE, ITR, ITRMAX, ICODE
0012                   COMMON  /INR1/     FSTR(9,11), FKV(9), HF(9), FLMAX(10), FVMAX(10),
                     *                    DEST,DESTV,DESTL, BTMS, RFLX,BOIL, PP(50), T(50),
                     *                    MU(50), SL(50), SV(50), FL(50), FLL(50,10),
                     *                    FV(50), FVV(50,10), ZCONVT, ZCONVF
0013                   COMMON  /INR2/     DFK(10,21), HL(50), HLL(50,10), CL(50), HHE(50),
                     *                    DEXH(50,11), HV(50), HVV(50,10), CV(50)
0014                   COMMON  /INR3/     AMAT(21,21), BMAT(50,21,21), D(50,21)
0015                   COMMON  /INR4/     VAPOR, LIQUID, FEED(11)
0016                   COMMON  /VLE/      XFK(10), GAM(10), X(10), Y(10), VP(10), FUG(10)
0017                   COMMON  /KNST/     XFKNST(10)
             C
0018                   DATA               SMALL /0.00005/
             C
0019                   NCR=5
             C
0020                   ITR=0
             C
0021               30  CALL MATRIX
0022                   CALL CORECT
0023                   CALL TEST
0024                   IF (ICODE) 30,160,40
             C
0025              160  CALL RESULT
0026                   GO TO 170
0027               40  WRITE(5,41)
```

```
)028          41  FORMAT(' IDCOE=1, TRIAL LIMIT REACHED PROBLEM NOT CONVERGED')
)029              CALL RESULT
            C
)030         170  RETURN
)031              END
```

```
      SUBROUTINE START
      IMPLICIT REAL    (M)
      INTEGER          COMPNT
      REAL             LIQUID
C
      COMMON /B2L/     FD(11),Z(10),FK(10,2),PF,TF,HI,XSAVE(10,2)
      COMMON  /CTRL/   NCR, NPRT, NSTART, TITLE(20)
      COMMON /CONTRL/  TDUM,P,NOBUB,NODEW,ISO,NLIQ
      COMMON  /NJIT0/  NC, NCM1, IDLL, IDLV, IDH, LDBUG, ISW,
     *                 NAME(2,10), L(10), NDIM, COMPNT(10)
      COMMON  /NJIT1/  CPL(10,4), CPV(10,4), ENP(10,10), ANT(6,10),
     *                 W(10)
      COMMON  /NJIT2/  C(180), ALPHA(45), VC(10), VOL(10), TC(10),
     *                 PC(10), QA(10), QB(10), AA(10,10), G(10,10),
     *                 THETA(10), THS(10), HFAC(10), HHFA(10), HM(10),
     *                 Q(10),R(10),XL(10),PHI(10),DUMMY(10)
      COMMON  /NJIT3/  TTC(10,10),PPC(10,10),VVC(10,10),ZZC(10,10),
     *                 AK(10,10), AVALUE(10,10), BVALUE(10,10),
     *                 BCROSS(10,10), OMEGA(10), DIPOLE(10), B(10,10)
      COMMON  /INR0/   NST, NSTM1, NK1, NK2, NK11, NK21, NCASE, KUNITS,
     *                 NFEED, LF(9), IDCODE, ITR, ITRMAX, ICODE
      COMMON  /INR1/   ESTR(9,11), FKV(9), HF(9), FLMAX(10), FVMAX(10),
     *                 DEST,DESTV,DESTL, BTMS, RFLX,BOIL, PP(50), T(50)
     *                 MU(50), SL(50), SV(50), FL(50), FLL(50,10),
     *                 FV(50), FVV(50,10), ZCONVT, ZCONVF
      COMMON  /INR2/   DFK(10,21), HL(50), HLL(50,10), CL(50), HHE(50),
     *                 DFXH(50,11), HV(50), HVV(50,10), CV(50)
      COMMON  /INR3/   AMAT(21,21), BMAT(50,21,21), D(50,21)
      COMMON  /INR4/   VAPOR, LIQUID, FEED(11)
      COMMON  /VLE/    XFK(10), GAM(10), X(10), Y(10), VP(10), FUG(10)
      COMMON  /KNST/   XFKNST(10)
C
      DATA             SMALL /0.00005/
C
      ICODE=0
      NST=0
C
      WRITE (NPRT,5)
    5 FORMAT ('1***  AZEOTROPIC DISTILLATION PROGRAM ***'/)
C
      READ (NCR,10) TITLE
   10 FORMAT (20A4)
      WRITE (NPRT,11) TITLE
   11 FORMAT ('0',19A4,A3)
C
C
C
C     BASIC CONTROL PARAMETERS
C
C        NC          NUMBER OF COMPONENTS
C        IDLL        LIQUID PHASE CLASSIFICATION CODE
C                        0    IDEAL
C                        1    NRTL
C                        2    WILSON
C                        3    UNIQUAC
C        IDLV        VAPOR PHASE CLASSIFICATION CODE
```

```
          C                                0     IDEAL
          C                                1     REDLICH-KWONG
          C                                2     VIRIAL-TSONOPOULOS'
          C            IDH        ENTHALPY CORRECTION
          C                                0     CORRECT BOTH PHASES
          C                                1     CORRECT VAPOR PHASE ONLY
          C                                2     NO CORRECTION
          C            LDBUG      DEBUG CODE
          C                                0     NO INTERMEDIATE PRINT
          C                                1     SUPERFICIAL TRACE
          C                                2     DETAILED TRACE
          C
          C
0028                READ (NCR,12) NC, IDLL, IDLV, IDH, LDBUG, NDIM
0029             12 FORMAT (20I2)
0030                NCM1=NC-1
0031                NDIM=0
0032                IF (IDLL.LT.0 .OR. IDLL.GT.4) IDLL=0
0033                IF (IDLV.LT.0 .OR. IDLV.GT.4) IDLV=0
0034                IF (IDLL.EQ.4 .AND. IDH.EQ.0) IDH=1
          C
0035                WRITE (NPRT,13) NC
0036             13 FORMAT ('0NUMBER OF COMPONENTS =', I3)
0037                WRITE (NPRT,14) IDLL,IDLV,IDH
0038             14 FORMAT ('0VAPOR-LIQUID EQUILIBRIUM DATA CODES:'/
               *          5X, 'LIQUID =', I4 /
               *          5X, 'VAPOR =', I5/
               *          5X, 'ENTHALPY =', I2/)
          C
          C
          C         READ IN THE PROGRAM CONTROL PARAMETERS, CALL SUBROUTINE
          C         PJIT FOR COMPONENT PROPERTIES, AND NLIQ,TF,PF FOR TWO-LIQ
          C        PROGRAM,ALSO THE INITIAL COMPOSITIONS IN EACH PHASE(XSAVE)
          C
          C
          C
          C         READ IN AZEOTROPIC DATA FOR REFLUX/PRODUCT SEPARATOR
          C
          C         TWO LIQUID PHASES  :   1= ORGANIC RICH (REFLUX)
          C                                2= AQUEOUS RICH (PURGE PRODUCT)
          C
0039                READ (5, 8) NLIQ,TF,PF
0040             8  FORMAT(I2,8X,6F10.5)
          C
          C         COMPONTIAL FLOW RATE IIN MOOLES/HR FD(I)-- TO BE ESTABLISHED
          C         BY DISTILLATION ALGORITHM , (FVV(NST,*),*=COOMPONENT # )
          C
          C
          C         READ IN THE INITIAL PHASE COMPOSITIONS 1=BZ,2=ETOH,3=WTR
          C         THEN NORMALIZE THE XSAVES
          C
          C
0041                READ (5,9) (XSAVE(I,1),I=1,NC)
0042             9  FORMAT(8F10.4)
0043                READ (5,9) (XSAVE(I,2),I=1,NC)
          C
```

```
0044                   CALL NJIT
                 C
0045              20 WRITE (NPRT,21) TITLE
0046              21 FORMAT ('1',19A4,A3)
0047                 RETURN
0048                 END
```

```
      SUBROUTINE TEST
      IMPLICIT REAL    (M)
      INTEGER          COMPNT
      REAL             LIQUID
C
      COMMON  /CTRL/   NCR, NPRT, NSTART, TITLE(20)
      COMMON /B2L/     FD(11),Z(10),EK(10,2),PF,TF,HI,XSAVE(10,2)
      COMMON /CONTRL/  IDUM,P,NOBUB,NODEW,ISO,NLTQ
      COMMON  /NJIT0/  NC, NCM1, IDLL, IDLV, IDH, LDBUG, ISW,
     *                 NAME(2,10), L(10), NDIM, COMPNT(10)
      COMMON  /NJIT1/  CPL(10,4), CPV(10,4), ENP(10,10), ANT(6,10),
     *                 N(10)
      COMMON  /NJIT2/  C(180), ALPHA(45), VC(10), VOL(10), TC(10),
     *                 PC(10), OA(10), OB(10), AA(10,10), G(10,10),
     *                 THETA(10), THS(10), HFAC(10), HHFA(10), HM(10),
     *                 W(10),R(10),XL(10),PHI(10),DUMMY(10)
      COMMON  /NJIT3/  TTC(10,10),PPC(10,10),VVC(10,10),ZZC(10,10),
     *                 AK(10,10), AVALUE(10,10), BVALUE(10,10),
     *                 BCROSS(10,10), OMEGA(10), DIPOLE(10), B(10,10)
      COMMON  /INR0/   NST, NSTM1, NK1, NK2, NK11, NK21, NCASE, KUNITS,
     *                 NFEED, LF(9), IDCODE, ITR, ITRMAX, TCODE
      COMMON  /INR1/   FSTR(9,11), FKV(9), HF(9), FLMAX(10), FVMAX(10),
     *                 DEST,DESTV,DESTL, BTMS, RFLX,BOIL, PP(50), T(50)
     *                 MU(50), SL(50), SV(50), FL(50), FLL(50,10),
     *                 FV(50), FVV(50,10), ZCONVT, ZCONVF
      COMMON  /INR2/   DFK(10,21), HL(50), HLL(50,10), CL(50), HHE(50),
     *                 DEXH(50,11), HV(50), HVV(50,10), CV(50)
      COMMON  /INR3/   AMAT(21,21), BMAT(50,21,21), D(50,21)
      COMMON  /INR4/   VAPOR, LIQUID, FEED(11)
      COMMON  /VLE/    XFK(10), GAM(10), X(10), Y(10), VP(10), FUG(10)
      COMMON  /KNST/   XFKNST(10)
C
      DATA             SMALL /0.00005/
C
      ITR=ITR+1
C
      WRITE (NPRT,75) ITR
   75 FORMAT ('0ITERATION # =', I4)
C
      IF (LDBUG.EQ.0) GO TO 110
      WRITE (NPRT,80)
   80 FORMAT (' STAGE    TEMP        PRES       LIQUID(MOLS)    VAPOR(MOL
     *)')
      DO 90 I=1,NST
      GO TO (81,85,85), KUNITS
   81 TDEG=(T(I)-273.16)*1.8+32.0
      PRES=PP(I)*14.696
      FLZ=FL(I)/453.59
      FVZ=FV(I)/453.59
      GO TO 90
   85 TDEG=T(I)
      PRES=PP(I)
      FLZ=FL(I)
      FVZ=FV(I)
   90 WRITE (NPRT,100) I,TDEG,PRES,FLZ,FVZ
  100 FORMAT (I5,F10.2,F12.3,F15.3,F14.3)
```

```
                C
                C      SUM OF SQUARES OF DISCREPANCY FUNCTIONS
                C
0039              110 REST=0.0
0040                  RESF=0.0
0041                  DTBIG=0.0
0042                  ITBIG=0
0043                  DLBIG=0.0
0044                  ILBIG=0
0045                  JLBIG=0
0046                  DVBIG=0.0
0047                  IVBIG=0
0048                  JVBIG=0
0049                  DO 120 I=1,NST
0050                  IF (ABS(D(I,NK1)).LT.DTBIG) GO TO 112
0051                  DTBIG=ABS(D(I,NK1))
0052                  ITBIG=I
0053              112 REST=REST+D(I,NK1)**2
0054                  DO 120 J=1,NC
0055                  IF (D(I,J).EQ.0.0) GO TO 115
0056                  IF (FLL(I,J)/FL(I).LT.SMALL) GO TO 115
0057                  IF (ABS(D(I,J))/FLL(I,J).LT.DLBIG) GO TO 113
0058                  DLBIG=ABS(D(I,J))/FLL(I,J)
0059                  ILBIG=I
0060                  JLBIG=J
0061              113 RESF=RESF+(D(I,J)/FLL(I,J))**2
0062              115 IF (D(I,J+NK1).EQ.0.0) GO TO 120
0063                  IF (FVV(I,J)/FV(I).LT.SMALL) GO TO 120
0064                  IF (ABS(D(I,J+NK1))/FVV(I,J).LT.DVBIG) GO TO 118
0065                  DVBIG=ABS(D(I,J+NK1))/FVV(I,J)
0066                  IVBIG=I
0067                  JVBIG=J
0068              118 RESF=RESF+(D(I,J+NK1)/FVV(I,J))**2
0069              120 CONTINUE
                C
0070                  WRITE (NPRT,130) REST,RESF
0071              130 FORMAT (' SUM DI**2 =',       G17.6, /
                    *               ' SUM (DF/F)**2 =', G13.6)
0072                  WRITE (NPRT,135) ITBIG,DTBIG,ILBIG,JLBIG,DLBIG,IVBIG,JVBIG,DVBIG
0073              135 FORMAT (5X,I5,G12.5,5X,2I5,G12.5,5X,2I5,G12.5)
                C
0074                  IF (ITR.EQ.ITRMAX) GO TO 160
                C
0075                  DO 150 I=1,NST
0076                  IF (ABS(D(I,NK1)).GT.ZCONVT) GO TO 160
0077                  DO 150 J=1,NC
0078                  IF (FLL(I,J)/FL(I).LT.SMALL) GO TO 140
0079                  IF (ABS(D(I,J))/FLL(I,J).GT.ZCONVF) GO TO 160
0080              140 IF (FVV(I,J)/FV(I).LT.SMALL) GO TO 150
0081                  IF (ABS(D(I,J+NK1))/FVV(I,J).GT.ZCONVF) GO TO 160
0082              150 CONTINUE
0083                  GO TO 190
                C
                C      SET ICODE=-1........ PROBLEM HAS NOT CONVERGED
0084              160 ICODE=-1
0085                  GO TO 200
```

```
               C
               C      SET ICODE=1..........TRIAL LIMIT REACHED OR BAD COLUMN DATA
0086             180  ICODE=1
0087                  GO TO 200
               C
               C      SET ICODE=0..........PROBLEM CONVERGED
0088             190  ICODE=0
               C
0089             200  RETURN
0090                  END
```

```
                SUBROUTINE NJIT
          C
                DOUBLE PRECISION EQNW, EQNU
                INTEGER          COMPNT, ID(10)
                REAL             TREF(10), HVAP(10), EK(10)
          C
                COMMON  /CTRL/   NCR, NPRT, NSTART, TITLE(20)
                COMMON  /NJIT0/  NC, NCM1, IDLL, IDLV, IDH, LDBUG, ISW,
               *                 NAME(4,10), L(10), NDIM, COMPNT(10)
                COMMON  /NJIT1/  CPL(10,4), CPV(10,4), ENP(10,10), ANT(6,10),
               *                 W(10)
                COMMON  /NJIT2/  C(180), ALPHA(45), VC(10), VOL(10), TC(10),
               *                 PC(10), OA(10), OB(10), AA(10,10), G(10,10),
               *                 THETA(10), THS(10), HFAC(10), HHFA(10), HM(10),
               *                 Q(10),R(10),XL(10),PHI(10),DUMMY(10)
                COMMON  /NJIT3/  TTC(10,10),PPC(10,10),VVC(10,10),ZZC(10,10),
               *                 AK(10,10), AVALUE(10,10), BVALUE(10,10),
               *                 BCROSS(10,10), OMEGA(10), DIPOLE(10), B(10,10)
          C
                DATA             EQNR /'NRTL'/
                DATA             EQNW /'WILSON'/
                DATA             EQNU /'UNIQUAC'/
          C
                DATA             OMA, OMB  /0.42748, 0.08664/
          C
                WRITE (NPRT,30)
             30 FORMAT ('0NOTE: ALL FLOWS ARE  PER UNIT TIME, AND ENERGY' /
               *        '       VALUES ARE IN UNITS OF K-BTU PER UNIT TIME.')
          C
          C
          C
          C        THE 1ST CARD IS THE PROBLEM TITLE CARD
          C        THE 2ND CARD IS THE CONTROL PARAMETERS CARD
          C        THE ABOVE TWO CARDS ARE SPECIFFIED IN MAIN PROGRAM
          C
          C     COMPONENT DATA, FOUR CARD(IDLV=2),THREE CARDS(IDLV=0,1)
          C
                CONTINUE
          C      CARD #1
          C         NAME       COMPONENT NAME
          C         L          COMPONENT TYPE
          C                           0     NORMAL
          C                           1     SUPER CRITICAL
          C                           2     NON CONDENSIBLE
          C                           3     NON VOLATILE
          C         W          MOLECULAR WEIGHT---G/G MOLE
          C         TC         CRITICAL TEMPERATURE---DEG K
          C         PC         CRITICAL PRESSURE----- ATM
          C         VC         CRITICAL VOLUME----CC/G MOLE
          C         VOL        MOLAR VOLUME---CC/G MOLE
          C         OB         REDLICH-KWONG PARAMETERS
          C
          C      CARD #2 (IF VIRIAL IS CHOSEN) TSONOPOULOS' PARAMETERS
          C         AVALUE----TSONOPOULOS' COMPONT PARAMETER 'A'
          C         BVALUE----                               'B'
```

```
C            ZZC-------CRITICAL COMPRESSIBILITY OF COMPONENT
C            OMEGA-----PITZER'S ACENTRIC FACTOR
C
C
C        CARD #2-A(OPTIONAL, USED IF UNIQUAC IS  CHOSEN)
C        COMPONENT SURFACE AREA AND VOLUME PARAMETERS
C            R(I)------COMPONENT SURFACE PARAMETER
C            Q(I)----- COMPONENT VOLUME PARAMETER
       CONTINUE
C
C        CARD #3 (IF VIRIAL IS CHOSEN,OTHERWISE #2) ENTHALPY  DATA
C
C            HVAP       HEAT OF VAPORIZATION---CAL/G MOLE
C            TREF       REFERENCE TEMPERATURE(NORMAL B.P.)--DEG K
C            CPL        SPECIFIC HEAT CONSTANTS       LIQUID
C            CPV      (CAL/G MOLE-K)                  VAPOR
C
       CONTINUE
C        CARD#4(IF VIRIAL IS CHOSEN,OTHERWISE #3) VAP PRESS CONSTANTS
C        ANTOINE'S EQ.   LN(VAP PRESS) =  C1 +  C2/(C3+TEMP); MMHG,K
C
C
C            INTERNAL CODE VALUES FOR COMPONENT TYPE
C                      -1    NON-VOLATILE
C                       0    NON-CONDENSIBLE
C                       1    NORMAL
C                       2    SUPERCRITICAL
C
C
C       AK(I,J) THE TSONOPOULOS' BINARY CONSTANTS ONE PER COMPONENT
C       MUST FOLLOW THE LAST COMPONENT PROPERTIES CARD, AND IF NRTL
C       OR OTHER ACTIVITY METHOS ARE USED THEN READ IN THE BINARY
C       PARAMETERS CARD AFTER THE LAST AK(I,J) CARD
C
C
C
C
      DO 250 I=1,NC
      READ (NCR,230) (NAME(J,I),J=1,2),L(I),W(I),TC(I),PC(I),VC(I),
     *                 VOL(I), OA(I),OB(I)
  230 FORMAT (2A4,I2,7F10.0)
C
      VVC(I,I)=VC(I)
      TTC(I,I)=TC(I)
      PPC(I,I)=PC(I)
      IF (IDLV.NE.2) GO TO 81
   75 READ (NCR,240)  AVALUE(I,I),BVALUE(I,I),ZZC(I,I),OMEGA(I)
C
C
C     READ  IN UNIQUAC COMPONENT MOLECULAR SURFACE  AREA AND VOLUME
C     PARAMETERS  R(I) AND Q(I) , IF IDLL=3
C
C
   81 IF (IDLL.NE.3) GO TO 82
      READ(NCR,240) R(I),Q(I)
      XL(I)=5.0*(R(I)-Q(I))-(R(I)-1.0)
```

```
  82  IF (L(I)-1) 150,160,170
  150 L(I)=1
      GO TO 200
  160 L(I)=2
      GO 10 200
  170 IF (L(I)-3) 180,190,150
  180 L(I)=0
      GO TO 200
  190 L(I)=-1
  200 CONTINUE
C
      IF (W(I).LE.0.0) W(I)=1.0
      READ (NCR,240) HVAP(I),TREF(I),(CPL(I,J),J=1,3),(CPV(I,J),J=1,3)
      CPL(I,4)=0.0
      CPV(I,4)=0.0
  240 FORMAT (8F10.5)
      READ (NCR,240) (ANT(J,I),J=1,6)
  250 CONTINUE
C
C
C    IF VIRIAL IS CHOSEN, THEN READ IN AK(I,J) IN THE ORDER OF
C     AK(1,1),AK(1,2),AK(1,3) PER COMPONENT #1 FOR NC=3, THEN
C     READ IN AK(21),AK(2,2),AK(2,3) ETC.
C
C
C     IF VIRIAL IS USED READ IN TSONOPOULOS'  BINARY CONSTANTS
C
      IF(IDLV.NE.2) GO TO  259
      DO 85 I=1,NC
  85  READ (NCR,240) (AK(I,J),J=1,NC)
C
C
C     CALL IN VIRMIX TO CALCULATE CRITICAL BINARY PROPERTES
C
      CALL VIRMIX
  259 WRITE (NPRT,260)  (J,J=1,NC)
C
  260 FORMAT ('0COMPONENT NO',23X,9(I1,9X))
      WRITE (NPRT,270) ((NAME(J,I),J=1,2),I=1,NC)
  270 FORMAT (' NAME',25X,9(2A4,2X))
      WRITE (NPRT,280) (W(J),J=1,NC)
  280 FORMAT (' MOLECULAR WEIGHT',16X,9(F5.1,5X))
      WRITE (NPRT,290) (TC(J),J=1,NC)
  290 FORMAT (' CRITICAL PROPERTIES'/' TEMPERATURE  (DEG K)',10X,
     *       9(F7.1,3X))
      WRITE (NPRT,300) (PC(J),J=1,NC)
  300 FORMAT (' PRESSURE       ( ATM)',11X,9(F7.1,3X))
      WRITE (NPRT,310) (VC(J),J=1,NC)
  310 FORMAT (' VOLUME          (CC/GMOL)',6X,9(F7.1,3X))
      IF (IDLL.NE.3) GO TO 314
      WRITE (NPRT,291) (R(I),I=1,NC)
  291 FORMAT('  UNIQUAC COMPONT R(I)      ',6X,9(F7.4,3X))
      WRITE (NPRT,292) (Q(I),I=1,NC)
  292 FORMAT('  UNIQUAC COMPONT Q(I)      ',6X,9(F7.4,3X))
  314 IF (IDLV.NE.2) GO TO 311
      WRITE(NPRT,315)  (ZZC(I,I),I=1,NC)
```

```
  315 FORMAT(' COMPRESSIBILITY  ',13X,9(F7.3,3X))
      WRITE (NPRT,316) (OMEGA(I),I=1,NC)
  316 FORMAT(' ACENTRIC FACTOR  ',13X,9(F7.3,3X))
      WRITE (NPRT,317) (AVALUE(I,I),I=1,NC)
  317 FORMAT(' TSONOPOULOS -A-  ',13X,9(F7.4,3X))
      WRITE (NPRT,318) (BVALUE(I,I),I=1,NC)
  318 FORMAT(' TSONOPOULOS -B-  ',13X,9(F7.4,3X))
      DO 319 I=1,NC
      DO 319 J=1,NC
  319 WRITE(NPRT,321) I,J,AK(I,J)
  321 FORMAT(' AK(',I1,',',I1,')= ',9(F7.3,3X))
 311  WRITE (NPRT,320) (ANT(1,J),J=1,NC)
  320 FORMAT (' VAPOR PRESSURE CONSTANTS'/' ( MMHG AND DEG K)'/
     *        ' C(1)',26X,9(F7.3,3X))
      DO 340 I=2,6
      WRITE (NPRT,330) I,(ANT(I,J),J=1,NC)
  330 FORMAT (' C(',I1,')',23X,9F10.2)
  340 CONTINUE
      WRITE (NPRT,350)
  350 FORMAT (' LIQUID MOLAR VOLUME CONSTANTS')
      I=1
      WRITE (NPRT,390) I,(VOL(J),J=1,NC)
      WRITE (NPRT,360) (HVAP(J),J=1,NC)
  360 FORMAT (' ENTHALPY CONSTANTS (CAL/GM)' /
     *        ' LATENT HEAT',19X,9(F7.1,3X))
      WRITE (NPRT,370) (TREF(J),J=1,NC)
  370 FORMAT (' AT DEG K',22X,9(F7.1,3X))
      WRITE (NPRT,380)
  380 FORMAT (' LIQUID SP. HEAT CONSTANTS')
      DO 400 I=1,4
      WRITE (NPRT,390) I,(CPL(J,I),J=1,NC)
  390 FORMAT (' C(',I1,')',23X,9F10.3)
  400 CONTINUE
      WRITE (NPRT,410)
  410 FORMAT (' VAPOR SP. HEAT CONSTANTS')
      DO 420 I=1,4
      WRITE (NPRT,390) I,(CPV(J,I),J=1,NC)
  420 CONTINUE
      DO 440 I=1,NC
      DO 430 J=1,4
      CPL(I,J)=CPL(I,J)*W(I)
  430 CPV(I,J)=CPV(I,J)*W(I)
      HVAP(I)=HVAP(I)*W(I)
      ENP(I,5)=CPL(I,4)/4.0
      ENP(I,4)=CPL(I,3)/3.0
      ENP(I,3)=CPL(I,2)/2.0
      ENP(I,2)=CPL(I,1)
      TR=TREF(I)
      ENP(I,1)=-(((ENP(I,5)*TR+ENP(I,4))*TR+ENP(I,3))*TR+ENP(I,2))*TR
      ENP(I,10)=CPV(I,4)/4.0
      ENP(I,9)=CPV(I,3)/3.0
      ENP(I,8)=CPV(I,2)/2.0
      ENP(I,7)=CPV(I,1)
  440 ENP(I,6)=HVAP(I)-(((ENP(I,10)*TR+ENP(I,9))*TR+ENP(I,8))*TR+
     *             ENP(I,7))*TR
C
```

```
C     LIQUID-LIQUID BINARY CONSTANTS
C         C          CONSTANTS FOR NRTL, WILSON, & UNIQUAC
C
C     RENON ALPHA PARAMETERS
C         ALPHA      NRTL CONSTANTS
C
      IF (IDLL.EQ.0) GO TO 520
C
  450 J=NC*NCM1*2
      DO 460 I=1,NC
      AA(I,I)=0.0
  460 G(I,I)=1.0
C
      READ (NCR,240) (C(I),I=1,J)
      IF (IDLL.EQ.3) GO TO 473
 469  WRITE(NPRT,470) EQNR
  470 FORMAT ('0',A6,' CONSTANTS, CAL/GMOL')
 473  WRITE(NPRT,462) EQNU
 462  FORMAT('0',A7,' PARAMETERS,CAL/G MOL')
      K=0
      DO 490 I=1,NCM1
      II=I+1
      DO 490 J=II,NC
      K=K+4
      IF (J.LE.9)  ID(1)=10*I+J
      IF (J.GE.10) ID(1)=100*I+J
      IF (I.LE.9)  ID(2)=10*J+I
      IF (I.GE.10) ID(2)=100*J+I
      WRITE (NPRT,480) ID(1),C(K-3),ID(1),C(K-2),ID(2),C(K-1),ID(2),C(K)
  480 FORMAT (4X,2(5X,'A',I4,' =',F9.2,5X,'B',I4,' =',F9.2,5X))
  490 CONTINUE
C
      IF (IDLL.NE.1) GO TO 520
C
      J=NC*NCM1/2
      READ (NCR,240) (ALPHA(I),I=1,J)
      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 (9X,4('ALPHA',I2,' =',F7.4,5X))
      KK=1
  510 CONTINUE
      IF (KK.EQ.1) GO TO 520
      KK=KK-1
      WRITE (NPRT,500) (ID(I),EK(I),I=1,KK)
C
  520 IF (IDLV.EQ.0) GO TO 640
```

```
      530 DO 580 I=1,NC
          IF (OA(I).NE.0.0) GO TO 550
          OA(I)=OMA
      550 IF (OB(I).NE.0.0) GO TO 570
          OB(I)=OMB
      570 OA(I)=SQRT(OA(I)*TC(I)**2.5/PC(I))
      580 OB(I)=OB(I)*TC(I)/PC(I)
    C
      640 RETURN
          END
```

```
               SUBROUTINE READIN
         C
               IMPLICIT REAL         (M)
               INTEGER               COMPNT
               REAL                  LIQUID, OUT(15,10)
               DIMENSION             TF(9), NN(9), SLSV(9), FCALC(11)
         C
               COMMON   /CTRL/       NCR, NPRT, NSTART, TITLE(20)
         C
               COMMON   /NJIT0/      NK, NCM1, IDLL, IDLV, IDH, LDBUG, ISW,
              *                      NAME(4,10), L(10), NDIM, COMPNT(10)
               COMMON   /NJIT1/      CPL(10,4), CPV(10,4), ENP(10,10), ANT(6,10),
              *                      W(10)
               COMMON   /INR0/       NST, NSTM1, NK1, NK2, NK11, NK21, NCASE, KUNITS,
              *                      NFEED, LF(9), IDCODE, ITR, ITRMAX, ICODE
               COMMON   /INR1/       FSTR(9,11), FKV(9), HF(9), FLMAX(10), FVMAX(10),
              *                      DEST,DESTV,DESTL, BTMS, RFLX,BOIL, PP(50), T(50),
              *                      MU(50), SL(50), SV(50), FL(50), FLL(50,10),
              *                      FV(50), FVV(50,10), ZCONVT, ZCONVF
               COMMON   /INR4/       VAPOR, LIQUID, FEED(11)
               COMMON   /VLE/        XFK(10), GAM(10), X(10), Y(10), VP(10), FUG(10)
               COMMON   /KNST/       XFKNST(10)
         C
               EQUIVALENCE           (WATER,VAPOR)
         C
               DATA                  CONVT /0.01/, CONVF /0.0001/
         C
         C     READ COLUMN SPECIFICATIONS
         C
         C          NCASE  ...  CALCULATION CODE
         C                1     ABSORBER/STRIPPER
         C                2     REBOILED ABSORBER/STRIPPER
         C                3     DISTILLATION COLUMN WITH PRODUCT RATES & REFLUX RATIO
         C                4     DISTILLATION COLUMN WITH PRODUCT RATES & BOILUP RATIO
         C                5     REBOIED ABSORBER
         C
         C          NSTART  ...  CALCULATION CODE
         C               -1     CHANGE MADE TO FEED AND/OR THE DESIGN PARAMETER
         C                0     NEW PROBLEM
         C               +1     NEW PROBLEM ... INPUT THE OVERHEAD AND BOTTOMS PRODUCTS
         C
         C          IDCODE  ...  DISTILLATE CODE
         C               -1     SUBCOOLED LIQUID
         C                0     VAPOR OR VAPOR/LIQUID
         C               +1     LIQUID AT THE BUBBLE POINT
         C
               RFLX=0.0
               BOIL=0.0
               NSAVE=NST
         C
               READ (NCR,10,END=700,ERR=700) NCASE,NSTART,NST,NFEED,NSL,NSV,
              *                             ITRMAX,KUNITS,IDCODE
            10 FORMAT (9I2)
         C
               IF (KUNITS.LE.0) KUNITS=2
               IF (ITRMAX.LE.0) ITRMAX=50
```

```
C
      READ (NCR,20) MUS,ZCONVT,ZCONVF
   20 FORMAT (8F10.0)
C
      NSTM1=NST-1
      ZCONVT=ABS(ZCONVT)
      ZCONVF=ABS(ZCONVF)
      IF (ZCONVT.EQ.0.0) ZCONVT=CONVT
      IF (ZCONVF.EQ.0.0) ZCONVF=CONVF
C
      IF (NCASE.EQ.0) NCASE=3
      GO TO (31,33,35,37,39), NCASE
   31 WRITE (NPRT,32)
   32 FORMAT ('0ABSORBER STRIPPER SIMULATION')
      IDCODE=0
      GO TO 45
   33 WRITE (NPRT,34)
   34 FORMAT ('0REBOILED ABSORBER STRIPPER SIMULATION')
      IDCODE=0
      GO TO 45
   35 WRITE (NPRT,36)
   36 FORMAT ('0DISTILLATION COLUMN; PRODUCT RATES & REFLUX RATIO SPECIF
     *IED')
      GO TO 45
   37 WRITE (NPRT,38)
   38 FORMAT ('0DISTILLATION COLUMN; PRODUCT RATES & BOILUP RATIO SPECIF
     *IED')
      GO TO 45
   39 WRITE (NPRT,40)
   40 FORMAT ('0 REBOILED  ABSORBER ')
      IDCODE=0
C
   45 NK1=NK+1
      NK2=2*NK+1
      NK11=NK1+1
      NK21=NK2-1
C
C     READ MURPHREE STAGE EFFICIENCIES.  IF 'MUS' IS POSITIVE,
C     ONE CONSTANT EFFICIENCY IS READ INTO 'MU'.
C
      IF (MUS.LT.10.0) GO TO 100
      DO 49 I=1,NST
   49 MU(I)=0.0
C
   50 READ (NCR,60) J,K,MUS
   60 FORMAT (2(I2,8X),F10.0)
C
      IF (J.EQ.0) GO TO 80
      IF (K.EQ.0) K=J
      IF (MUS.LE.0.0) MUS=1.0
      DO 70 I=J,K
   70 MU(I)=MUS
      GO TO 50
   80 DO 90 I=1,NST
      IF (MU(I).EQ.0.0) MU(I)=1.0
   90 CONTINUE
```

```
            GO TO 120
        100 IF (MUS.LE.0.0) MUS=1.0
            DO 110 I=1,NST
        110 MU(I)=MUS
        120 CONTINUE
      C
            IF (NCASE.NE.1) MU(1)=1.0
            IF (NCASE.GE.3) MU(NST)=1.0
      C
      C     TEMPERATURE AT COLUMN TOP (TT) AND COLUMN BOTTOM (TB) ARE
      C     IN DEGREES K.  PRESSURE AT TOP OF COLUMN (PP-NST) AND THE
      C     STAGE PRESSURE DROP (DPATM) ARE IN MMHG ABS.
      C
      C     REBOILER IS STAGE 1
      C
            READ (NCR,20) DESTV,DESTL,DUMMY,TT,TB,PP(NST),DPATM
            DPATM=ABS(DPATM)
      C
            GO TO (121,125,125), KUNITS
        121 TT=(TT-32.0)/1.8+273.16
            TB=(TB-32.0)/1.8+273.16
            PP(NST)=PP(NST)/14.696
            DPATM=DPATM/14.696
            DESTV=DESTV*453.59
            DESTL=DESTL*453.59
      C
        125 IF (NCASE.EQ.3) RFLX=DUMMY
            IF (NCASE.EQ.4) BOIL=DUMMY
            IF (NCASE.EQ.5) BOIL=DUMMY
      C
            DEST=DESTV+DESTL
            IF (IDCODE.EQ.0) GO TO 129
            DESTV=DEST
            DESTL=0.0
            DO 126 J=1,NK
            ZVP=EXP(ANT(1,J)+ANT(2,J)/(ANT(3,J)+TT)+ANT(4,J)*TT+ANT(5,J)*
           *        TT*TT+ANT(6,J)*ALOG(TT))
        126 XFKNST(J)=ZVP/PP(NST)
      C
      C     ASSUME CONSTANT PRESSURE DROP ACROSS THE COLUMN
      C
        129 PP(1)=PP(NST)+NSTM1*DPATM
            DO 130 I=2,NST
        130 PP(I)=PP(I-1)-DPATM
      C
      C     GUESS OF THE TEMPERATURE PROFILE IN THE COLUMN.
      C
            IF (NSTART.LT.0) GO TO 140
            DO 131 I=1,NST
        131 T(I)=TB+(I-1)*(TT-TB)/NSTM1
      C
      C
        140 DO 141 J=1,NK1
        141 FEED(J)=0.0
            DO 144 I=1,NST
            SL(I)=0.0
```

```
  144 SV(I)=0.0
      NFTOP=0
      NFBTM=0
C
      DO 145 I=1,10
      DO 145 J=1,15
  145 OUT(J,I)=0.0
C
      WRITE (NPRT,150)
  150 FORMAT ('0FEED STREAMS:')
C
C     READ FEED SPECIFICATIONS ... INTERNAL UNITS
C         FEED / EXTERNAL HEAT STREAM
C                   LF          STAGE
C                   QIN         ENERGY INPUT, K-CAL/UNIT TIME
C                   TF          TEMPERATURE, DEG K
C                   FKV         FRACTION VAPOR
C                   FSTR        FEED RATE .. COMPONENTS, MOLES/UNIT TIME
C                   HF          COMPUTED FEED STREAM ENERGY, CAL
C
      DO 206 I=1,NFEED
C
      READ (NCR,155) LF(I),QIN,TF(I),FKV(I),(FSTR(I,J),J=1,5)
  155 FORMAT (I2,F8.0,7F10.0)
      IF (NK.GT.5) READ (NCR,20) (FSTR(I,J),J=6,NK)
      GO TO (156,165,165), KUNITS
  156 TF(I)=(TF(I)-32.0)/1.8+273.16
      QIN=QIN*252.16*1.0E3
      DO 157 J=1,NK
C 157 FSTR(I,J)=FSTR(I,J)*453.59
  165 IF (LF(I).EQ.1)    NFBTM=I
      IF (LF(I).EQ.NST) NFTOP=I
      FSTR(I,NK1)=0.0
      HF(I)=0.0
      TK=TF(I)
C
      IF (QIN.NE.0.0) GO TO 190
C
      DO 169 J=1,NK
      HF(I)=HF(I) + FSTR(I,J)*FKV(I)*(((((ENP(J,10)*TK+ENP(J,9))*TK+
     *      ENP(J,8))*TK+ENP(J,7))*TK+ENP(J,6)) + FSTR(I,J)*(1.0-FKV(I))
     *      *((((ENP(J,5)*TK+ENP(J,4))*TK+ENP(J,3))*TK+ENP(J,2))*TK+
     *      ENP(J,1))
  169 FSTR(I,NK1)=FSTR(I,NK1)+FSTR(I,J)
C
      IF (FKV(I).EQ.0.0) GO TO 178
C
      IF (IDLV.EQ.0) GO TO 188
      IF (IDH.EQ.2) GO TO 188
      ISTAGE=LF(I)
      DO 170 J=1,NK
      VP(J)=PP(ISTAGE)
  170 Y(J)=FSTR(I,J)/FSTR(I,NK1)
      CALL FUGCTY (TF(I),PP(ISTAGE),Y,VP,FUG,DHV)
      HF(I)=HF(I)+DHV*FSTR(I,NK1)
```

```
      GO TO 188
C
  178 IF (IDLL.EQ.0) GO TO 188
      IF (IDH.GT.0) GO TO 188
      DO 179 J=1,NK
  179 X(J)=FSTR(I,J)/FSTR(I,NK1)
      ISW=0
      CALL XSHLIN (TF(I),X,XSH)
      HF(I)=HF(I)+XSH*FSTR(I,NK1)
C
  188 DO 189 J=1,NK1
  189 FEED(J)=FEED(J)+FSTR(I,J)
C
  190 HF(I)=HF(I)+QIN
      GO TO (191,195,195), KUNITS
  191 TDEG=(TF(I)-273.16)*1.8+32.0
      H=HF(I)/252.16/1.0E3
      QINQ=QIN/252.16/1.0E3
      DO 192 J=1,NK1
  192 FCALC(J)=FSTR(I,J)/453.59
      GO TO 201
  195 TDEG=TF(I)
      H=HF(I)
      QINQ=QIN
      DO 196 J=1,NK1
  196 FCALC(J)=FSTR(I,J)
C
  201 IF (QIN.EQ.0.0) GO TO 202
      OUT(1,I)=LF(I)
      OUT(4,I)=QINQ
      GO TO 206
C
  202 OUT(1,I)=LF(I)
      OUT(2,I)=TDEG
      OUT(3,I)=FKV(I)
      OUT(4,I)=H
      DO 205 J=1,NK
  205 OUT(J+4,I)=FCALC(J)
      OUT(NK1+4,I)=FCALC(NK1)
C
  206 CONTINUE
C
      NFP1=NFEED+1
      DO 207 J=1,NK
  207 OUT(J+4,NFP1)=FEED(J)
      OUT(NK1+4,NFP1)=FEED(NK1)
C
      GO TO (208,210,210), KUNITS
  208 DO 209 J=1,NK
  209 OUT(J+4,NFP1)=FEED(J)/453.59
      OUT(NK1+4,NFP1)=FEED(NK1)/453.59
C
  210 WRITE (NPRT,211) (OUT(1,I),I=1,NFEED)
  211 FORMAT (' STAGE', 15X, 10F12.0)
      WRITE (NPRT,212) (OUT(2,I),I=1,NFEED)
  212 FORMAT (' TEMP ', 15X, 10F12.2)
```

```
      WRITE (NPRT,213) (OUT(3,I),I=1,NFEED)
  213 FORMAT (' FRACV', 15X, 10F12.4)
      WRITE (NPRT,214) (OUT(4,I),I=1,NFEED)
  214 FORMAT (' H    ', 15X, 1P10E12.4)
      DO 215 J=1,NK
  215 WRITE (NPRT,216) J,(NAME(K,J),K=1,2),(OUT(J+4,I),I=1,NFP1)
  216 FORMAT (' COMP', I2, 2X,2A4,5X, F11.3, 9F12.3)
      WRITE (NPRT,217) (OUT(NK1+4,I),I=1,NFP1)
  217 FORMAT (' TOTAL', 15X, 10F12.3)
C
  225 IF (NSL.EQ.0) GO TO 265
      DO 235 J=1,NSL
  235 READ (NCR,240) NN(J),SLSV(J)
  240 FORMAT (I2,8X,F10.0)
      GO TO 265
  250 WRITE (NPRT,251)
  251 FORMAT ('OLIQUID SIDE STREAMS'/' STAGE',3X,'MOLES')
      DO 264 J=1,NSL
      N=NN(J)
      SL(N)=SLSV(J)
      WRITE (NPRT,260) N,SL(N)
  260 FORMAT (I5,F11.3)
      GO TO (261,264,264), KUNITS
  261 SL(N)=SL(N)*453.59
  264 CONTINUE
      GO TO 270
C
  265 IF (DESTL.EQ.0.0 .AND.NSL.EQ.0) GO TO 270
      NSL=NSL+1
      NN(NSL)=NST
      SLSV(NSL)=DESTL/453.59
      GO TO 250
C
  270 IF (NSV.EQ.0) GO TO 300
      WRITE (NPRT,280)
  280 FORMAT ('OVAPOR SIDE STREAMS'/' STAGE',3X,'MOLES')
      DO 285 J=1,NSV
  285 READ (NCR,240) NN(J),SLSV(J)
      DO 299 J=1,NSV
      N=NN(J)
      SV(N)=SLSV(J)
      WRITE (NPRT,260) N,SV(N)
      GO TO (291,299,299), KUNITS
  291 SV(N)=SV(N)*453.59
  299 CONTINUE
C
C     FIRST GUESS OF THE COMPONENT FLOWS AND THE TOTAL FLOWS.
C
  300 XDEST=0.0
      DO 310 I=1,NST
  310 XDEST=XDEST+SV(I)+SL(I)
      BTMS=FEED(NK1)-DESTV-XDEST
      IF (BTMS.LE.0.0) GO TO 680
C
      IF (NSTART.LE.0) GO TO 320
C
```

```
      READ (NCR,20) (FVV(NST,J),J=1,NK)
      READ (NCR,20) (FVV(1,J),J=1,NK)
      READ (NCR,20) (FLL(NST,J),J=1,NK)
      READ (NCR,20) (FLL(1,J),J=1,NK)
      GO TO (301,320,320), KUNITS
  301 DO 302 J=1,NK
      FVV (NST,J)=FVV(NST,J)*453.59
  302 FLL(1,J)=FLL(1,J)*453.59
C
  320 GO TO (330,330,410,410,410), NCASE
C
C     ABSORBER / STRIPPER
C
C     SET MAX DEVIATIONS IN COMPONENT FLOWS BETWEEN ITERATIONS
  330 DO 340 J=1,NK
      FVMAX(J)=FEED(J)
  340 FLMAX(J)=FEED(J)
C
      IF (NSTART) 521,380,350
C
  350 FV(NST)=0.0
      FL(1)=0.0
      DO 360 J=1,NK
      FVV(1,J)=FSTR(NFBTM,J)
      FLL(NST,J)=FSTR(NFTOP,J)
      FV(NST)=FV(NST)+FVV(NST,J)
  360 FL(1)=FL(1)+FLL(1,J)
C     FV(1)=FSTR(NFBTM,NK1)
C     FL(NST)=FSTR(NFTOP,NK1)
      DO 370 I=2,NSTM1
      FV(I)=FV(I-1)+(FV(NST)-FV(1))/NSTM1
      FL(I)=FL(I-1)+(FL(NST)-FL(1))/NSTM1
      DO 370 J=1,NK
      FVV(I,J)=FVV(I-1,J)+(FVV(NST,J)-FVV(1,J))/NSTM1
      FLL(I,J)=FLL(I-1,J)+(FLL(NST,J)-FLL(1,J))/NSTM1
  370 CONTINUE
      GO TO 530
C
  380 DO 390 I=1,NST
      FV(I)=FSTR(NFBTM,NK1)
      FL(I)=FSTR(NFTOP,NK1)
      DO 390 J=1,NK
      FVV(I,J)=FSTR(NFBTM,J)
      FLL(I,J)=FSTR(NFTOP,J)
      IF (FVV(I,J).LE.0.0) FVV(I,J)=1.0E-20
      IF (FLL(I,J).LE.0.0) FLL(I,J)=1.0E-20
  390 CONTINUE
      DO 400 J=1,NK
      FVV(NST,J)=FVV(NST,J)/FV(NST)*DEST
  400 FLL(1,J)=FLL(1,J)/FL(1)*BTMS
      FV(NST)=DEST
      FL(1)=BTMS
      GO TO 530
C
C     DISTILLATION COLUMN (REFLUX OR BOTLUP SPECIFIED)
C
```

```
C     SET MAX DEVIATIONS IN COMPONENT FLOWS BETWEEN ITERATIONS
  410 DO 420 J=1,NK
      FVMAX(J)=FEED(J)*(1.0+DUMMY)
  420 FLMAX(J)=FEED(J)*(1.0+DUMMY)
C
      IF (NSTART.LT.0) GO TO 521
C
      FV(NST)=DESTV
      FL(1)=BTMS
      IF (NCASE.EQ.3) FL(NST)=DEST*RFLX
      IF (NCASE.EQ.4) FV(1)=BTMS*BOIL
      IF (NCASE.EQ.5) FV(1)= BTMS*BOIL
      SS=0.0
      S=0.0
      DO 430 I=1,NFEED
      IF (LF(I).EQ.NST) S=FSTR(I,NK1)*FKV(I)
      IF (LF(I).EQ.1) SS=FSTR(I,NK1)*(1.0-FKV(I))
  430 CONTINUE
      FV(NSTM1)=FL(NST)-S+SV(NST)+SL(NST)+DESTV
      DO 440 II=3,NST
      IF (NST.LE.2) GO TO 440
      I=NST+2-II
      FL(I)=FL(I+1)-SL(I)
      FV(I-1)=FV(I)+SV(I)
  440 CONTINUE
      DO 460 I=1,NFEED
      J=LF(I)
      S=(1.0-FKV(I))*FSTR(I,NK1)
      SSS=FKV(I)*FSTR(I,NK1)
      DO 450 II=2,J
      FL(II)=FL(II)+S
  450 FV(II-1)=FV(II-1)-SSS
  460 CONTINUE
      FL(1)=BTMS
C
      IF (NSTART.GT.0) GO TO 480
C
      DO 470 I=1,NST
      DO 470 J=1,NK
      FVV(I,J)=FEED(J)/FEED(NK1)*FV(I)
  470 FLL(I,J)=FEED(J)/FEED(NK1)*FL(I)
      GO TO 530
C
  480 S=0.0
      SS=0.0
      DO 490 J=1,NK
      S=S+FVV(NST,J)
  490 SS=SS+FLL(1,J)
      DO 500 J=1,NK
      FVV(NST,J)=FVV(NST,J)/S
      FLL(NST,J)=FVV(NST,J)
      FLL(1,J)=FLL(1,J)/SS
  500 FVV(1,J)=FLL(1,J)
      DO 510 I=2,NSTM1
      DO 510 J=1,NK
      FVV(I,J)=FVV(I-1,J)+(FVV(NST,J)-FVV(1,J))/NSTM1
```

```
  510 FLL(I,J)=FLL(I-1,J)+(FLL(NST,J)-FLL(1,J))/NSTM1
      DO 520 I=1,NST
      DO 520 J=1,NK
      FVV(I,J)=FVV(I,J)*FV(I)
  520 FLL(I,J)=FLL(I,J)*FL(I)
      GO TO 530
C
C     FOR NSTART=-1 CHECK FOR ZERO FLOWS
C
  521 IF (NST.LE.NSAVE) GO TO 525
      DO 522 I=NSAVE,NST
      FL(I)=FL(NSAVE)
      FV(I)=FV(NSAVE)
      DO 522 J=1,NK
      FLL(I,J)=FLL(NSAVE,J)
  522 FVV(I,J)=FVV(NSAVE,J)
      GO TO 530
  525 FV(NST)=DESTV
      FL(1)=BTMS
C
C     SCREEN COMPONENT TYPE AND ADJUST INITIAL FLOW MAP
C
  530 DO 538 J=1,NK
      IF (L(J).NE.-1) GO TO 534
C     NON-VOLATILE COMPONENT, VAPOR FLOW = 0.0
      DO 532 I=1,NST
  532 FVV(I,J)=0.0
      GO TO 538
  534 IF (L(J).NE.0) GO TO 538
C     NON-CONDENSABILE COMPONENT, LIQUID FLOW = 0.0
      DO 536 I=1,NST
  536 FLL(I,J)=0.0
  538 CONTINUE
      DO 1030 I=1,NST
      SUMV=0.0
      SUML=0.0
      DO 1010 J=1,NK
      SUMV=SUMV+FVV(I,J)
 1010 SUML=SUML+FLL(I,J)
      DO 1020 J=1,NK
      FVV(I,J)=FVV(I,J)/SUMV*FV(I)
 1020 FLL(I,J)=FLL(I,J)/SUML*FL(I)
 1030 CONTINUE
C
      GO TO (1031,1035,1035), KUNITS
 1031 PRES=PP(NST)*14.696
      DPRES=DPATM*14.696
      DESTZ=DEST/453.59
      BTMSZ=BTMS/453.59
      GO TO 539
 1035 PRES=PP(1)
      DPRES=DPATM
      DESTZ=DEST
      BTMSZ=BTMS
C
  539 WRITE (NPRT,540) NST,DESTZ,BTMSZ,PRES,DPRES
```

```
      540 FORMAT ('0NUMBER OF STAGES', I9 //
         *         ' ESTIMATED OVERHEAD PRODUCT RATE', F12.4 /
         *         ' ESTIMATED BOTTOMS PRODUCT RATE', F13.4 //
         *         ' PRESSURE AT TOP OF COLUMN', F18.5 /
         *         ' CONSTANT DELTA P PER STAGE', F17.5  )
          GO TO (590,590,550,570,570), NCASE
      550 WRITE (NPRT,560) RFLX
      560 FORMAT ('0REFLUX RATIO', F15.6)
          GO TO 590
      570 WRITE (NPRT,580) BOIL
      580 FORMAT ('0BOILUP RATIO', F15.6)
    C
    C     FOR NSTART=-1 CHECK FOR ZERO TEMPERATURE
    C
      590 IF (NSTART.GE.0) GO TO 610
          IF (NST.LE.NSAVE) GO TO 610
          DO 607 I=NSAVE,NST
      607 T(I)=T(NSAVE)
    C
      610 IF (LDBUG.EQ.0) GO TO 800
          WRITE (NPRT,620)
      620 FORMAT ('0INITIAL COLUMN PROFILES:' /
         *  ' STAGE     TEMP          PRES        LIQUID(MOLS)    VAPOR(MOLS)' )
          DO 630 I=1,NST
      621 [illegible]
          PRES=PP(I)*14.696
          FLZ=FL(I)/453.59
          FVZ=FV(I)/453.59
          GO TO 629
      625 TDEG=T(I)
          PRES=PP(I)
          FLZ=FL(I)
          FVZ=FV(I)
      629 WRITE (NPRT,640) I,TDEG,PRES,FLZ,FVZ
      630 CONTINUE
      640 FORMAT (I5,F10.2,F12.3,F15.3,F14.3)
          GO TO 800
    C
      680 WRITE (NPRT,690)
      690 FORMAT (' MATERIAL BALANCE ERROR ... BOTTOMS RATE IS LT/EQ ZERO')
    C
      700 ICODE=1
    C
      800 RETURN
          END
```

```
      SUBROUTINE TEST
      IMPLICIT REAL     (M)
      INTEGER           COMPNT
      REAL              LIQUID
C
      COMMON /CTRL/     NCR, NPRT, NSTART, TITLE(20)
      COMMON /NJIT0/    NC, NCM1, IDLL, IDLV, IDH, LDBUG, ISW,
     *                  NAME(4,10), L(10), NDIM, COMPNT(10)
      COMMON /NJIT1/    CPL(10,4), CPV(10,4), ENP(10,10), ANT(6,10),
     *                  W(10)
      COMMON /NJIT2/    C(180), ALPHA(45), VC(10), VOL(10), TC(10),
     *                  PC(10), OA(10), OB(10), AA(10,10), G(10,10),
     *                  THETA(10), THS(10), HFAC(10), HHFA(10), HM(10),
     *                  Q(10),R(10),XL(10),PHI(10),DUMMY(10)
      COMMON /NJIT3/    TTC(10,10),PPC(10,10),VVC(10,10),ZZC(10,10),
     *                  AK(10,10), AVALUE(10,10), BVALUE(10,10),
     *                  BCROSS(10,10), OMEGA(10), DIPOLE(10), B(10,10)
      COMMON /INR0/     NST, NSTM1, NK1, NK2, NK11, NK21, NCASE, KUNITS,
     *                  NFEED, LF(9), IDCODE, ITR, ITRMAX, ICODE
      COMMON /INR1/     FSTR(9,11), FKV(9), HF(9), FLMAX(10), FVMAX(10),
     *                  DEST,DESTV,DESTL, BTMS, RFLX,BOIL, PP(50), T(50),
     *                  MU(50), SL(50), SV(50), FL(50), FLL(50,10),
     *                  FV(50), FVV(50,10), ZCONVT, ZCONVF
      COMMON /INR2/     DFK(10,21), HL(50), HLL(50,10), CL(50), HHE(50),
     *                  DEXH(50,11), HV(50), HVV(50,10), CV(50)
      COMMON /INR3/     AMAT(21,21), BMAT(50,21,21), D(50,21)
      COMMON /INR4/     VAPOR, LIQUID, FEED(11)
      COMMON /VLE/      XFK(10), GAM(10), X(10), Y(10), VP(10), FUG(10)
      COMMON /KNST/     XFKNST(10)
C
      DATA              SMALL /0.00005/
C
      ITR=ITR+1
C
      WRITE (NPRT,75) ITR
   75 FORMAT ('0ITERATION # =', I4)
C
      IF (LDBUG.EQ.0) GO TO 110
      WRITE (NPRT,80)
   80 FORMAT (' STAGE    TEMP        PRES      LIQUID(MOLS)   VAPOR(MOL
     *)')
      DO 90 I=1,NST
      GO TO (81,85,85), KUNITS
   81 TDEG=(T(I)-273.16)*1.8+32.0
      PRES=PP(I)*14.696
      FLZ=FL(I)/453.59
      FVZ=FV(I)/453.59
      GO TO 90
   85 TDEG=T(I)
      PRES=PP(I)
      FLZ=FL(I)
      FVZ=FV(I)
   90 WRITE (NPRT,100) I,TDEG,PRES,FLZ,FVZ
  100 FORMAT (I5,F10.2,F12.3,F15.3,F14.3)
C
C     SUM OF SQUARES OF DISCREPANCY FUNCTIONS
```

```
C
  110 REST=0.0
      RESF=0.0
      DTBIG=0.0
      ITBIG=0
      DLBIG=0.0
      ILBIG=0
      JLBIG=0
      DVBIG=0.0
      IVBIG=0
      JVBIG=0
      DO 120 I=1,NST
      IF (ABS(D(I,NK1)).LT.DTBIG) GO TO 112
      DTBIG=ABS(D(I,NK1))
      ITBIG=I
  112 REST=REST+D(I,NK1)**2
      DO 120 J=1,NC
      IF (D(I,J).EQ.0.0) GO TO 115
      IF (FLL(I,J)/FL(I).LT.SMALL) GO TO 115
      IF (ABS(D(I,J))/FLL(I,J).LT.DLBIG) GO TO 113
      DLBIG=ABS(D(I,J))/FLL(I,J)
      ILBIG=I
      JLBIG=J
  113 RESF=RESF+(D(I,J)/FLL(I,J))**2
  115 IF (D(I,J+NK1).EQ.0.0) GO TO 120
      IF (FVV(I,J)/FV(I).LT.SMALL) GO TO 120
      IF (ABS(D(I,J+NK1))/FVV(I,J).LT.DVBIG) GO TO 118
      DVBIG=ABS(D(I,J+NK1))/FVV(I,J)
      IVBIG=I
      JVBIG=J
  118 RESF=RESF+(D(I,J+NK1)/FVV(I,J))**2
  120 CONTINUE
C
      WRITE (NPRT,130) REST,RESF
  130 FORMAT (' SUM DT**2 =',      G17.6, /
     *          ' SUM (DF/F)**2 =', G13.6)
      WRITE (NPRT,135) ITBIG,DTBIG,ILBIG,JLBIG,DLBIG,IVBIG,JVBIG,DVBIG
  135 FORMAT (5X,I5,G12.5,5X,2I5,G12.5,5X,2I5,G12.5)
C
      IF (ITR.EQ.ITRMAX) GO TO 160
C
      DO 150 I=1,NST
      IF (ABS(D(1,NK1)).GT.ZCONVT) GO TO 160
      DO 150 J=1,NC
      IF (FLL(I,J)/FL(I).LT.SMALL) GO TO 140
      IF (ABS(D(I,J))/FLL(I,J).GT.ZCONVF) GO TO 160
  140 IF (FVV(I,J)/FV(I).LT.SMALL) GO TO 150
      IF (ABS(D(I,J+NK1))/FVV(I,J).GT.ZCONVF) GO TO 160
  150 CONTINUE
      GO TO 190
C
C     SET ICODE=-1........ PROBLEM HAS NOT CONVERGED
  160 ICODE=-1
      GO TO 200
C
C     SET ICODE=1..........TRIAL LIMIT REACHED OR BAD COLUMN DATA
```

```
0084            180 ICODE=1
0085                GO TO 200
              C
              C     SET ICODE=0..........PROBLEM CONVERGED
0086            190 ICODE=0
              C
0087            200 RETURN
0088                END
```

```
0001                SUBROUTINE EDWARD
             C      THIS IS THE OLD MAIN PROGRAM OF EXXON
             C      THE READ IN PORTION FOR FD(I),TF,PF,NLIQ HAS BEEN RELOCTED
             C
             C      THE ISOTHERMAL FLASH IS THE ONLY ACTIVE SUBR IN USE ISO=0
             C
             C
             C      VAPOR LIQUID FLASH PROGRAM FOR NON IDEAL SYSTEMS
             C
             C**** IMPLICIT REAL*8 (A-H,O-Z), INTEGER*2 (I-N)
             C
0002                DIMENSION          DEWC(9), BUBC(9),  HLIQD(2)
0003                COMMON /B2L/      FD(11),Z(10),FK(10,2),PF,TF,HI,XSAVE(10,2)
0004                COMMON /CONTRL/   T,P,NOBUB,NODEW,ISO,NLIQ
0005                COMMON /VAPOR/    Y(10),VP(10),FUG(10),DHV,HIDLV,HREALV,FRACV
0006                COMMON /LIQUID/    X(10,2),GAM(10,2),DHL(2),HIDLL(2),HREALL(2),
                +                     FRACL
0007                COMMON /DUMMY/     XX(10,2),SX(10,2),XC(10,2),YY(10),SY(10),
                +                     YC(10),RMAX,RMIN
0008                COMMON   /CTRL/   NCR, NPRT, NSTART, TITLE(20)
0009                COMMON   /NJIT0/  NC, NCM1, IOLL, IOLV, IOH, LDBUG, ISW,
                *                     NAME(2,10),L(10),COMPNT(10)
0010                COMMON   /NJIT1/  CPL(10,4), CPV(10,4), ENP(10,10), ANT(6,10),
                *                     W(10)
0011                COMMON   /NJIT2/  C(180), ALPHA(45), VC(10), VOL(10), TC(10),
                *                     PC(10), QA(10), QB(10), AZ(10,10), G(10,10),
                *                     THETA(10), THS(10), HFAC(10), HHFA(10), HM(10),
                *                     Q(10),RR(10),XL(10),PHI(10),DUMMY(10)
0012                COMMON   /NJIT3/  TTC(10,10),PPC(10,10),VVC(10,10),ZZC(10,10),
                *                     AK(10,10), AVALUE(10,10), BVALUE(10,10),
                *                     BCROSS(10,10), OMEGA(10), DIPOLE(10), BZ(10,10)
             C
             C
0013             10 DO 15 I=1,NC
0014                Y(I)=0.0
0015                YY(I)=0.0
0016                X(I,1)=0.0
0017                X(I,2)=0.0
0018                XX(I,1)=0.0
0019             15 XX(I,2)=0.0
0020                SUM=0.0
0021                DO 25 I=1,NC
0022             25 SUM = SUM + FD(I)
0023                DO 30 I=1,NC
0024             30 Z(I)= FD(I)/SUM
             C
             C
             C
0025                WRITE (6,40)
0026             40 FORMAT('1',/// '********* TWO-LIQUID FLASH PROGRAM *****'///)
0027                WRITE (6,50)SUM,PF,TF
0028             50 FORMAT ('0FD MOL =',F8.4,' MOLES',8X,'PRESS = ',
                * F8.2,' MMHG',8X,'TEMP =',F8.2,' DEG K')
0029                WRITE (6,60)((NAME(J,I),J=1,2),I=1,NC)
0030             60 FORMAT(25X,9(2A4,2X))
0031                WRITE (6,70)(Z(I),I=1,NC)
```

```
 0032             70 FORMAT(' FEED MOLEFRACTIONS',4X,9F10.5)
              C
 0033                ISO=0
              C
 0034                RMIN=0.0
 0035                RMAX=1.0
 0036                DO100I=1,NC
 0037                IF (L(I))80,90,100
 0038             80 RMAX=RMAX-Z(I)
 0039                GO TO 100
 0040             90 RMIN=RMIN+Z(I)
 0041            100 CONTINUE
              C
 0042                NODEW=0
 0043                NOBUB=0
              C
 0044                DO140I=1,NC
 0045                IF (FD(I))140,140,110
 0046            110 IF (L(I))120,130,140
 0047            120 NODEW=1
 0048                GO TO 140
 0049            130 NOBUB=1
 0050            140 CONTINUE
              C
 0051            150 WRITE (6,151)
 0052            151 FORMAT ('1RESULTS OF DEW POINT CALCULATION')
 0053                IF (NODEW.EQ.0) GO TO 170
 0054                WRITE (6,160)
 0055            160 FORMAT('0NO DEW POINT SINCE NONVOLATILE COMPONENTS ARE PRESENT')
 0056                TDEW=1.D6
 0057                DO 165 I=1,NC
 0058            165 DEWC(I)=0.0
 0059                GO TO 220
              C
 0060            170 DO180I=1,NC
 0061            180 Y(I)=Z(I)
 0062                T=TF
 0063                NHOLD=NLIQ
 0064                NLIQ=1
 0065                CALL DEWPT
 0066                TDEW=T
 0067                DO190I=1,NC
 0068            190 DEWC(I)=X(I,1)
 0069                WRITE (6,200) P,TDEW
 0070            200 FORMAT('0DEW POINT OF FEED AT',F7.2,' MMHG IS',F7.2,' DEG K')
 0071                WRITE (6,60)((NAME(J,I),J=1,2),I=1,NC)
 0072                WRITE (6,210)(DEWC(I),I=1,NC)
 0073            210 FORMAT (' DEW PT LIQ MOLE FRAC', 2X, 9F10.5)
 0074                CALL PRINT
 0075                NLIQ=NHOLD
              C
              C
              C      BUBBLE POINT CALCULATION
              C
              C
 0076            220 WRITE (6,221)
```

```
0077          221 FORMAT (////'0RESULTS OF BUBBLE POINT CALCULATION')
0078              IF (NOBUB.EQ.0) GO TO 240
0079              WRITE (6,230)
0080          230 FORMAT('0NO BUBBLE POINT SINCE NONCONDENSIBLE COMPONENTS ARE PRES
                 *NT')
0081          231 TBUB=0.1
0082              DO 235 I=1,NC
0083          235 BUBC(I)=0.0
0084              GO TO 320
           C
0085          240 IF (NLIQ.EQ.2) GO TO 280
0086              DO 241 I=1,NC
0087          241 X(I,1)=Z(I)
0088              T=TF
0089              FRACL=1.0
0090              CALL BUBPT1
           C
0091          245 IF (NOBUB.EQ.0) GO TO 255
0092              WRITE (6,250)
0093          250 FORMAT('0FEED REPRESENTS A HYPOTHETICAL LIQUID OR IS IN THE RETRO
                 +RADE REGION, BUBBLE POINT CALCULATIONS TERMINATED.')
0094              GO TO 231
           C
0095          255 TBUB=T
0096              WRITE (6,260) P,TBUB
0097          260 FORMAT('0BUBBLE POINT OF FEED AT',F7.2,' MMHG IS',F7.2,' DEG K')
0098              DO 265 I=1,NC
0099          265 BUBC(I)=Y(I)
0100              WRITE (6,60)((NAME(J,I),J=1,2),I=1,NC)
0101              WRITE (6,270) (BUBC(I),I=1,NC)
0102          270 FORMAT (' BUB PT VAP MOLE FRAC', 2X, 9F10.5)
0103              CALL PRINT
0104              GO TO 320
           C
0105          280 DO 281 I=1,NC
0106              DO 281 J=1,NLIQ
0107          281 X(I,J) = XSAVE(I,J)
           C
           C THE XSAVE(I,J) VALUES ARE INITIALIZED IN THE NEW SUBROUTINE 'START'
           C FOR THE ABOVE X(I,J)
           C      TWO LIQUID PHASE BUBBLE POINT INITIALIZATION
           C           * COMPONENT #1(ORGANIC) PREDOMINATELY IN PHASE #1(ORGANIC)
           C           * COMPONENT #NC PREDOMINATELY IN PHASE #2(AQUEOUS)
           C
           C
           C           INITIALIZE LIQUID COMPOSITION XSAVE FOR NLLIQ=2
           C
           C 280 X(1,1)=Z(1)
           C     X(1,2)=1.0E-12
           C     X(NC,1)=1.0E-12
           C     X(NC,2)=Z(NC)
           C     DO 281 I=2,NC-1
           C     X(I,1)=Z(I)/2.0
           C 281 X(I,2)=X(I,1)
0108              DO 284 N=1,2
0109              SUM=0.0
```

```
      DO 282 I=1,NC
  282 SUM=SUM+X(I,N)
      DO 283 I=1,NC
  283 X(I,N)=X(I,N)/SUM
  284 CONTINUE
      T=TF
      FRACL=0.5
      CALL BUBPT2
      IF (NLIQ.EQ.1) GO TO 245
      WRITE (6,285) FRACL
  285 FORMAT ('0TWO LIQ PHASE REGION, LIQUID PHASE MOLE RATIO', F12.6)
      GO TO 245
C
  320 IF (ISO.NE.0) GO TO 440
C
      IF (TF-TDEW) 380,340,330
  330 T=TF
  340 WRITE (6,350)
  350 FORMAT('0FEED AT OR ABOVE DEW POINT')
      CALL PRINT
      DO360I=1,NC
  360 Y(I)=Z(I)
      CALL VAPH
      H=HREALV
      WRITE (6,370)HIDLV,DHV
  370 FORMAT('0IDEAL VAP ENTHALPY =',E15.6,5X,'DELTA H =',E15.6)
      GO TO 650
C
  380 IF (TF-TBUB) 390,400,440
  390 T=TF
  400 WRITE (6,410)
  410 FORMAT('0FEED AT OR BELOW BUBBLE POINT')
      GO TO (415,420), NLIQ
  415 DO 416 I=1,NC
  416 X(I,1)=Z(I)
      CALL LIQH
      H=HREALL(1)
      GO TO 429
  420 CALL TWOLIQ
      CALL LIQH
C
C          FRACL= PHASE#1/(PHASE#1 + PHASE#2)
C
C
      H=HREALL(1)*FRACL+HREALL(2)*(1.0-FRACL)
      WRITE (6,285) FRACL
      DO 428 I=1,NC
  428 Y(I)=0.00
  429 CALL PRINT
      WRITE (6,430) (HIDLL(N),DHL(N),N=1,NLIQ)
  430 FORMAT('0IDEAL LIQ ENTHALPY =',E15.6,5X,'DELTA H =',E15.6)
      GO TO 650
C
C     INITIALIZE VAPOR & LIQUID PHASES FOR FLASH
C
  440 FRACV=(RMAX+RMIN)/2.0
```

```
              C
0156                 IF (NOBUB.EQ.0) GO TO 460
0157                 IF (NODEW.EQ.0) GO TO 550
0158                 GO TO480
              C
0159             460 DO470I=1,NC
0160             470 Y(I)=BUBC(I)
0161                 GO TO 570
              C
              C  480 GO TO (490,520), NLIQ
0162             480 GO TO (490,539),NLIQ
0163             490 DO 500 I=1,NC
0164                 IF (L(I)) 492,494,496
0165             492 Y(I)=0.0
0166                 X(I,1)=Z(I)
0167                 GO TO 500
0168             494 Y(I)=Z(I)
0169                 X(I,1)=0.0
0170                 GO TO 500
0171             496 Y(I)=Z(I)/2.0
0172                 X(I,1)=Y(I)
0173             500 CONTINUE
0174                 UY=0.0
0175                 UX=0.0
0176                 DO 505 I=1,NC
0177                 UY=UY+Y(I)
0178             505 UX=UX+X(I,1)
0179                 DO 510 I=1,NC
0180                 Y(I)=Y(I)/UY
0181             510 X(I,1)=X(I,1)/UX
0182                 GO TO 570
              C  520 DO 540 I=1,NC
              C      IF (L(I)) 522,528,530
              C  522 Y(I)=0.0
              C      IF (I.EQ.1) GO TO 524
              C      IF (I.EQ.NC) GO TO 526
              C      X(I,1)=Z(I)/2.0
              C      X(I,2)=X(I,1)
              C      GO TO 540
              C  524 X(I,1)=Z(I)
              C      X(I,2)=1.0E-12
              C      GO TO 540
              C  526 X(I,1)=1.0E-12
              C      X(I,2)=Z(I)
              C      GO TO 540
              C  528 Y(I)=Z(I)
              C      X(I,1)=0.0
              C      X(I,2)=0.0
              C      GO TO 540
              C  530 Y(I)=Z(I)/2.0
              C      IF (I.EQ.1) GO TO 532
              C      IF (I.EQ.NC) GO TO 534
              C      X(I,1)=Z(I)/4.0
              C      X(I,2)=X(I,1)
              C      GO TO 540
              C  532 X(I,1)=Z(I)/2.0
```

```
C      X(I,2)=1.0E-12
C      GO TO 540
C 534  X(I,1)=1.0E-12
C      X(I,2)=Z(1)/2.0
C 540  CONTINUE
  539  DO 543 I=1,NC
       Y(I) =Z(I)
       DO 543 J=1,NLIQ
  543  X(I,J)=XSAVE(I,J)
       SUM=0.0
       UY=0.0
       UX=0.0
       DO 542 I=1,NC
       SUM=SUM+Y(I)
       UY=UY+X(I,1)
  542  UX=UX+X(I,2)
       DO 544 I=1,NC
       Y(I)=Y(I)/SUM
       X(I,1)=X(I,1)/UY
  544  X(I,2)=X(I,2)/UX
       GO TO 570
C
  550  DO 552 I=1,NC
  552  Y(I)=Z(I)
       GO TO (554,558), NLIQ
  554  DO 556 I=1,NC
  556  X(I,1)=DEWC(I)
       GO TO 570
C 558  X(1,1)=DEWC(1)
C      X(1,2)=1.0E-12
C      X(NC,1)=1.0E-12
C      X(NC,2)=DEWC(NC)
C      DO 560 I=2,NC-1
C      X(I,1)=DEWC(I)/2.0
C 560  X(I,2)=X(I,1)
  558  DO 561 I=1,NC
       DO 561 J=1,NLIQ
  561  X(I,J)=XSAVE(I,J)
       DO 566 N=1,2
       SUM=0.0
       DO 562 I=1,NC
  562  SUM=SUM+X(I,N)
       DO 564 I=1,NC
  564  X(I,N)=X(I,N)/SUM
  566  CONTINUE
C
  570  I=IF
       IF (ISO)580,590,580
  580  WRITE (6,581)
  581  FORMAT ('1RESULTS OF ADBIATIC FLASH CALCULATION')
       CALL AFLASH
       GO TO 600
  590  WRITE (6,591)
  591  FORMAT ('1RESULTS OF ISOTHERMAL FLASH CALCULATION')
       GO TO (592,593), NLIQ
  592  CALL FLASH1
```

```
0225                GO TO 600
0226           593  CALL FLASH2
           C
0227           600  WRITE (6,610)T,P,FRACV
0228           610  FORMAT('0SYSTEM IS IN THE V/L PHASE REGION AT',F7.2,' DEG K AND',
                  * F7.2,' MMHG.    VAPOR/FEED MOLE RATIO =',F9.6)
0229                IF (NLIQ.EQ.2) WRITE (6,285) FRACL
           C
0230                CALL PRINT
           C
0231                CALL LIQH
0232                CALL VAPH
0233                WRITE (6,430) (HIDLL(N),DHL(N),N=1,NLIQ)
0234                WRITE (6,370)HIDLV,DHV
0235                HVAPOR=HREALV*FRACV
0236                GO TO (631,632),NLIQ
0237       631      HLIQD(1)=HREALL(1)*(1.0-FRACV)
0238                HLIQD(2)=0.0
0239                GO TO 633
0240       632      HLIQD(1)=HREALL(1)*(1.0-FRACV)*FRACL
0241                HLIQD(2)=HREALL(2)*(1.0-FRACV)*(1.0-FRACL)
0242       633      WRITE (6,640) HVAPOR,(HLIQD(N),N=1,NLIQ)
0243           640  FORMAT('0ENTHALPY OF VAPOR PHASE/LBMOL OF FEED  =',F10.2,' CAL'/
                  *( ' ENTHALPY OF LIQUID PHASE/LBMOL OF FEED =',F10.2,' BTU'))
0244                H=HVAPOR+HLIQD(1)
0245                IF (NLIQ .EQ. 2) H=H+HLIQD(2)
           C
0246           650  WRITE (6,660)TREF,H
0247           660  FORMAT('0ENTHALPY OF SYSTEM WITH REFERENCE TO PURE LIQUID AT',
                  *F7.2,' DEG K ',F10.2,' BTU/LBMOL')
           C
0248                DO 670 I=1,2
0249                DO 670 J=1,NC
0250           670  XSAVE(J,I)=X(J,I)
0251                RETURN
           C
0252                END
```

```
                SUBROUTINE    DEWPT
      C
      C         DEW POINT PROGRAM SOLVING FOR THE TEMPERATURE
      C
      C****     IMPLICIT REAL*8 (A-H,O-Z), INTEGER*2 (I-N)
      C
                COMMON /B2L/      FD(11),Z(10),EK(20),PF,TF,HI,XSAVE(10,2)
                COMMON /CONTRL/   T,P,NOBUB,NODEW,ISO,NLIQ
                COMMON /VAPOR/    Y(10),VP(10),FUG(10),DHV,HIIDLV,HREALV,FRACV
                COMMON /LIQUID/    X(20),GAM(20),DHL(2),HIDLL(2),HREALL(2),
               +                   FRACL
                COMMON /DUMMY/     XX(20),SX(20),XC(20),YY(10),SY(10),
               +                   YC(10),RMAX,RMIN
                COMMON  /CTRL/    NCR, NPRT, NSTART, TITLE(20)
                COMMON  /NJIT0/   NC, NCM1, IDLL, IDLV, IDH, LDBUG, ISW, NDIM,
               *                  NAME(2,10),L(10),COMPNT(10)
                COMMON  /NJIT1/   CPL(10,4), CPV(10,4), ENP(10,10), ANT(6,10),
               *                  W(10)
                COMMON  /NJIT2/   C(180), ALPHA(45), VC(10), VOL(10), TC(10),
               *                  PC(10), OA(10), OB(10), AZ(10,10), G(10,10),
               *                  THETA(10), THS(10), HFAC(10), HHFA(10), HM(10),
               *                  Q(10),RP(10),XL(10),PHI(10),DUMMY(10)
                COMMON  /NJIT3/   TTC(10,10),PPC(10,10),VVC(10,10),ZZC(10,10),
               *                  AK(10,10), AVALUE(10,10), BVALUE(10,10),
               *                  BCROSS(10,10), OMEGA(10), DIPOLE(10), BZ(10,10)
      C
                DATA                 CONV/1.0E-5/,  CONV2/1.0E-4/
                DATA                 STEP/20.0/
      C
      C         CALLING PROGRAM MUST PROVIDE INITIAL GUESS FOR T
      C
                KNT=0
                ISTR=IDLL
                IDLL=0
                ISW=0
                IDX=1
                HD=0.0
                DO 5 I=1,NC
                X(I)=0.0
                EK(I)= 0.0
              5 XX(I)=0.0
      C
             10 ID=1
                IF (LDBUG.GE.1) WRITE (6,20) T,(X(I),I=1,9),(EK(I),I=1,9)
             20 FORMAT ('0DEWPT  T/X-K', F12.4/(9E14.5))
                S=T
                K=0
      C
             30 CALL KCALC
                V=-1.0
                DO60I=1,NC
                IF (L(I)) 50,40,50
             40 XX(I)=0.0
                GO TO 60
             50 XX(I)=Y(I)/EK(I)
                V=V+XX(I)
```

```
   60 CONTINUE
      K=K+1
C
      IF (LDBUG.GE.2) WRITE (6,70) T,V
   70 FORMAT ('      T&SUM', F12.4,E14.5)
      IF (LDBUG.GE.2) WRITE (6,75) (X(I),I=1,9)
   75 FORMAT ('0X-ASS  ',9E13.5)
C
      IF (K.LT.20) GO TO 80
   71 WRITE (6,72)
   72 FORMAT ('0DEW POINT CALCULATION TERMINATED'/
     +           ' CALCULATION CONTINUING' ///)
      SUM=0.0
      DO 74 I=1,NC
   74 SUM=SUM+XX(I)
      GO TO 175
C
   80 IF (ABS(V).LT.CONV) GO TO 130
C
      GO TO (90,100), ID
   90 T=S+SIGN(5.0,V)
      HD=V
      ID=2
      GO TO 30
  100 HD=V*(S-T)/(HD-V)
      S=T
      IF (ABS(HD)-STEP)120,120,110
  110 HD=SIGN(STEP,HD)
  120 T=T-HD
      HD=V
      GO TO 30
C
  130 IDLL=ISTR
      IF (IDLL)170,170,140
  140 GO TO (200,150,150),IDX
  150 DO160I=1,NC
      IF ( (L(I) .EQ. 0) .OR. (Z(I) .LT. 1.0E-12) ) GO TO 160
      IF (ABS(X(I)-XX(I))/X(I) .GT. CONV2) GO TO 190
  160 CONTINUE
  170 SUM=V+1.0
  175 DO 180 I=1,NC
  180 X(I)=XX(I)/SUM
      RETURN
C
  190 KNT=KNT+1
      IF (KNT.EQ.50) GO TO 71
      GO TO (200,220,240), IDX
C
  200 IDX=2
      DO210I=1,NC
  210 X(I)=XX(I)
  215 SUM=V+1.0
      GO TO 255
  220 IDX=3
      DO230I=1,NC
      SX(I)=X(I)
```

```
            XC(I)=XX(I)
        230 X(I)=XX(I)
            GO TO 215
        240 SUM=0.0
            DO250I=1,NC
            IF (L(I).EQ.0 .OR. Z(I).LT.1.0E-12) GO TO 250
            CALL WEGS (X(I),XX(I),SX(I),XC(I))
            SUM=SUM+X(I)
        250 CONTINUE
      C
        255 DO 260 I=1,NC
        260 X(I)=X(I)/SUM
            GO TO 10
      C
            END
```

```
      SUBROUTINE    BUBPT1
C
C     BUBBLE POINT PROGRAM SOLVING FOR THE TEMPERATURE *** ONE LIQUID
C
C**** IMPLICIT REAL*8 (A-H,O-Z), INTEGER*2 (I-N)
C
      COMMON /B2L/      FD(11),Z(10),EK(20),PF,TF,HI,XSAVE(10,2)
      COMMON /CONTRL/   T,P,NOBUB,NODEW,ISO,NLIQ
      COMMON /VAPOR/    Y(10),VP(10),FUG(10),DHV,HIIDLV,HREALV,FRACV
      COMMON /LIQUID/    X(20),GAM(20),DHL(2),HIDLL(2),HREALL(2),
     +                   FRACL
      COMMON /DUMMY/     XX(20),SX(20),XC(20),YY(10),SY(10),
     +                   YC(10),RMAX,RMIN
      COMMON  /CTRL/    NCR, NPRT, NSTART, TITLE(20)
      COMMON  /NJIT0/   NC, NCM1, IDLL, IDLV, IDH, LDBUG, ISW, NDIM,
     *                  NAME(2,10),L(10),COMPNT(10)
      COMMON  /NJIT1/   CPL(10,4), CPV(10,4), ENP(10,10), ANT(6,10),
     *                  W(10)
      COMMON  /NJIT2/   C(180), ALPHA(45), VC(10), VOL(10), TC(10),
     *                  PC(10), OA(10), OB(10), AZ(10,10), G(10,10),
     *                  THETA(10), THS(10), HFAC(10), HHFA(10), HM(10),
     *                  Q(10),RR(10),XL(10),PHI(10),DUMMY(10)
      COMMON  /NJIT3/   TTC(10,10),PPC(10,10),VVC(10,10),ZZC(10,10),
     *                  AK(10,10), AVALUE(10,10), BVALUE(10,10),
     *                  BCROSS(10,10), OMEGA(10), DIPOLE(10), BZ(10,10)
C
      DATA                 CONV/1.0E-5/,  CONV2/1.0E-4/
      DATA                 STEP/20.0/
C
C     CALLING PROGRAM MUST PROVIDE INITIAL GUESS FOR T
C
      KNT=0
      ISTR=IDLV
      IDLV=0
      ISW=0
      IDX=1
      HD=0.0
      DO 5 I=1,NC
      Y(I)=0.0
      YY(I)=0.0
    5 EK(I)=0.0
C
   10 ID=1
      IF (LDBUG.GE.1) WRITE (6,20) T,(Y(I),I=1,9),(EK(I),I=1,9)
   20 FORMAT ('0BUBPT#1  T/Y-K', F12.4/(9E14.5))
      S=T
      K=0
C
   30 CALL KCALC
      V=-1.0
      DO60I=1,NC
      IF (L(I)) 40,50,50
   40 YY(I)=0.0
      GO TO 60
   50 YY(I)=EK(I)*X(I)
      V=V+YY(I)
```

```
   60 CONTINUE
      K=K+1
C
      IF (LDBUG.GE.1) WRITE (6,70) T,V
   70 FORMAT (5X, 'T&SUM', F12.4,E15.5)
      IF (LDBUG.GE.2) WRITE (6,75) (Y(I),I=1,9)
   75 FORMAT ('0Y-ASS  ',9E13.5)
C
      IF (K.LT.20) GO TO 80
   71 WRITE (6,72)
   72 FORMAT('0BUBBLE POINT (1 LIQUID PHASE) CALCULATION TERMINATED'/
     +      ' CALCULATION CONTINUING' ///)
      SUM=0.0
      DO 74 I=1,NC
   74 SUM=SUM+YY(I)
      GO TO 195
C
   80 IF (ABS(V).LT.CONV) GO TO 150
C
      GO TO (90,100), ID
   90 T=S-SIGN(5.0,V)
      HD=V
      ID=2
      GO TO 30
  100 SLOPE=(HD-V)/(S-T)
      IF (SLOPE.GT.0.0) GO TO 120
      NOBUB=2
      IDLV=ISTR
      RETURN
  120 HD=V/SLOPE
      S=T
      IF (ABS(HD)-STEP)140,140,130
  130 HD=SIGN(STEP,HD)
  140 T=T-HD
      HD=V
      GO TO 30
C
  150 IDLV=ISTR
      IF (IDLV)190,190,160
  160 GO TO (220,170,170),IDX
  170 DO180I=1,NC
      IF (L(I).LT.0 .OR. Z(I).LT.1.0E-12) GO TO 180
      IF (ABS(Y(I)-YY(I))/Y(I)-CONV2)180,180,210
  180 CONTINUE
  190 SUM=V+1.0
  195 DO 200 I=1,NC
  200 Y(I)=YY(I)/SUM
      IDLV=ISTR
      RETURN
C
  210 KNT=KNT+1
      IF (KNT.EQ.50) GO TO 71
      GO TO (220,240,260), IDX
C
  220 IDX=2
      DO230I=1,NC
```

```
  230 Y(I)=YY(I)
  235 SUM=V+1.0
      GO TO 275
  240 IDX=3
      DO250I=1,NC
      SY(I)=Y(I)
      YC(I)=YY(I)
  250 Y(I)=YY(I)
      GO TO 235
  260 SUM=0.0
      DO270I=1,NC
      IF (L(I).LT.0 .OR. Z(I).LT.1.0E-12) GO TO 270
      CALL WEGS(Y(I),YY(I),SY(I),YC(I))
      SUM=SUM+Y(I)
  270 CONTINUE
C
  275 DO 280 I=1,NC
  280 Y(I)=Y(I)/SUM
      GO TO 10
C
      END
```

```
      SUBROUTINE    BUBPT2
C
C      BUBBLE POINT PROGRAM SOLVING FOR THE TEMPERATURE *** TWO LIQUIDS
C
C**** IMPLICIT REAL*8 (A-H,O-Z), INTEGER*2 (I-N)
C
C
      COMMON /B2L/      FD(11),Z(10),EK(10,2),PF,TF,HI,XSAVE(10,2)
      COMMON /CONTRL/   T,P,NOBUB,NODEW,ISO,NLIQ
      COMMON /VAPOR/    Y(10),VP(10),FUG(10),DHV,HIIDLV,HREALV,FRACV
      COMMON /LIQUID/    X(10,2),GAM(10,2),DHL(2),HIDLL(2),HREALL(2),
     +                   FRACL
      COMMON /DUMMY/     XX(10,2),SX(10,2),XC(10,2),YY(10),SY(10),
     +                   YC(10),RMAX,RMIN
      COMMON  /CTRL/    NCR, NPRT, NSTART, TITLE(20)
      COMMON  /NJIT0/   NC, NCM1, IDLL, IDLV, IDH, LDBUG, ISW, NDIM,
     *                  NAME(2,10),L(10),COMPNT(10)
      COMMON  /NJIT1/   CPL(10,4), CPV(10,4), ENP(10,10), ANT(6,10),
     *                  W(10)
      COMMON  /NJIT2/   C(180), ALPHA(45), VC(10), VOL(10), TC(10),
     *                  PC(10), OA(10), OB(10), AZ(10,10), G(10,10),
     *                  THETA(10), THS(10), HFAC(10), HHFA(10), HM(10),
     *                  Q(10),RR(10),XL(10),PHI(10),DUMMY(10)
      COMMON  /NJIT3/   TTC(10,10),PPC(10,10),VVC(10,10),ZZC(10,10),
     *                  AK(10,10), AVALUE(10,10), BVALUE(10,10),
     *                  BCROSS(10,10), OMEGA(10), DIPOLE(10), BZ(10,10)
      DATA                CONV/1.0E-5/,  CONV2/1.0E-4/
      DATA                STEP/20.0/
C
C      CALLING PROGRAM MUST INITIALIZE T & FRACL
C
      KNT=0
      ISTR=IDLV
      IDLV=0
      ISW=0
      IDX=1
      HD=0.0
      DO 5 I=1,NC
      Y(I)=0.0
      YY(I)=0.0
      DO 5 N=1,2
    5 EK(I,N)=0.0
C
   10 ID=1
      IF (LDBUG.GE.1) WRITE (6,20) T,(Y(I),I=1,9),(EK(I,1),I=1,9),
     +                           (EK(I,2),I=1,9)
   20 FORMAT('0BUBPT#2  T/Y-K1-K2', F12.4/(9E14.5))
      S=T
      K=0
C
   30 CALL TWOLIQ
   40 CALL KCALC
      V=-1.0
      DO60I=1,NC
      IF (L(I).GE.0) GO TO 50
      YY(I)=0.0
```

```
      GO TO 60
   50 YY(I)=FK(I,1)*X(I,1)
      V=V+YY(I)
   60 CONTINUE
      K=K+1
C
      IF (LDBUG.GE.1) WRITE (6,70) T,V
   70 FORMAT ('0', 4X, 'T&SUM', F12.4,E14.5)
      IF (LDBUG.GE.2) WRITE (6,75) (Y(I),I=1,9)
   75 FORMAT ('0Y-ASS  ',9E13.5)
C
      IF (K.LT.20) GO TO 80
   71 WRITE (6,72)
   72 FORMAT ('0BUBBLE POINT (2 LIQUID PHASE) CALCULATION TERMINATED'/
     +        ' CALCULATION CONTINUING' ///)
      SUM=0.0
      DO 74 I=1,NC
   74 SUM=SUM+YY(I)
      GO TO 195
C
   80 IF (ABS(V).LT.CONV) GO TO 150
C
      GO TO (90,100), ID
   90 T=S-SIGN(5.0,V)
      HD=V
      ID=2
      GO TO 40
  100 HD=(HD-V)/(S-T)
      HD=V/HD
      S=T
      IF (ABS(HD)-STEP)140,140,130
  130 HD=SIGN(STEP,HD)
  140 T=T-HD
      HD=V
      GO TO 30
C
  150 IDLV=ISTR
      IF (IDLV)190,190,160
  160 GO TO (220,170,170),IDX
  170 DO180I=1,NC
      IF (L(I).LT.0 .OR. Z(I).LT.1.0E-12) GO TO 180
      IF (ABS(Y(I)-YY(I))/Y(I)-CONV2)180,180,210
  180 CONTINUE
  190 SUM=V+1.0
  195 DO 200 I=1,NC
  200 Y(I)=YY(I)/SUM
      IDLV=ISTR
      RETURN
C
  210 KNT=KNT+1
      IF (KNT.EQ.50) GO TO 71
      GO TO (220,240,260), IDX
C
  220 IDX=2
      DO230I=1,NC
  230 Y(I)=YY(I)
```

```
  235 SUM=V+1.0
      GO TO 275
  240 IDX=3
      DO250I=1,NC
      SY(I)=Y(I)
      YC(I)=YY(I)
  250 Y(I)=YY(I)
      GO TO 235
  260 SUM=0.0
      DO270I=1,NC
      IF (L(I).LT.0 .OR. Z(I).LT.1.0E-12) GO TO 270
      CALL WEGS(Y(I),YY(I),SY(I),YC(I))
      SUM=SUM+Y(I)
  270 CONTINUE
C
  275 DO 280 I=1,NC
  280 Y(I)=Y(I)/SUM
      GO TO 10
C
      END
```

```
      SUBROUTINE    TWOLIQ
C
C     TWO PHASE MATERIAL BALANCE USED FOR
C         *  BUBBLE POINT
C         *  SUBCOOLED LIQUID
C
C**** IMPLICIT REAL*8 (A-H,O-Z), INTEGER*2 (I-N)
C
      DIMENSION          R(9)
C
      COMMON /B2L/      FD(11),Z(10),EK(10,2),PF,TF,HI,XSAVE(10,2)
      COMMON /CONTRL/   T,P,NOBUB,NODEW,ISO,NLIQ
      COMMON /VAPOR/    Y(10),VP(10),FUG(10),DHV,HIDLV,HREALV,FRACV
      COMMON /LIQUID/    X(10,2),GAM(10,2),DHL(2),HIDLL(2),HREALL(2),
     +                   FRACL
      COMMON /DUMMY/     XX(10,2),SX(10,2),XC(10,2),YY(10),SY(10),
     +                   YC(10),RMAX,RMIN
      COMMON  /CTRL/    NCR, NPRT, NSTART, TITLE(20)
      COMMON  /NJIT0/   NC, NCM1, IDLL, IDLV, IDH, LDBUG, ISW, NDIM,
     *                  NAME(2,10),L(10),COMPNT(10)
      COMMON  /NJIT1/   CPL(10,4), CPV(10,4), ENP(10,10), ANT(6,10),
     *                  W(10)
      COMMON  /NJIT2/   C(180), ALPHA(45), VC(10), VOL(10), TC(10),
     *                  PC(10), OA(10), OB(10), A7(10,10), G(10,10),
     *                  THETA(10), THS(10), HFAC(10), HHFA(10), HM(10),
     *                  Q(10),RR(10),XL(10),PHI(10),DUMMY(10)
      COMMON  /NJIT3/   TTC(10,10),PPC(10,10),VVC(10,10),ZZC(10,10),
     *                  AK(10,10), AVALUE(10,10), BVALUE(10,10),
     *                  BCROSS(10,10), OMEGA(10), DIPOLE(10), BZ(10,10)
C
      DATA               CONV/1.0E-5/,  CONV1/1.0E-4/
C   .
      KNT=0
      IDX=1
      ISAVE=ISW
      ISW=0
      CALL ACTVTY (T,X(1,1),GAM(1,1))
      CALL ACTVTY (T,X(1,2),GAM(1,2))
      ISW=1
      GO TO 30
C
   20 CALL ACTVTY (T,X(1,1),GAM(1,1))
      CALL ACTVTY (T,X(1,2),GAM(1,2))
   30 DO 40 I=1,NC
   40 R(I)=GAM(I,1)/GAM(I,2)
      K=0
C
      IF (LDBUG.GE.2) WRITE (6,45) (X(I,1),I=1,9),(X(I,2),I=1,9)
   45 FORMAT ('0X1-ASS ',9E13.5/' X2-ASS ',9E13.5)
C
   50 F2=0.0
      DF2=0.0
      DDF2=0.0
      DO 60 I=1,NC
      IF (L(I).EQ.0 .OR. Z(I).LT.1.0E-12) GO TO 60
      B=Z(I)*(1.0-R(I))
```

```
      WW=FRACL+(1.0-FRACL)*R(I)
      DWW=1.0-R(I)
      F2=F2+B/WW
      DF2=DF2-B/WW**2*DWW
      DDF2=DDF2+2.0*B/WW**3*DWW**2
   60 CONTINUE
      CC=2.0*F2*DF2
C     FF=2.0*DF2**2+4.0*F2*DDF2
      FF=2.0*DF2**2-F2*DDF2
      DEL=-CC/FF
      K=K+1
C
      IF (LDBUG.GE.1) WRITE (6,62) T,F2,FRACL,DEL
   62 FORMAT (5X, 'T-F2-FRACL-DEL', F12.4,3E14.5)
C
      IF (K.LT.50) GO TO 70
   63 WRITE (6,64)
   64 FORMAT ('0TWOLIQ CALCULATION TERMINATED'/
     +           ' CALCULATION CONTINUING' ///)
      DO 66 I=1,NC
      WW=FRACL+(1.0-FRACL)*R(I)
      X(I,1)=Z(I)/WW
   66 X(I,2)=X(I,1)*R(I)
      DO 69 N=1,2
      SUM=0.0
      DO 67 I=1,NC
   67 SUM=SUM+X(I,N)
      DO 68 I=1,NC
   68 X(I,N)=X(I,N)/SUM
   69 CONTINUE
      ISW=ISAVE
      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/2.0
      GO TO 75
C
   80 IF (FRACL.LT.0.99) GO TO 85
      FRACL=1.0-FRACL
      DO 81 I=1,NC
      HOLD=X(I,1)
      X(I,1)=X(I,2)
      X(I,2)=HOLD
      HOLD=XX(I,1)
      XX(I,1)=XX(I,2)
      XX(I,2)=HOLD
      HOLD=SX(I,1)
      SX(I,1)=SX(I,2)
      SX(I,2)=HOLD
      HOLD=XC(I,1)
      XC(I,1)=XC(I,2)
      XC(I,2)=HOLD
      HOLD=GAM(I,1)
      GAM(I,1)=GAM(I,2)
```

```
            GAM(I,2)=HOLD
   81 CONTINUE
   85 IF (FRACL.LT.1.E-10) GO TO 166
C
   90 IF (ABS(F2).LT.CONV .AND. ABS(DEL).LT.CONV .AND. NCVRG.EQ.0)
     +     GO TO 95
      FRACL=FRACL+DEL
      GO TO 50
C
   95 DO 100 I=1,NC
      WW=FRACL+(1.0-FRACL)*R(I)
      XX(I,1)=Z(I)/WW
  100 XX(I,2)=XX(I,1)*R(I)
C
      KNT=KNT+1
      IF (KNT.EQ.50) GO TO 63
      GO TO (110,150), IDX
C
  110 IDX=2
      DO 140 N=1,2
      SUM=0.0
      DO 120 I=1,NC
      SX(I,N)=X(I,N)
      XC(I,N)=XX(I,N)
      X(I,N)=(X(I,N)+XX(I,N))/2.0
  120 SUM=SUM+X(I,N)
      DO 130 I=1,NC
  130 X(I,N)=X(I,N)/SUM
  140 CONTINUE
      GO TO 20
C
  150 DO 160 I=1,NC
      IF (L(I).EQ.0 .OR. Z(I).LT.1.0E-12) GO TO 160
C     IF (ABS(X(I,1)*GAM(I,1)-X(I,2)*GAM(I,2))/(X(I,2)*GAM(I,2)) .GT.
C    +     CONV1) GO TO 190
      IF (ABS(X(I,1)-XX(I,1))/X(I,1) .GT. CONV1 .OR.
     *(ABS(X(I,2)-XX(I,2))/X(I,2)) .GT. CONV1) GO TO 190
  160 CONTINUE
      GO TO 170
C
  166 DO 167 I=1,NC
      X(I,1)=Z(I)
  167 X(I,2)=0.0
      NLIQ=1
      WRITE (6,168)
  168 FORMAT (// 5X, 'LIQUID HAS GONE TO A ONE PHASE SYSTEM' //)
      RETURN
C
  170 DO 180 N=1,2
      SUM=0.0
      DO 172 I=1,NC
  172 SUM=SUM+X(I,N)
      DO 176 I=1,NC
  176 X(I,N)=X(I,N)/SUM
  180 CONTINUE
      ISW=ISAVE
```

```
      RETURN
C
  190 DO 220 N=1,2
      SUM=0.0
      DO 200 I=1,NC
      IF (L(I).EQ.0 .OR. Z(I).LT.1.0E-12) GO TO 200
      CALL WEGS (X(I,N),XX(I,N),SX(I,N),XC(I,N))
      SUM=SUM+X(I,N)
  200 CONTINUE
      DO 210 I=1,NC
  210 X(I,N)=X(I,N)/SUM
  220 CONTINUE
      GO TO 20
C
      END
```

```
      SUBROUTINE    FLASH1
C
C     ISOTHERMAL FLASH *** ONE LIQUID
C
C**** IMPLICIT REAL*8 (A-H,O-Z), INTEGER*2 (I-N)
C
      COMMON /B2L/      FD(11),Z(10),EK(20),PF,TF,HI,XSAVE(10,2)
      COMMON /CONTRL/   T,P,NOBUB,NODEW,ISO,NLIQ
      COMMON /VAPOR/    Y(10),VP(10),FUG(10),DHV,HIDLV,HREALV,FRACV
      COMMON /LIQUID/    X(20),GAM(20),DHL(2),HIDLL(2),HREALL(2),
     +                   FRACL
      COMMON /DUMMY/     XX(20),SX(20),XC(20),YY(10),SY(10),
     +                   YC(10),RMAX,RMIN
      COMMON  /CTRL/    NCR, NPRT, NSTART, TITLE(20)
      COMMON  /NJIT0/   NC, NCM1, IDLL, IDLV, IDH, LDBUG, ISW, NDIM,
     *                  NAME(2,10),L(10),COMPNT(10)
      COMMON  /NJIT1/   CPL(10,4), CPV(10,4), ENP(10,10), ANT(6,10),
     *                  W(10)
      COMMON  /NJIT2/   C(180), ALPHA(45), VC(10), VOL(10), TC(10),
     *                  PC(10), OA(10), OB(10), AZ(10,10), G(10,10),
     *                  THETA(10), THS(10), HFAC(10), HHFA(10), HM(10),
     *                  U(10),RR(10),XL(10),PHI(10),DUMMY(10)
      COMMON  /NJIT3/   TTC(10,10),PPC(10,10),VVC(10,10),ZZC(10,10),
     *                  AK(10,10), AVALUE(10,10), BVALUE(10,10),
     *                  BCROSS(10,10), OMEGA(10), DIPOLE(10), BZ(10,10)
C
      EQUIVALENCE         (R,FRACV)
C
      DATA                CONV/1.0E-4/,  CONV1/1.0E-5/,  CONV2/1.0E-5/
C
C     R IS VAPOR FRACTION
C     CALLING PROGRAM MUST SUPPLY INITIAL VALUE FOR R,X,Y
C
      KNT=0
      IDX=1
      ISW=0
      CALL KCALC
      ISW=1
      IF (NC.GT.1) GO TO  21
C
      Y(1)=1.0
      X(1)=1.0
      ISO=0
      RETURN
C
   20 CALL KCALC
C
   21 IF (LDBUG.GE.1) WRITE (6,25) T,R
   25 FORMAT ('0FLASH#1  T&R', F12.4,E14.5)
      IF (LDBUG.GE.2) WRITE (6,26) (Y(I),I=1,9),(X(I),I=1,9)
   26 FORMAT ('0Y-ASS  ',9E13.5/' X-ASS  ',9E13.5)
C
   29 K=0
   30 AMAX=RMAX
      AMIN=RMIN
      F1=0.0
```

```
0033              DF=0.0
0034              DO80I=1,NC
0035              IF (L(I))40,50,60
0036           40 S=1.0/(1.0-R)
0037              GO TO 70
0038           50 S=-1.0/R
0039              GO TO 70
0040           60 S=(1.0-EK(I))/(1.0+R*(EK(I)-1.0))
0041           70 F1=F1+Z(I)*S
0042           80 DF=DF+Z(I)*S*S
0043              K=K+1
            C
0044              IF (LDBUG.GE.2) WRITE (6,90) F1,DF1,R
0045           90  FORMAT (5X, 'F1-DF1-R',3E14.5)
            C
0046              IF (K.LT.20) GO TO 99
0047           91 WRITE (6,92)
0048           92 FORMAT ('0FLASH#1 CALCULATION TERMINATED'/
             +          ' CALCULATION CONTINUING' ///)
0049              GO TO 320
            C
0050           99 IF (ABS(F1).LT.CONV2) GO TO 190
            C   99 IF (F1) 100,190,110
            C 100 AMIN=R
            C     GO TO 120
            C 110 AMAX=R
            C 120 IF ((AMAX-AMIN).LT.CONV1) GO TO 170
            C     DF1=-F1/DF1
            C 130 F1=R+DF1
            C     IF (F1-AMIN)140,150,150
            C 140 DF=DF*0.5
            C     GO TO 130
            C 150 IF (F1-AMAX)160,160,140
            C 160 R=F1
0051              IF (ABS(R-AMIN).LT.CONV1 .OR. ABS(R-AMAX).LT.CONV1) GO TO 190
0052              DR=-F1/DF1
0053          130 RNEXT=R + DR
0054              IF (RNEXT.GE.AMIN) GO TO 150
0055          140 DR=DR/2.0
0056              GO TO  130
0057          150 IF (RNEXT.GT.AMAX) GO TO 140
0058              R=RNEXT
            C
            C     IF (ABS(DF)-CONV1)190,30,30
0059              IF (ABS(DR).GT. CONV1) GO TO 30
            C
            C 170 DO180I=1,NC
            C 180 X(I)=(X(I)+SX(I))/2.0
            C     GO TO 20
            C
0060          190 IF (LDBUG.GE.2) WRITE (6,200) R
0061          200 FORMAT (5X, 'R', E14.5)
0062              DO240I=1,NC
0063              IF (L(I))210,220,230
0064          210 XX(I)=Z(I)/(1.0-R)
0065              YY(I)=0.0
```

```
          GO TO 240
      220 XX(I)=0.0
          YY(I)=Z(I)/R
          GO TO 240
      230 XX(I)=Z(I)/(1.0+R*(EK(I)-1.0))
          YY(I)=EK(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
          DO280I=1,NC
          IF ((L(I).EQ.0).OR.(Z(I).LT.1.0E-12)) GO TO 280
          IF (ABS(X(I)-XX(I))/X(I) .GT. CONV) GO TO 410
      280 CONTINUE
C
      290 IF (IDLV.EQ.0) GO TO 320
          DO310I=1,NC
          IF ((L(I).LT.0).OR.(Z(I).LT.1,0E-12)) GO TO 310
          IF (ABS(Y(I)-YY(I))/Y(I)-CONV)310,410,410
      310 CONTINUE
C
      320 UX=0.0
          UY=0.0
          DO 330 I=1,NC
          X(I)=XX(I)
          Y(I)=YY(I)
          UX=UX+X(I)
      330 UY=UY+Y(I)
          WRITE (6,331) UX,UY
      331 FORMAT(' FLASH1 SUM UX/UY',2G20.6)
          DO 335 I=1,NC
          X(I)=X(I)/UX
      335 Y(I)=Y(I)/UY
          ISW=0
          RETURN
C
      340 IF (IDLL.EQ.0) GO TO 370
          DO 360 I=1,NC
          SX(I)=X(I)
          XC(I)=XX(I)
      360 X(I)=(XX(I)+X(I))/2.0
      370 IF (IDLV.EQ.0) GO TO 400
          DO 390 I=1,NC
          SY(I)=Y(I)
          YC(I)=YY(I)
      390 Y(I)=(YY(I)+Y(I))/2.0
      400 IDX=2
          GO TO 20
C
      410 IF (IDLL.EQ.0) GO TO 450
          SUM=0.0
          DO430I=1,NC
```

```
0116                IF ((L(I).EQ.0).OR.(Z(I).LT.1.0E-12)) GO TO 430
0117                CALL WEGS (X(I),XX(I),SX(I),XC(I))
0118                SUM=SUM+X(I)
0119            430 CONTINUE
0120                DO440I=1,NC
0121            440 X(I)=X(I)/SUM
          C
0122            450 IF (IDLV.EQ.0) GO TO 20
0123                SUM=0.0
0124                DO470I=1,NC
0125                IF ((L(I).LT.0).OR.(Z(I).LT.1.0E-12)) GO TO 470
0126                CALL WEGS(Y(I),YY(I),SY(I),YC(I))
0127                SUM=SUM+Y(I)
0128            470 CONTINUE
0129                DO480I=1,NC
0130            480  Y(I)=Y(I)/SUM
0131                GO TO 20
          C
0132                END
```

```
      SUBROUTINE    FLASH2
C
C     ISOTHERMAL FLASH *** TWO LIQUIDS
C
C**** IMPLICIT REAL*8 (A-H,O-Z), INTEGER*2 (I-N)
C
      DIMENSION           R(9), ZJ(2,2), RHS(2)
C
      COMMON /B2L/      FD(11),Z(10),EK(10,2),PF,TF,HI,XSAVE(10,2)
      COMMON /CONTRL/   T,P,NOBUB,NODEW,ISO,NLIQ
      COMMON /VAPOR/    Y(10),VP(10),FUG(10),DHV,HIIDLV,HREALV,FRACV
      COMMON /LIQUID/    X(10,2),GAM(10,2),DHL(2),HIDLL(2),HREALL(2),
     +                   FRACL
      COMMON /DUMMY/     XX(10,2),SX(10,2),XC(10,2),YY(10),SY(10),
     +                   YC(10),RMAX,RMIN
      COMMON  /CTRL/    NCR, NPRT, NSTART, TITLE(20)
      COMMON  /NJIT0/   NC, NCM1, IDLL, IDLV, IDH, LDBUG, ISW, NDIM,
     *                  NAME(2,10),L(10),COMPNT(10)
      COMMON  /NJIT1/   CPL(10,4), CPV(10,4), ENP(10,10), ANT(6,10),
     *                  W(10)
      COMMON  /NJIT2/   C(180), ALPHA(45), VC(10), VOL(10), TC(10),
     *                  PC(10), OA(10), OB(10), AZ(10,10), G(10,10),
     *                  THETA(10), THS(10), HFAC(10), HHFA(10), HM(10),
     *                  Q(10),RR(10),XL(10),PHI(10),DUMMY(10)
      COMMON  /NJIT3/   TTC(10,10),PPC(10,10),VVC(10,10),ZZC(10,10),
     *                  AK(10,10), AVALUE(10,10), BVALUE(10,10),
     *                  BCROSS(10,10), OMEGA(10), DIPOLE(10), B7(10,10)
C
      EQUIVALENCE         (U,FRACV), (V,FRACL)
C
      DATA                CONV/1.0E-4/,  CONV1/1.0E-5/,  CONV2/1.0E-5/
C
      KNT=0
      IDX=1
      ISW=0
      CALL KCALC
      ISW=1
      IF (NC.GT.2) GO TO 26
C
      CALL TWOLIQ
      CALL KCALC
      DO 11 I=1,NC
   11 Y(I)=EK(I,1)*X(I,1)
      IF (IDLV.EQ.0) GO TO 240
      GO TO 13
   12 CALL KCALC
   13 CALL TWOLIQ
      GO TO (14,17), IDX
   14 SUM=0.0
      DO 15 I=1,NC
      YY(I)=EK(I,1)*X(I,1)
      SY(I)=Y(I)
      YC(I)=YY(I)
      Y(I)=(Y(I)+YY(I))/2.0
   15 SUM=SUM+Y(I)
      DO 16 I=1,NC
```

```
   16 Y(I)=Y(I)/SUM
      IDX=2
      GO TO 12
   17 DO 18 I=1,NC
      IF (L(I).LT.0 .OR. Z(I).LT.1.0E-12) GO TO 18
      IF (ABS(Y(I)-YY(I))/Y(I).GT.CONV) GO TO 19
   18 CONTINUE
      GO TO 240
   19 SUM=0.0
      DO 21 I=1,NC
      IF (L(I).LT.0 .OR. Z(I).LT.1.0E-12) GO TO 21
      CALL WEGS (Y(I),YY(I),SY(I),YC(I))
      SUM=SUM+Y(I)
   21 CONTINUE
      DO 22 I=1,NC
   22 Y(I)=Y(I)/SUM
      GO TO 12
C
   25 CALL KCALC
   26 DO 27 I=1,NC
   27 R(I)=EK(I,1)/EK(I,2)
      K=0
C
      IF (LDBUG.GE.1) WRITE (6,28) T,U,V
   28 FORMAT ('OFLASH#2   T-U-V', F12.4,2E14.5)
      IF (LDBUG.GE.2) WRITE (6,29) (Y(I),I=1,9),(X(I,1),I=1,9),
     +                            (X(I,2),I=1,9)
   29 FORMAT ('0Y-ASS  ',9E13.5/' X1-ASS ',9E13.5/' X2-ASS ',9E13.5)
C
   30 F1=0.0
      F2=0.0
      DF1U=0.0
      DF2U=0.0
      DF1V=0.0
      DF2V=0.0
      DDF1UU=0.0
      DDF1VV=0.0
      DDF1UV=0.0
      DDF2UU=0.0
      DDF2VV=0.0
      DDF2UV=0.0
C
      DO 50 I=1,NC
C
      AA=Z(I)*(1.0-EK(I,1))
      BB=Z(I)*(1.0-R(I))
      WW=V*(1.0-U)+(1.0-V)*(1.0-U)*R(I)+U*EK(I,1)
      F1=F1+AA/WW
      F2=F2+BB/WW
C
      DWU=V*(R(I)-1.0)-R(I)+EK(I,1)
      DWV=(1.0-U)*(1.0-R(I))
      DDWUV=R(I)-1.0
C
      DF1U=DF1U-AA/WW**2*DWU
      DF2U=DF2U-BB/WW**2*DWU
```

```
      DF1V=DF1V-AA/WW**2*DWV
      DF2V=DF2V-BB/WW**2*DWV
C
      DDF1UU=DDF1UU+2.0*AA/WW**3*DWU**2
      DDF2UU=DDF2UU+2.0*BB/WW**3*DWU**2
      DDF1VV=DDF1VV+2.0*AA/WW**3*DWV**2
      DDF2VV=DDF2VV+2.0*BB/WW**3*DWV**2
      DDF1UV=DDF1UV+2.0*AA/WW**3*DWU*DWV-AA/WW**2*DDWUV
      DDF2UV=DDF2UV+2.0*BB/WW**3*DWU*DWV-BB/WW**2*DDWUV
C
   50 CONTINUE
C
      RHS(1)=-F1
      RHS(2)=-F2
      ZJ(1,1)=DF1U
      ZJ(1,2)=DF1V
      ZJ(2,1)=DF2U
      ZJ(2,2)=DF2V
C
C     RHS(1)=2.0*(F1*DF1U+F2*DF2U)
C     RHS(2)=2.0*(F1*DF1V+F2*DF2V)
C     ZJ(1,1)=2.0*(DF1U**2+F1*DDF1UU+DF2U**2+F2*DDF2UU)
C     ZJ(2,2)=2.0*(DF1V**2+F1*DDF1VV+DF2V**2+F2*DDF2VV)
C     ZJ(1,2)=2.0*(DF1U*DF1V+F1*DDF1UV+DF2U*DF2V+F2*DDF2UV)
C     ZJ(2,1)=ZJ(1,2)
C
      DETRM=ZJ(1,1)*ZJ(2,2)-ZJ(1,2)*ZJ(2,1)
      DU=(RHS(1)*ZJ(2,2)-RHS(2)*ZJ(1,2))/DETRM
      DV=(ZJ(1,1)*RHS(2)-ZJ(2,1)*RHS(1))/DETRM
      K=K+1
C
      IF (LDBUG.GE.2) WRITE (6,55) F1,F2,U,DU,V,DV
   55 FORMAT ( 5X,'F1-F2-U-DU-V-DV', 6E14.5)
C
      IF (K.LT.20) GO TO 59
   57 WRITE (6,58)
   58 FORMAT ('0FLASH2 CALCULATION TERMINATED' /
     +         ' CALCULATION CONTINUING' ///)
      GO TO 240
C
C     COMPUTE NEW VALUES OF U & V
C
   59 NCVRG=0
      GO TO (60,70), ID
   60 SDU=DU
      SDV=DV
      ID=2
      GO TO 80
   70 SSDU=SDU
      SSDV=SDV
      SDU=DU
      SDV=DV
      TOP=SSDU*SSDV+SDU*SDV
      BTM=(SSDU**2+SSDV**2)*(SDU**2+SDV**2)
      COSANG=TOP/SQRT(BTM)
      BETA=1.0+COSANG
```

```
      BETA=1.0
      DU=BETA*DU
      DV=BETA*DV
C
C     CHECK TO INSURE THAT U & V ARE .LT. 1.0 AND .GT. 0.0
C
   80 IF ((U+DU.LT.1.0 .AND. U+DU.GT.0.0) .AND.
     +    (V+DV.LE.1.0 .AND. V+DV.GE.0.0)) GO TO 90
      NCVRG=1
      DU=DU/2.0
      DV=DV/2.0
      GO TO 80
C
   90 IF (V.LT.0.99) GO TO 94
      V=1.0-V
      DO 91 I=1,NC
      HOLD=X(I,1)
      X(I,1)=X(I,2)
      X(I,2)=HOLD
      HOLD=XX(I,1)
      XX(I,1)=XX(I,2)
      XX(I,2)=HOLD
      HOLD=SX(I,1)
      SX(I,1)=SX(I,2)
      SX(I,2)=HOLD
      HOLD=XC(I,1)
      XC(I,1)=XC(I,2)
      XC(I,2)=HOLD
      HOLD=EK(I,1)
      EK(I,1)=EK(I,2)
      EK(I,2)=HOLD
      R(I)=EK(I,1)/EK(I,2)
      HOLD=GAM(I,1)
      GAM(I,1)=GAM(I,2)
      GAM(I,2)=HOLD
   91 CONTINUE
C
   94 IF (V.LT.1.E-10) GO TO 231
      IF (ABS(DU).LT.CONV1 .AND. ABS(DV).LT.CONV1 .AND. NCVRG.EQ.0)
     +    GO TO 110
C
   95 U=U+DU
      V=V+DV
      GO TO 30
C
  110 IF (ABS(F1).LT.CONV2.AND.ABS(F2).LT.CONV2) GO TO 120
      GO TO 95
C
C     CALCULATE COMPOSITIONS
C
  120 DO 180 I=1,NC
      IF (Z(I).LT.1.0E-12) GO TO 170
      IF (L(I)) 130,140,150
C     NONVOLATILE
  130 WW=V+(1.0-V)*R(I)
      YY(I)=0.0
```

```
      XX(I,1)=Z(I)/WW
      XX(I,2)=XX(I,1)*R(I)
      GO TO 180
C     NONCONDENSIBLE
  140 YY(I)=Z(I)/U
      XX(I,1)=0.0
      XX(I,2)=0.0
      GO TO 180
C     NORMAL AND SUPERCRITCAL
  150 WW=V*(1.0-U)+(1.0-V)*(1.0-U)*R(I)+U*EK(I,1)
      XX(I,1)=Z(I)/WW
      XX(I,2)=X(I,1)*R(I)
      YY(I)=EK(I,1)*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), IOX
C
  190 IF (IDLL.EQ.0) GO TO 220
      DO 210 I=1,NC
      IF (L(I).EQ.0 .OR. Z(I).LT.1.0E-12) GO TO 210
C     IF (ABS(X(I,1)*GAM(I,1)-X(I,2)*GAM(I,2))/(X(I,2)*GAM(I,2))
      IF (ABS(X(I,1)-XX(I,1))/X(I,1) .GT. CONV .OR.
     *(ABS(X(I,2)-XX(I,2))/X(I,2)) .GT. CONV) GO TO 360
C    *.GT.CONV) GO TO 360
  210 CONTINUE
  220 IF (IDLV.EQ.0) GO TO 240
      DO 230 I=1,NC
      IF (L(I).LT.0 .OR. Z(I).LT.1.0E-12) GO TO 230
      IF (ABS(Y(I)-YY(I))/Y(I).GT.CONV) GO TO 360
  230 CONTINUE
      GO TO 240
C
  231 DO 232 I=1,NC
      HOLD=X(I,1)
      X(I,1)=X(I,2)
  232 X(I,2)=HOLD
      WRITE (6,238)
  238 FORMAT (// 5X, 'LIQUID HAS GONE TO A ONE PHASE SYSTEM' //)
      NLIQ=1
      CALL FLASH1
C
  240 SUM=0.0
      SUM1=0.0
      SUM2=0.0
      DO260I=1,NC
      Y(I)=YY(I)
      SUM=SUM+Y(I)
      DO 250 N=1,2
  250 X(I,N)=XX(I,N)
      SUM1=SUM1+X(I,1)
```

```
      SUM2=SUM2+X(I,2)
  260 CONTINUE
      DO270I=1,NC
      Y(I)=Y(I)/SUM
      X(I,1)=X(I,1)/SUM1
  270 X(I,2)=X(I,2)/SUM2
      ISW=0
      RETURN
C
  280 IF (IDLL.EQ.0) GO TO 320
      DO 310 N=1,2
      SUM=0.0
      DO290I=1,NC
      SX(I,N)=X(I,N)
      XC(I,N)=XX(I,N)
      X(I,N)=(X(I,N)+XX(I,N))/2.0
  290 SUM=SUM+X(I,N)
      DO300 I=1,NC
  300 X(I,N)=X(I,N)/SUM
  310 CONTINUE
  320 IF (IDLV.EQ.0) GO TO 350
      SUM=0.0
      DO 330 I=1,NC
      SY(I)=Y(I)
      YC(I)=YY(I)
      Y(I)=(Y(I)+YY(I))/2.0
  330 SUM=SUM+Y(I)
      DO 340 I=1,NC
  340 Y(I)=Y(I)/SUM
  350 IDX=2
      GO TO 25
C
  360 IF (IDLL.EQ.0) GO TO 400
      DO 390 N=1,2
      SUM=0.0
      DO 370 I=1,NC
      IF (L(I).EQ.0 .OR. Z(I).LT.1.0E-12) GO TO 370
C     WRITE (6,365) N,I,X(I,N),XX(I,N),SX(I,N),XC(I,N)
C 365 FORMAT(/' #365', 2I5,4G20.5)
      CALL WEGS(X(I,N),XX(I,N),SX(I,N),XC(I,N))
      SUM=SUM+X(I,N)
  370 CONTINUE
      DO 380 I=1,NC
  380 X(I,N)=X(I,N)/SUM
  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 WEGS (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)
```

```
      430 SUM=SUM+Y(I)
      440 DO 450 I=1,NC
      450 Y(I)=Y(I)/SUM
          GO TO 25
    C
          END
```

```
      SUBROUTINE    AFLASH
C
C     ADIABATIC FLASH
C
C**** IMPLICIT REAL*8 (A-H,O-Z), INTEGER*2 (I-N)
C
      COMMON /B2L/      FD(11),Z(10),EK(10,2),PF,TF,HI,XSAVE(10,2)
      COMMON /CONTRL/  T,P,NOBUB,NODEW,ISO,NLIQ
      COMMON /VAPOR/   Y(10),VP(10),FUG(10),DHV,HIIDLV,HREALV,FRACV
      COMMON /LIQUID/   X(10,2),GAM(10,2),DHL(2),HIDLL(2),HREALL(2),
     +                  FRACL
      COMMON /DUMMY/    XX(10,2),SX(10,2),XC(10,2),YY(10),SY(10),
     +                  YC(10),RMAX,RMIN
      COMMON  /CTRL/   NCR, NPRT, NSTART, TITLE(20)
      COMMON  /NJIT0/  NC, NCM1, IDLL, IDLV, IDH, LDBUG, ISW, NDIM,
     *                 NAME(2,10),L(10),COMPNT(10)
      COMMON  /NJIT1/  CPL(10,4), CPV(10,4), ENP(10,10), ANT(6,10),
     *                 W(10)
      COMMON  /NJIT2/  C(180), ALPHA(45), VC(10), VOL(10), TC(10),
     *                 PC(10), OA(10), OB(10), AZ(10,10), G(10,10),
     *                 THETA(10), THS(10), HFAC(10), HHFA(10), HM(10),
     *                 W(10),RR(10),XL(10),PHI(10),DUMMY(10)
      COMMON  /NJIT3/  TTC(10,10),PPC(10,10),VVC(10,10),ZZC(10,10),
     *                 AK(10,10), AVALUE(10,10), BVALUE(10,10),
     *                 BCROSS(10,10), OMEGA(10), DIPOLE(10), BZ(10,10)
C
      DATA STEP,TINC,CONV/30.0,10.0,1.0E-4/
C
      ID=1
      S=T
   10 GO TO (11,12), NLIQ
   11 CALL FLASH1
      FRACL=1.0
      GO TO 15
   12 CALL FLASH2
   15 CALL LIQH
      CALL VAPH
      H=HREALV*FRACV+HREALL(1)*(1.0-FRACV)*FRACL+HREALL(2)*(1.0-FRACV)
     +  *(1.0-FRACL)-HI
      IF (ABS(H/HI)-CONV)70,20,20
   20 GO TO (30,40),ID
   30 T=S-SIGN(TINC,H)
      HD=H
      ID=2
      GO TO 10
   40 HD=H*(S-T)/(HD-H)
      S=T
      IF (ABS(HD)-STEP)60,60,50
   50 HD=SIGN(STEP,HD)
   60 T=T-HD
      HD=H
      GO TO 10
   70 WRITE (6,80)
   80 FORMAT('0FOLLOWING IS THE RESULT OF AN ADIABATIC FLASH.')
      RETURN
C
```

```
0039              END
```

```
      SUBROUTINE    LIQH
C
C     ENTHALPY OF A REAL LIQUID
C
C**** IMPLICIT REAL*8 (A-H,O-Z), INTEGER*2 (I-N)
C
      COMMON /B2L/      FD(11),Z(10),EK(10,2),PF,TF,HI,XSAVE(10,2)
      COMMON /CONTRL/   T,P,NOBUB,NODEW,ISO,NLIQ
      COMMON /VAPOR/    Y(10),VP(10),FUG(10),DHV,HIIDLV,HREALV,FRACV
      COMMON /LIQUID/    X(10,2),GAM(10,2),DHL(2),HIDLL(2),HREALL(2),
     +                   FRACL
      COMMON /DUMMY/     XX(10,2),SX(10,2),XC(10,2),YY(10),SY(10),
     +                   YC(10),RMAX,RMIN
      COMMON  /CTRL/    NCR, NPRT, NSTART, TITLE(20)
      COMMON  /NJIT0/   NC, NCM1, IDLL, IDLV, IDH, LDBUG, ISW, NDIM,
     *                  NAME(2,10),L(10),COMPNT(10)
      COMMON  /NJIT1/   CPL(10,4), CPV(10,4), ENP(10,10), ANT(6,10),
     *                  W(10)
C
      ISW=0
      IF (IDLL)20,10,20
   10 DHL(1)=0.0
      DHL(2)=0.0
      GO TO 50
   20 DO 40 I=1,NLIQ
      CALL ACTVTY (T,X(1,NLIQ),GAM(1,NLIQ))
   40 CALL XSHLIQ(T,X(1,NLIQ),DHL(NLIQ))
   50 DO 60 N=1,NLIQ
      HIDLL(N)=0.0
      DO 55 I=1,NC
 55   HIDLL(N)=HIDLL(N)+X(I,N)*(((ENP(I,4)*T+ENP(I,3))*T + ENP(I,2))*T
     1           +ENP(I,1))
      HREALL(N)=HIDLL(N)
      IF (IDH.EQ.0) HREALL(N)=HREALL(N)+DHL(N)
   60 CONTINUE
      RETURN
C
      END
```

```
                 SUBROUTINE    VAPH
           C
           C     ENTHALPY OF REAL VAPOR
           C
           C**** IMPLICIT REAL*8 (A-H,O-Z), INTEGER*2 (I-N)
           C
                 COMMON  /NJIT0/  NC, NCM1, IDLL, IDLV, IDH, LDBUG, ISW, NDIM,
                *                 NAME(2,10),L(10),COMPNT(10)
                 COMMON  /NJIT1/  CPL(10,4), CPV(10,4), ENP(10,10), ANT(6,10),
                *                 W(10)
                 COMMON   /VAPOR/   Y(9), VP(9), FUG(9), DHV, HIDLV, HREALV, FRACV
                 COMMON /CONTRL/  T,P,NOBUB,NODEW,ISO,NLIQ
           C
                 ISW=0
                 IF (IDLV)20,10,20
              10 DHV=0.0
                 GO TO 30
              20 CALL XSHVAP(T,P,Y,DHV)
            30   HIDLV=0.0
                 DO 40 I=1,NC
            40   HIDLV=HIDLV + Y(I)*(((ENP(I,4)*T+ENP(I,3))*T + ENP(I,2))*T
                1        +ENP(I,1))
                 HREALV=HIDLV
                 IF (IDH.EQ.0)HREALV=HREALV+DHV
                 RETURN
           C
                 END
```

```
                SUBROUTINE   XSHVAP (T,P,Y,DHV)
                COMMON  /NJITO/  NC, NCM1, IDLL, IDLV, IDH, LDBUG, ISN, NDIM,
               *                 NAME(2,10),L(10),COMPNT(10)
                GO TO (10,20),IDLV
         10     CALL RKDHV(T,P,Y,DHV)
                GO TO 99
         20     CALL VIRDHV(T,P,Y,DHV)
         99     RETURN
                END
```

```
001                  SUBROUTINE    TEMPCV(ITF,T)
               C
               C      TEMPERATURE CONVERSION
               C
               C**** IMPLICIT REAL*8 (A-H,O-Z), INTEGER*2 (I-N)
               C
002                  GO TO (20,10,30,40),ITF
003               10 T=T*1.8+32.0
004               20 RETURN
005               30 T=T-459.69
006                  RETURN
007               40 T=(T*1.8)-459.69
008                  RETURN
               C
009                  END
```

```
001                 SUBROUTINE    PRESS(IPF,P)
              C
              C     PRESSURE CONVERSION
              C
              C**** IMPLICIT REAL*8 (A-H,O-Z), INTEGER*2 (I-N)
              C
002                 GO TO (20,10,30),IPF
003              10 P=P*0.0193421
004              20 RETURN
005              30 P=P*14.70
006                 RETURN
              C
007                 END
```

```
      SUBROUTINE    PRINT
C
C**** IMPLICIT REAL*8 (A-H,O-Z), INTEGER*2 (I-N)
C
      DIMENSION          ACT(9)
C
      COMMON /B2L/     FD(11),Z(10),EK(10,2),PF,TF,HI,XSAVE(10,2)
      COMMON /CONTRL/  T,P,NOBUB,NODEW,ISO,NLIQ
      COMMON /VAPOR/   Y(10),VP(10),FUG(10),DHV,HIIDLV,HREALV,FRACV
      COMMON /LIQUID/   X(10,2),GAM(10,2),DHL(2),HIDLL(2),HREALL(2),
     +                  FRACL
      COMMON /DUMMY/    XX(10,2),SX(10,2),XC(10,2),YY(10),SY(10),
     +                  YC(10),RMAX,RMIN
      COMMON   /CTRL/  NCR, NPRT, NSTART, TITLE(20)
      COMMON   /NJIT0/ NC, NCM1, IDLL, IDLV, IDH, LOBUG, ISW, NDIM,
     *                 NAME(2,10),L(10),COMPNT(10)
      COMMON   /NJIT1/ CPL(10,4), CPV(10,4), ENP(10,10), ANT(6,10),
     *                 W(10)
      COMMON   /NJIT2/ C(180), ALPHA(45), VC(10), VOL(10), TC(10),
     *                 PC(10), OA(10), OB(10), AZ(10,10), G(10,10),
     *                 THETA(10), THS(10), HFAC(10), HHFA(10), HM(10),
     *                 Q(10),RR(10),XL(10),PHI(10),DUMMY(10)
      COMMON   /NJIT3/ TTC(10,10),PPC(10,10),VVC(10,10),ZZC(10,10),
     *                 AK(10,10), AVALUE(10,10), BVALUE(10,10),
     *                 BCROSS(10,10), OMEGA(10), DIPOLE(10), BZ(10,10)
C
      DO80 N=1,NLIQ
      WRITE (6,5) N
    5 FORMAT (/'0"VLE" DATA FOR VAPOR AND LIQUID PHASE #', I3)
      WRITE (6,1) ((NAME(J,I),J=1,2),I=1,NC)
    1 FORMAT (/25X,9(2A4,2X))
      WRITE (6,6) (Y(I),I=1,NC)
    6 FORMAT (' VAP MOLE FRAC', 9X, 9F10.5)
      WRITE (6,7) (X(I,N),I=1,NC)
    7 FORMAT (' LIQ MOLE FRAC', 9X, 9F10.5)
      WRITE (6,10) (EK(I,N),I=1,NC)
   10 FORMAT(' VALUES OF K=Y/X',7X,9F10.5)
      WRITE (6,20)(VP(I),I=1,NC)
   20 FORMAT(' VAPOR PRESSURES',7X,9F10.3)
      IF (IDLV)30,50,30
   30 WRITE (6,40)(FUG(I),I=1,NC)
   40 FORMAT(' FUGACITY FACTORS',6X,9F10.5)
   50 IF (IDLL)60,80,60
   60 WRITE (6,70) (GAM(I,N),I=1,NC)
   70 FORMAT(' ACTIVITY COEFFICIENTS ',9F10.4)
      DO 71 I=1,NC
   71 ACT(I)=GAM(I,N)*X(I,N)
      WRITE (6,72) (ACT(I),I=1,NC)
   72 FORMAT (' ACTIVITY', 14X, 9F10.4)
   80 CONTINUE
      RETURN
C
      END
```

```
0001               SUBROUTINE    WEGS(G,F,OG,OF)
             C
             C     WEGSTEIN CONVERGENCE
             C
             C**** IMPLICIT REAL*8 (A-H,O-Z), INTEGER*2 (I-N)
             C
0002               SL=(OF-F)/(OG-G)
0003               OG=G
0004               OF=F
0005               SL=1.0/(1.0-SL)
0006               IF (SL.LE.0.0)SL=0.5
0007            10 V=SL*F+(1.0-SL)*G
0008               IF (V.GT.0.0) GO TO 20
0009               SL=SL*0.5
0010               GO TO 10
0011            20 G=V
0012               RETURN
             C
0013               END
```

```
              SUBROUTINE    RKDHV(T,P,Y,DHV)
       C
       C      ENTHALPY DEPARTURE FROM IDEAL GAS -- EVALUATED
       C           USING REDLICH-KWONG EQUATION
       C
       C**** IMPLICIT REAL*8 (A-H,O-Z), INTEGER*2 (I-N)
       C
              DIMENSION  Y(20)
              COMMON  /NJIT0/  NC, NCM1, IDLL, IDLV, IDH, LDBUG, ISW, NDIM,
             *                 NAME(2,10),L(10),COMPNT(10)
              COMMON  /NJIT2/  C(180), ALPHA(45), VC(10), VOL(10), TC(10),
             *                 PC(10), OA(10), OB(10), AZ(10,10), G(10,10),
             *                 THETA(10), THS(10), HFAC(10), HHFA(10), HM(10),
             *                 W(10),RR(10),XL(10),PHI(10),DUMMY(10)
       C
              TE=T
              A=0.0
              B=0.0
              DO10J=1,NC
              A=A+OA(J)*Y(J)
           10 B=B+OB(J)*Y(J)
              A=A/TE**1.25
              B=B/TE
              CALL ZCALC  ( A,B,P,ZZ)
              DHV=1.9872*TE*(ZZ-1.0-1.5*A*A*ALOG(1.0+B*P/ZZ)/B)
              RETURN
       C
              END
```

```
                 SUBROUTINE       KCALC
           C
                 IMPLICIT REAL    (M)
                 INTEGER          COMPNT
           C
                 COMMON /B2L/     FD(11),Z(10),EK(10,2),PF,TF,HI,XSAVE(10,2)
                 COMMON /CONTRL/  T,P,NOBUB,NODEW,ISO,NLIQ
                 COMMON /VAPOR/   Y(10),VP(10),FUG(10),DHV,HIIDLV,HREALV,FRACV
                 COMMON /LIQUID/   X(10,2),GAM(10,2),DHL(2),HIDLL(2),HREALL(2),
                +                  FRACL
                 COMMON /DUMMY/    XX(10,2),SX(10,2),XC(10,2),YY(10),SY(10),
                +                  YC(10),RMAX,RMIN
                 COMMON  /CTRL/   NCR, NPRT, NSTART, TITLE(20)
                 COMMON  /NJIT0/  NC, NCM1, IDLL, IDLV, IDH, LDBUG, ISW, NDIM,
                *                 NAME(2,10),L(10),COMPNT(10)
                 COMMON  /NJIT1/  CPL(10,4), CPV(10,4), EMP(10,10), ANT(6,10),
                *                 W(10)
           C
           C
                 TT=T
                  P=PF
           C
               8 DO 9 J=1,NC
                 GAM(J,1)=1.0
                 GAM(J,2)=1.0
                 FUG(J)=1.0
                 VP(J)=EXP(ANT(1,J)+ANT(2,J)/(ANT(3,J)+TT)+ANT(4,J)*TT+ANT(5,J)*
                *      TT*TT+ANT(6,J)*ALOG(TT))
               9 CONTINUE
           C
           C
              11 IF (IDLL.EQ.0) GO TO 20
                 ISW=0
                 DO 12 I=1,NLIQ
            12   CALL ACTVTY (TT,X(1,I),GAM(1,I))
           C
              20 IF (IDLV.EQ.0) GO TO 40
                 CALL FUGCTY (TT,P,Y,VP,FUG,DHV)
           C
              40 DO 50 I=1,NLIQ
                  DO 50 J=1,NC
              50 EK(J,I)=VP(J)/P*GAM(J,I)*FUG(J)
           C
           C
             250 RETURN
                 END
```

```
                   SUBROUTINE        VIRDHV (T,P,Y,DHV)
            C
                   REAL              Y(1),VP(1),FUG(1)
            C
                   COMMON   /NJIT0/  NC, NCM1, IDLL, IDLV, IDH, LDBUG, ISW, NDIM,
                 *                   NAME(2,10),L(10),COMPNT(10)
                   COMMON   /NJIT2/  C(180), ALPHA(45), VC(10), VOL(10), TC(10),
                 *                   PC(10), OA(10), OB(10), AZ(10,10), G(10,10)
                   COMMON   /NJIT3/  TTC(10,10),PPC(10,10),VVC(10,10),ZZC(10,10),
                 *                   AK(10,10), AVALUE(10,10), BVALUE(10,10),
                 *                   ACROSS(10,10), OMEGA(10), DIPOLE(10), BZ(10,10)
                   P=P/760.0
            C
            C
            C      SUBROUTINE TSONOP GENERATES BZ(I,J) FOR VIRFUG
                   CALL TSONOP(T,P,MARK)
            C
                   RT=82.057*T
                   PORT=P/RT
                   SUMY=0.0
                   BMIX=0.0
                   DO 15 I=1,NC
                   VP(I)=VP(I)/760.0
                   SUMY=SUMY+Y(I)
                   DO 10 J=1,NC
                   BMIX=BMIX+Y(I)*Y(J)*BZ(I,J)
                10 CONTINUE
                15 CONTINUE
                   BMIX=BMIX /SUMY**2
                   IF (MARK) 20,20,22
                20 SQARG=0.25 + BMIX*PORT
            C
            C   IF BMIX*P/RT IS MORE NEGATIVE THAN 0.25, THE PRESSURE SERIES VIRIAL
            C   EQ. MUST BE USED. THE ARGUMENT MARK IS USED TO COMUNICATE THIS
            C   TO THE MAIN PROGRAM
            C
                   IF (SQARG) 22,25,25
                22 VMIX=BMIX +1. /PORT
                   ZMIX=PORT*VMIX
                   MARK=MARK+1
                   GO TO 50
                25 VMIX=(0.5+SQRT (SQARG))/PORT
                   ZMIX=PORT*VMIX
            C
            C   CALCULATION OF FUGACITY COEFFICIENTS
            C
              50   DHV=1.9872*T*(ZMIX-1.0)
            C      PRINT 400,DHV,T,P
             400   FORMAT(5X,'DHV=',G15.6,'TEMP=',G15.6,'PRESS=',G15.6)
            C      DO 51 I=1,NC
            C      DO 51 J=1,NC
            C 51   WRITE(6,401) I,J,BZ(I,J)
             401   FORMAT(5X,'B(',I2,',',I2,')=',G15.5)
                   DO 52 I=1,NC
              52   VP(I)=VP(I)*760.0
                   P=P*760.0
```

```
035                 RETURN
036                 END
```

```
      SUBROUTINE MATRIX
C
      IMPLICIT REAL     (M)
      INTEGER           COMPNT
      REAL              LIQUID
C
      COMMON  /CTRL/    NCR, NPRT, NSTART, TITLE(20)
      COMMON  /NJITO/   NK, NCM1, IDLL, IDLV, IDH, LDBUG, ISW,
     *                  NAME(4,10), L(10), NDIM, COMPNT(10)
      COMMON  /INR0/    NST, NSTM1, NK1, NK2, NK11, NK21, NCASE, KUNITS,
     *                  NFEED, LF(9), IDCODE, ITR, ITRMAX, ICODE
      COMMON  /INR1/    FSTR(9,11), FKV(9), HF(9), FLMAX(10), FVMAX(10),
     *                  DEST,DESTV,DESTL, BTMS, RFLX,BOIL, PP(50), T(50),
     *                  MU(50), SL(50), SV(50), FL(50), FLL(50,10),
     *                  FV(50), FVV(50,10), ZCONVT, ZCONVF
      COMMON  /INR2/    DFK(10,21), HL(50), HLL(50,10), CL(50), HHE(50),
     *                  DEXH(50,11), HV(50), HVV(50,10), CV(50)
      COMMON  /INR3/    AMAT(21,21), BMAT(50,21,21), D(50,21)
      COMMON  /INR4/    VAPOR, LIQUID, FEED(11)
      COMMON  /VLE/     XFK(10), GAM(10), X(10), Y(10), VP(10), FUG(10)
C
      EQUIVALENCE       (WATER,VAPOR)
C
C
C     D(I,J) IS THE MATRIX CONSISTING OF THE CALCULATED
C     DISCREPANCY  FUNCTIONS ON PLATE I FOR COMPONENT J.
C
C     FOR PLATE I, D(I,J) CONSISTS OF
C         EQNS      1-NC              COMPONENTIAL MATERIAL BALANCES
C         EQNS      NC+1-2*NC         EQUILIBRIUM RELATION WITH MURPHREE EFF
C         EQN       2*NC+1            ENERGY BALANCE
C
C     NOTE THAT FOR I=1 AND I=NST (NST=NUMBER OF STAGES) THERE ARE
C     SPECIAL RELATIONS USED TO REPLACE THE ENTHALPY BALANCES.
C
C     PROBLEM TYPE CONTROLLED BY 'NCASE'
C         1     ABSORBER / STRIPPER
C         2     REBOILED ABSORBER / STRIPPER
C         3     FRACTIONATOR --- REFLUX GIVEN
C         4     FRACTIONATOR --- BOILUP GIVEN
C         5     FRACTIONATOR --- REBOILED ABSORBER
C
      IF (IDCODE.EQ.0)  GO TO 9
C
C     LOCATE THE LARGEST COMPONENT # IN THE LIQUID DISTILLATE
C
      JBIG=0
      BIG=0.0
      DO 5 J=1,NK
      IF (FLL(NST,J).LE.BIG) GO TO 5
      JBIG=J
      BIG=FLL(NST,J)
    5 CONTINUE
C
    9 GO TO (10,10,30,30,30), NCASE
   10 ASSIGN  70 TO NSV1
```

```
      ASSIGN 170 TO NSV2
      GO TO 50
   30 ASSIGN  80 TO NSV1
      ASSIGN 160 TO NSV2
C
   50 DO 219 I=1,NST
C
      CALL KFAC(I)
      IF (I.NE.NST) GO TO 59
      IF (IDCODE.NE.1) GO TO 59
      IF (ITR.EQ.0) GO TO 59
C     THIS  IS A BUBBLE POINT CALCULATION FOR ONE LIQUID PHASE
C     TO PRE-ESTABLISH THE TEMPERATURE IN THE ACCUMULATOR(DISTILLATE
C     DRUM).  METHOD OF SOLVING THE DESIGN EQUATIONS
C     FN(T)=SUM OF KX -1.0=0 WHICH(SUM OF KL)-L=0 IS SECANT METHOD
C
C
      ID=1
      KNT=0
   51 FN=-FL(NST)
      DO 52 J=1,NK
   52 FN=FN+XFK(J)*FLL(NST,J)
C     WRITE (NPRT,53) JBIG,BIG,T(NST),FN
C  53 FORMAT (5X,I5,G12.5,10X,2G15.5)
      KNT=KNT+1
      IF (KNT.EQ.20) GO TO 59
      IF (ABS(FN)/FL(NST).LT.0.00005) GO TO 59
      GO TO (54,55), ID
   54 ID=2
      SFN=FN
      ST=T(NST)
      T(NST)=T(NST)-SIGN(2.0,FN)
      CALL KFAC(NST)
      GO TO 51
   55 DTNST=-FN/(FN-SFN)*(T(NST)-ST)
      DTNST=SIGN(AMIN1(ABS(DTNST),10.0),DTNST)
      SFN=FN
      ST=T(NST)
      T(NST)=T(NST)+DTNST
      CALL KFAC(NST)
      GO TO 51
C
C
C
C
   59 UA=1.0+SV(I)/FV(I)
C
C     UA=1.0+SV(I)/FV(I)
      UB=1.0+SL(I)/FL(I)
      UC=MU(I)*FV(I)/FL(I)
      UD=SL(I)/FL(I)**2
      UE=SV(I)/FV(I)**2
C
      DO 60 J=1,NK
      N=NK+J
      D(I,J)=FVV(I,J)*UA+FLL(I,J)*UB
```

```
      D(I,N)=UC*XFK(J)*FLL(I,J)-FVV(I,J)
      IF (I.GT.1) D(I,J)=D(I,J)-FVV(I-1,J)
      IF (I.GT.1) D(I,N)=D(I,N)+(1.0-MU(I))*FVV(I-1,J)*FV(I)/FV(I-1)
      IF (NCASE.EQ.1 .AND. I.EQ.1) D(1,N)=D(1,N)+(1.0-MU(1))*FSTR(1,J)*
     *                                 FV(1)/FSTR(1,NK1)
      IF (I.LT.NST) D(I,J)=D(I,J)-FLL(I+1,J)
   60 CONTINUE
C
C     SPECIAL EQUATIONS ... STAGES 1 & NST
C
      GO TO NSV1, (70,80)
C
C           ABSORBER / STRIPPER
   70 D(I,NK2)=UA*HV(I)+UB*HL(I)+(FL(I)+SL(I))*HHE(I)
      IF (I.EQ.1) GO TO 130
      D(I,NK2)=D(I,NK2)-HV(I-1)
      D(I-1,NK2)=D(I-1,NK2)-HL(I)-FL(I)*HHE(I)
      GO TO 130
C           DISTILLATION COLUMN
   80 IF (I.EQ.1) GO TO 90
      IF (I.EQ.NST) GO TO 110
      D(I,NK2)=UA*HV(I)+UB*HL(I)-HV(I-1)+(FL(I)+SL(I))*HHE(I)
      IF (I.GT.2) D(I-1,NK2)=D(I-1,NK2)-HL(I)-FL(I)*HHE(I)
      GO TO 130
C
C     REBOILER ... STAGE 1
   90 IF (NCASE.EQ.3) GO TO 91
      IF (NCASE.EQ.4) GO TO 100
      IF (NCASE.EQ.5) GO TO 106
C
C     REFLUX RATIO SPECIFIED ... BOTTOMS DRAWOFF PRODUCT RATE FIXED
   91 D(1,NK2)=BTMS
   92 DO 95 J=1,NK
   95 D(1,NK2)=D(1,NK2)-FLL(1,J)
      GO TO 130
C
C     BOILUP RATIO SPECIFIED ... FIX VAPOR RATE FROM REBOILER
  100 D(1,NK2)=BOIL*BTMS
  101 DO 105 J=1,NK
  105 D(1,NK2)=D(1,NK2)-FVV(1,J)
      GO TO 130
C
C     BOILUP RATIO SPECIFIED ... FIX VAPOR RATE FROM REBOILER
  106 GO TO 100
C
C     CONDENSER ... STAGE NST
  110 IF (NCASE.EQ.3) GO TO 111
      IF (NCASE.EQ.4) GO TO 121
      IF (NCASE.EQ.5) GO TO 129
C
C          DISTILLATE CODE    ...    "IDCODE"
C               -1   SUBCOOLED LIQUID (T-NST HELD CONSTANT)
C                0   ALL VAPOR / VAPOR-LIQUID PRODUCT
C                1   BUBBLE POINT LIQUID
C
C     REFLUX RATIO SPECIFIED ... CHECK DISTILLATE CODE
```

```
   111 IF (IDCODE) 116,112,116
C      VAPOR OR VAPOR/LIQUID DISTILLATE ... FIX REFLUX LIQUID RATE
   112 D(NST,NK2)=RFLX*DEST
   113 DO 114 J=1,NK
   114 D(NST,NK2)=D(NST,NK2)-FLL(NST,J)
   115 D(NSTM1,NK2)=D(NSTM1,NK2)-HL(NST)-FL(NST)*HHE(NST)
       GO TO 130
C      LIQUID DISTILLATE ... FVV/FV=FLL/FL PLUS BUBBLE POINT EQUATION
C      FOR SUBCOOLED LIQUID BUBBLE POINT EQUATION REPLACED BY DT-NST=0.0
   116 DO 117 J=1,NK
       N=J+NK
   117 D(NST,N)=FVV(NST,J)*FL(NST)-FLL(NST,J)*FV(NST)
       N=JBIG+NK
       D(NST,N)=-FL(NST)
       DO 118 J=1,NK
   118 D(NST,N)=D(NST,N)+XFK(J)*FLL(NST,J)
       IF (IDCODE.LT.0) D(NST,N)=0.0
       GO TO 112
C
C      BOILUP RATIO SPECIFIED ... CHECK DISTILLATE CODE
   121 IF (IDCODE) 126,122,126
C      VAPOR OR VAPOR/LIQUID DISTILLATE ... FIX DISTILLATE VAPOR RATE
   122 D(NST,NK2)=DESTV
       DO 124 J=1,NK
   124 D(NST,NK2)=D(NST,NK2)-FVV(NST,J)
       GO TO 115
C      LIQUID DISTILLATE ... FVV/FV=FLL/FL PLUS BUBBLE POINT EQUATION
C      FOR SUBCOOLED LIQUID BUBBLE POINT EQUATION REPLACED BY DT-NST=0.0
   126 DO 127 J=1,NK
       N=J+NK
   127 D(NST,N)=FVV(NST,J)*FL(NST)-FLL(NST,J)*FV(NST)
       N=JBIG+NK
       D(NST,N)=-FL(NST)
       DO 128 J=1,NK
   128 D(NST,N)=D(NST,N)+XFK(J)*FLL(NST,J)
       IF (IDCODE.LT.0) D(NST,N)=0.0
       GO TO 122
C
C      BOILUP RATIO SPECIFIED ... CHECK DISTILLATE CODE
   129 GO TO 121
C
   130 CONTINUE
C
C      DEFINITION OF THE JACOBIAN MATRIX.  IT CONSISTS OF PARTIAL
C      DERIVATIVES OF THE PLATE CORRECTION FUNCTIONS WITH RESPECT
C      TO THE VARIABLES ON PLATE I.
C
C      IN THE DESCRIPTION OF THE JACOBIAN MATRIX (B-MATRIX) THE
C      CORRECTION FUNCTIONS WILL BE STATED AS F AND THE INDEPENDENT
C      VARIABLES WILL BE STATED AS V.
C
       DO 150 J=1,NK
       JJ=J+NK
       DO 140 K=1,NK
       KK=NK1+K
C
```

```
      C           F(V)=MATERIAL BALANCES
      C           V=COMPONENT FLOW IN VAPOR PHASE
      C
                BMAT(I,J,KK)=-FVV(I,J)*UE
      C
      C           F(V)=EQUILIBRIUM RELATIONSHIPS
      C           V=COMPONENT FLOW IN VAPOR PHASE
      C
                BMAT(I,JJ,KK)=MU(I)*FLL(I,J)*(XFK(J)+DFK(J,KK)*FV(I))/FL(I)
                IF (I.GT.1) BMAT(I,JJ,KK)=BMAT(I,JJ,KK)+(1.0-MU(I))*FVV(I-1,J)/
               *             FV(I-1)
                IF (NCASE.EQ.1 .AND. I.EQ.1) BMAT(1,JJ,KK)=BMAT(1,JJ,KK)+
               *                 (1.0-MU(1))*FSTR(1,J)/FSTR(1,NK1)
      C
      C           F(V)=EQUILIBRIUM RELATIONSHIPS
      C           V=COMPONENT FLOW IN LIQUID PHASE
      C
                BMAT(I,JJ,K)=UC*FLL(I,J)*(DFK(J,K)-XFK(J)/FL(I))
      C
      C           F(V)=MATERIAL BALANCES
      C           V=COMPONENT FLOW IN LIQUID PHASE
      C
            140 BMAT(I,J,K)=-FLL(I,J)*UD
                BMAT(I,J,J)=BMAT(I,J,J)+UB
      C
      C           F(V)=MATERIAL BALANCES
      C           V=TEMPERATURE
      C
                BMAT(I,J,NK1)=0.0
      C
      C           F(V)=MATERIAL BALANCES
      C           V=COMPONENT FLOW IN VAPOR PHASE
      C
                BMAT(I,J,J+NK1)=BMAT(I,J,J+NK1)+UA
      C
      C           F(V)=EQUILIBRIUM RELATIONSHIPS
      C           V=COMPONENT FLOW IN LIQUID PHASE
      C
                BMAT(I,J+NK,J)=BMAT(I,J+NK,J)+UC*XFK(J)
      C
      C           F(V)=EQUILIBRIUM RELATIONSHIPS
      C           V=TEMPERATURE
      C
                BMAT(I,JJ,NK1)=UC*FLL(I,J)*DFK(J,NK1)
      C
      C           F(V)=EQUILIBRIUM RELATIONSHIP
      C           V=COMPONENT FLOW IN VAPOR PHASE
      C
                BMAT(I,J+NK,J+NK1)=BMAT(I,J+NK,J+NK1)-1.0
      C
            150 CONTINUE
      C
      C                     NOTE THE SPECIAL EQUATION FOR I=1 AND I=NST
      C
      C
                GO TO NSV2, (170,160)
```

```
C
  160 IF (I.EQ.1) GO TO 190
      IF (I.EQ.NST) GO TO 200
C
  170 DO 180 K=1,NK
C
C          F(V)=ENTHALPY BALANCES
C          V=COMPONENT FLOW IN VAPOR PHASE
C
      KK=NK1+K
      BMAT(I,NK2,KK)=-HV(I)*UE+UA*HVV(I,K)
C
C          F(V)=ENTHALPY BALANCES
C          V=COMPONENT FLOW IN LIQUID PHASE
C
  180 BMAT(I,NK2,K)=-HL(I)*UD+UB*HLL(I,K)+HHE(I)+(FL(I)+SL(I))*DEXH(I,K)
C
C          F(V)=ENTHALPY BALANCES
C          V=TEMPERATURE
C
      BMAT(I,NK2,NK1)=CV(I)*UA+CL(I)*UB+(FL(I)+SL(I))*DEXH(I,NK1)
      GO TO 219
C
C     SPECIAL EQUATIONS FOR STAGES 1 & NST
C
C     REBOILER ... STAGE 1
  190 IF (NCASE.EQ.3) GO TO 192
      IF (NCASE.EQ.4) GO TO 196
      IF (NCASE.EQ.5) GO TO 198
C
C     REFLUX RATIO SPECIFIED ... NCASE=3
C       (1) BOTTOMS PRODUCT RATE FIXED
C       (2) PUMPBACK REFLUX RATE FIXED
  192 DO 194 K=1,NK
      KK=K+NK1
      BMAT(I,NK2,KK)=0.0
  194 BMAT(I,NK2,K)=-1.0
      BMAT(I,NK2,NK1)=0.0
      GO TO 219
C
C     BOILUP RATIO SPECIFIED ... NCASE=4
C       (1) VAPOR FROM REBOILER FIXED
C       (2) VAPOR DISTILLATE FIXED
  196 DO 197 K=1,NK
      KK=K+NK1
      BMAT(I,NK2,KK)=-1.0
  197 BMAT(I,NK2,K)=0.0
      BMAT(I,NK2,NK1)=0.0
      GO TO 219
C
C     BOILUP RATIO SPECIFIED ... NCASE=5
  198 GO TO 196
C
C     CONDENSER ... STAGE NST
  200 IF (NCASE.EQ.3) GO TO 201
      IF (NCASE.EQ.4) GO TO 215
```

```
                IF (NCASE.EQ.5) GO TO 218
      C
      C         REFLUX SPECIFIED ... CHECK DISTILLATE CODE
          201   IF (IDCODE) 204,202,204
      C         VAPOR OR VAPOR/LIQUID DISTILLATE ... FIX LIQUID REFLUX
          202   GO TO 192
      C         LIQUID DISTILLATE ... FVV/FV=FLL/FL PLUS BUBBLE POINT EQUATION
      C         FOR SUBCOOLED LIQUID BUBBLE POINT EQUATION REPLACED BY DT-NST=0.0
          204   DO 205 J=1,NK
                N=J+NK
                BMAT(NST,N,NK1)=0.0
                DO 205 K=1,NK
                KK=K+NK
                BMAT(NST,N,K)=FVV(NST,J)
          205   BMAT(NST,N,KK)=-FLL(NST,J)
                DO 206 J=1,NK
                K=J
                N=J+NK
                KK=K+NK1
                BMAT(NST,N,K)=BMAT(NST,N,K)-FV(NST)
          206   BMAT(NST,N,KK)=BMAT(NST,N,KK)+FL(NST)
                N=JBIG+NK
                DO 207 K=1,NK
                J=K
                KK=K+NK1
                BMAT(NST,N,K)=XFK(J)-1.0
                BMAT(NST,N,KK)=0.0
          207   BMAT(NST,N,NK1)=BMAT(NST,N,NK1)+DFK(J,NK1)*FLL(NST,J)
                DO 209 J=1,NK
                DO 209 K=1,NK
                KK=K+NK1
                BMAT(NST,N,K)=BMAT(NST,N,K)+DFK(J,K)*FLL(NST,J)
          209   BMAT(NST,N,KK)=BMAT(NST,N,KK)+DFK(J,KK)*FLL(NST,J)
                IF (IDCODE.NE.-1) GO TO 214
                DO 213 K=1,NK2
          213   BMAT(NST,N,K)=0.0
                BMAT(NST,N,NK1)=1.0
          214   IF (NCASE.EQ.3) GO TO 192
                IF (NCASE.EQ.4) GO TO 195
      C
      C         BOILUP SPECIFIED ... CHECK DISTILLATE CODE
          215   IF (IDCODE) 217,216,217
      C         VAPOR OR VAPOR/LIQUID DISTILLATE ... FIX DISTILLATE VAPOR RATE
          216   GO TO 196
      C         LIQUID DISTILLATE ... FVV/FV=FLL/FL PLUS BUBBLE POINT EQUATION
      C         FOR SUBCOOLED LIQUID BUBBLE POINT EQUATION REPLACED BY DT-NST=0.0
          217   GO TO 204
      C
      C         BOILUP SPECIFIED ... CHECK DISTILLATE CODE
          218   GO TO 215
      C
          219   CONTINUE
      C
      C              FEED STREAMS ARE HANDLED HERE
      C
                DO 230 I=1,NFEED
```

```
      J=LF(I)
      DO 220 K=1,NK
  220 D(J,K)=D(J,K)-FSTR(I,K)
      IF (NCASE.EQ.5.AND.J.EQ.NST) GO TO 230
      D(J,NK2)=D(J,NK2)-HF(I)
  230 CONTINUE
C
C                        NOTE: SIGN BEFORE D(I,J) IS CHANGED
C                              DUE TO NEWTON-RAPHSON EQUATION
C
      DO 240 I=1,NST
      DO 240 J=1,NK2
  240 D(I,J)=-D(I,J)
C
C         AT THIS POINT THE B-MATRIX AND D-VECTOR ARE DEFINED FOR THE
C         ENTIRE COLUMN, STAGE=1,NST.
C
C         GENERATION OF THE A-MATRIX FOR STAGE 2 IS ACCOMPLISHED HERE.
C         A-MATRIX FOR STAGE 1 IS UNDEFINED.
C
      DO 290 J=1,NK2
      DO 290 K=1,NK2
  290 AMAT(J,K)=0.0
C
C          F(V)=MATERIAL BALANCES
C          V=COMPONENT FLOW IN VAPOR PHASE
C
      DO 300 J=1,NK
  300 AMAT(J,J+NK1)=-1.0
C
C          F(V)=ENTHALPY BALANCES
C          V=TEMPERATURE
C
      AMAT(NK2,NK1)=-CV(1)
C
C          F(V)=EQUILIBRIUM RELATIONSHIPS
C          V=COMPONENT FLOW IN VAPOR PHASE
C
      YX=(1.0-MU(2))*FV(2)/(FV(1)**2)
      DO 320 JJ=NK1,NK21
      J=JJ-NK
      DO 310 KK=NK11,NK2
  310 AMAT(JJ,KK)=-YX*FVV(1,J)
      JJJ=J+NK1
  320 AMAT(JJ,JJJ)=AMAT(JJ,JJJ)+YX*FV(1)
C
C          F(V)=ENTHALPY BALANCES
C          V=COMPONENT FLOW IN VAPOR PHASE
C
      DO 330 KK=NK11,NK2
      K=KK-NK1
  330 AMAT(NK2,KK)=-HVV(1,K)
C
C     MODIFY EQUILIBRIUM RELATIONSHIP TO REFLECT NON-VOLATILE (L=-1)
C     AND NON-CONDENSABILE (L=0) COMPONENTS
C
```

```
      DO 370 J=1,NK
      IF (L(J).GT.0) GO TO 370
      JJ=J+NK
      DO 340 K=1,NK2
  340 AMAT(JJ,K)=0.0
      DO 360 I=1,NST
      D(I,JJ)=0.0
      DO 350 K=1,NK2
  350 BMAT(I,JJ,K)=0.0
C     NON-VOLATILE COMPONENT ... VAPOR FLOW = 0.0
      IF (L(J).EQ.-1) BMAT(I,JJ,J+NK1)=1.0
C     NON-CONDENSABILE COMPONENT ... LIQUID FLOW = 0.0
      IF (L(J).EQ.0) BMAT(I,JJ,J)=1.0
  360 CONTINUE
  370 CONTINUE
C
      RETURN
      END
```

```
C     SUBROUTINE CORECT
      IMPLICIT REAL      (M)
      INTEGER            COMPNT
      REAL*8             CM(21,42)
      REAL               LIQUID
C
      COMMON  /CTRL/   NCR, NPRT, NSTART, TITLE(20)
      COMMON  /NJIT0/  NK, NCM1, IDLL, IDLV, IDH, LDBUG, ISW,
     *                 NAME(4,10), L(10), NDIM, COMPNT(10)
      COMMON  /INR0/   NST, NSTM1, NK1, NK2, NK11, NK21, NCASE, KUNITS,
     *                 NFEED, LF(9), IDCODE, ITR, ITRMAX, ICODE
      COMMON  /INR1/   FSTR(9,11), FKV(9), HF(9), FLMAX(10), FVMAX(10),
     *                 DEST,DESTV,DESTL, BTMS, RFLX,BOIL, PP(50), T(50),
     *                 MU(50), SL(50), SV(50), FL(50), FLL(50,10),
     *                 FV(50), FVV(50,10), ZCONVT, ZCONVF
      COMMON  /INR2/   DFK(10,21), HL(50), HLL(50,10), CL(50), HHE(50),
     *                 DFXH(50,11), HV(50), HVV(50,10), CV(50)
      COMMON  /INR3/   AMAT(21,21), BMAT(50,21,21), D(50,21)
      COMMON  /INR4/   VAPOR, LIQUID, FFED(11)
C
      DATA             TMAX /10.0/
C
      GO TO (10,10,30,30,30), NCASE
   10 ASSIGN 180 TO NSW1
      ASSIGN 230 TO NSW2
      ASSIGN 270 TO NSW3
      ASSIGN 390 TO NSW4
      GO TO 50
   30 ASSIGN 170 TO NSW1
      ASSIGN 220 TO NSW2
      ASSIGN 260 TO NSW3
      ASSIGN 380 TO NSW4
C
C     SOLUTION OF THE BLOCK TRIDIAGONAL EQUATION.
C
   50 DO 350 I=2,NST
C
C     THE B-MATRIX AND THE A-MATRIX ARE STORED IN THE MATRIX CM.
C     NOTE THAT BOTH A AND B ARE STORED IN THE TRANSPOSED FORM.
C
      DO 120 K=1,NK2
      KK=K+NK2
      DO 110 J=1,NK2
      CM(J,K)=BMAT(I-1,K,J)
      CM(J,KK)=AMAT(K,J)
  110 CONTINUE
  120 CONTINUE
C
C     FORMATION OF THE NEXT A-MATRIX  ...  STAGE I+1
C
      IF (I.EQ.NST) GO TO 200
      DO 130 J=1,NK2
      DO 130 K=1,NK2
  130 AMAT(J,K)=0.0
C
```

```
C          F(V)=MATERIAL BALANCES
C          V=COMPONENT FLOW IN VAPOR PHASE
C
      DO 140 J=1,NK
  140 AMAT(J,J+NK1)=-1.0
C
C          F(V)=EQUILIBRIUM RELATIONSHIPS
C          V=COMPONENT FLOW IN VAPOR PHASE
C
      XY=(1.0-MU(I+1))*FV(I+1)/(FV(I)**2)
      DO 160 JJ=NK1,NK21
      J=JJ-NK
      DO 150 KK=NK11,NK2
  150 AMAT(JJ,KK)=-XY*FVV(I,J)
      JJJ=J+NK1
  160 AMAT(JJ,JJJ)=AMAT(JJ,JJJ)+XY*FV(I)
C
C     NOTE: SPECIAL EQUATIONS FOR STAGE 'NST' ... THE TOP OF THE COLUMN
C
      GO TO NSW1, (180,170)
C
  170 IF (I.EQ.NSTM1) GO TO 191
C
C          F(V)=ENTHALPY BALANCES
C          V=TEMPERATURE
C
  180 AMAT(NK2,NK1)=-CV(I)
C
C          F(V)=ENTHALPY BALANCES
C          V=COMPONENT FLOW IN VAPOR PHASE
C
      DO 190 KK=NK11,NK2
      K=KK-NK1
  190 AMAT(NK2,KK)=-HVV(I,K)
C
C     MODIFY EQUILIBRIUM RELATIONSHIP TO REFLECT COMPONENT TYPE
C             L=-1  NON-VOLATILE
C             L=0   NON-CONDENSABLE
C
  191 DO 198 J=1,NK
      IF (L(J).GT.0) GO TO 198
      JJ=J+NK
      DO 194 K=1,NK2
  194 AMAT(JJ,K)=0.0
  198 CONTINUE
C
  200 CONTINUE
C
C     SOLUTION TO    Q=A *B   (INVERSE).
C                       I  I-1
C
C     NOTE THAT THE SOLUTION IS TRANSPOSED.
C
      CALL GAUSL (21,42,NK2,NK2,CM)
      DO 210 J=1,NK2
      DO 210 K=1,NK2
```

```
            KK=NK2+K
            CM(K,J)=CM(J,KK)
   210      CONTINUE
C
C           FORMATION OF THE MATRICES ACCORDING TO THE THOMAS PROCEDURE.
C
C           DERIVATIVES ON STAGE 'I' ARE STORED AS FOLLOWS:
C                     * STAGE 'I-1' IN 'AMAT'
C                     * STAGE 'I' IN 'BMAT'
C                     * STAGE 'I+1' GENERATED AS NEEDED ... FTN STM 220-400
C
            DO 250 J=1,NK2
            DO 250 K=1,NK
C
            GO TO NSW2, (230,220)
C
   220      IF (I.GT.2) GO TO 230
            BMAT(I,J,K)=BMAT(I,J,K)+CM(J,K)
            GO TO 240
   230      BMAT(I,J,K)=BMAT(I,J,K)+CM(J,K)+CM(J,NK2)*(HLL(I,K)+HHE(I)+FL(I)*
           *              DEXH(I,K))
   240      CONTINUE
   250      CONTINUE
C
            GO TO NSW3, (270,260)
C
   260      IF (I.EQ.2) GO TO 290
   270      DO 280 J=1,NK2
   280      BMAT(I,J,NK1)=BMAT(I,J,NK1)+CM(J,NK2)*(CL(I)+FL(I)*DEXH(I,NK1))
   290      CONTINUE
C
            DO 300 J=1,NK2
            DO 300 K=1,NK2
   300      D(I,J)=D(I,J)-CM(J,K)*D(I-1,K)
C
   350      CONTINUE
C
C           CORRECTION OF THE VARIABLES ACCORDING TO THE NEWTON-RAPHSON METHO
C           THE SIMPLE STRUCTURE OF THE COMPLETE JACOBIAN MATRIX IS UTILIZED.
C
            DO 550 KK=1,NST
            I=NST+1-KK
C
            DO 360 J=1,NK2
            CM(J,NK2+1)=D(I,J)
            DO 360 K=1,NK2
   360      CM(J,K)=BMAT(I,J,K)
            IF (I.EQ.NST) GO TO 410
C
            DO 370 J=1,NK
   370      CM(J,NK2+1)=CM(J,NK2+1)+D(I+1,J)
C
            GO TO NSW4, (390,380)
C
   380      IF (I.EQ.1) GO TO 410
   390      DO 400 J=1,NK
```

```
  400 CM(NK2,NK2+1)=CM(NK2,NK2+1)+D(I+1,J)*(HLL(I+1,J)+HHE(I+1)+FL(I+1)*
     *                  DEXH(I+1,J))
      CM(NK2,NK2+1)=CM(NK2,NK2+1)+D(I+1,NK1)*(CL(I+1)+FL(I+1)*DEXH(I+1,N
     *                  K1))
C
  410 CALL GAUSL (21,42,NK2,1,CM)
      DO 460 J=1,NK2
  460 D(I,J)=CM(J,NK2+1)
C
C     EVALUATE SIZE OF COMPUTED CORRECTIONS
C             * MAX CHANGE SET BY FLMAX, TMAX, & FVMAX
C             * NEGATIVE FLOWS ARE NOT PERMITTED
C
      DO 490 J=1,NK
      IF (D(I,J).EQ.0.0) GO TO 485
      SAVE=FLL(I,J)
      QQ=1.0
      IF (ABS(D(I,J)).LT.FLMAX(J)) GO TO 480
      QQ=FLMAX(J)/ABS(D(I,J))
  480 FLL(I,J)=FLL(I,J)+QQ*D(I,J)
      IF (FLL(I,J).LE.0.0) FLL(I,J)=SAVE/10.0
  485 IF (L(J).EQ.0) FLL(I,J)=0.0
  490 CONTINUE
C
      IF (ITR.EQ.0) D(I,NK1)=0.0
      IF (D(I,NK1).EQ.0.0) GO TO 510
      QQ=1.0
      IF (ABS(D(I,NK1)).LT.TMAX) GO TO 500
      QQ=TMAX/ABS(D(I,NK1))
  500 T(I)=T(I)+D(I,NK1)*QQ
C
  510 IF (I.EQ.NST .AND. FV(I).EQ.0.0) GO TO 550
      DO 540 JJ=NK11,NK2
      J=JJ-NK1
      IF (D(I,JJ).EQ.0.0) GO TO 535
      SAVE=FVV(I,J)
      QQ=1.0
      IF (ABS(D(I,JJ)).LT.FVMAX(J)) GO TO 530
      QQ=FVMAX(J)/ABS(D(I,JJ))
  530 FVV(I,J)=FVV(I,J)+D(I,JJ)*QQ
      IF (FVV(I,J).LE.0.0) FVV(I,J)=SAVE/10.0
  535 IF (L(J).EQ.-1) FVV(I,J)=0.0
  540 CONTINUE
C
  550 CONTINUE
C
C     GENERATE THE REVISED TOTAL FLOW
C
      DO 560 I=1,NST
      FL(I)=0.0
      FV(I)=0.0
      DO 560 J=1,NK
      FL(I)=FL(I)+FLL(I,J)
  560 FV(I)=FV(I)+FVV(I,J)
C
      RETURN
```

```
0135                END
```

```
0001                  SUBROUTINE GAUSL (ND,NCOL,N,NS,A)
                C
0002                  IMPLICIT REAL*8  (A-H,O-Z)
0003                  DIMENSION        A(21,42)
                C
                C     GAUSS SOLVES A*X=B, WHERE A IS N*N , BY GAUSSIAN ELIMINATION
                C     WITH ROW PIVOTING.  THE VECTOR B IS PLACED IN COLUMN N+1 OF A
                C     WITH A BEING DESTROYED.
                C
0004                  N1=N+1
0005                  NT=N+NS
0006                  IF (N.EQ.1) GO TO 50
                C     START ELIMINATION
0007                  DO 40 I=2,N
0008                  IP=I-1
0009                  I1=IP
0010                  X=DABS(A(I1,I1))
0011                  DO 10 J=I,N
0012                  IF (DABS(A(J,I1)).LT.X) GO TO 10
0013                  X=DABS(A(J,I1))
0014                  IP=J
0015               10 CONTINUE
0016                  IF (IP.EQ.I1) GO TO 30
                C     ROW INTERCHANGE
0017                  DO 20 J=I1,NT
0018                  X=A(I1,J)
0019                  A(I1,J)=A(IP,J)
0020               20 A(IP,J)=X
0021               30 DO 40 J=I,N
0022                  X=A(J,I1)/A(I1,I1)
0023                  DO 40 K=I,NT
0024               40 A(J,K)=A(J,K)-X*A(I1,K)
                C     ELIMINATION FINISHED, NOW COMPLETE THE BACK SUBSTITUTION
0025               50 DO 70 IP=1,N
0026                  I=N1-IP
0027                  DO 70 K=N1,NT
0028                  A(I,K)=A(I,K)/A(I,I)
0029                  IF (I.EQ.1) GO TO 70
0030                  I1=I-1
0031                  DO 60 J=1,I1
0032               60 A(J,K)=A(J,K)-A(I,K)*A(J,I)
0033               70 CONTINUE
                C
0034                  RETURN
0035                  END
```

```
      SUBROUTINE RESULT
C
      IMPLICIT REAL        (M)
      INTEGER              COMPNT
      DIMENSION            OUT(15,10), PROD(10)
C
      COMMON  /CTRL/       NCR, NPRT, NSTART, TITLE(20)
C
      COMMON  /NJITO/      NK, NCM1, IDLL, IDLV, IDH, LDBUG, ISW,
     *                     NAME(4,10), L(10), NDIM, COMPNT(10)
      COMMON  /INRO/       NST, NSTM1, NK1, NK2, NK11, NK21, NCASE, KUNITS,
     *                     NFEED, LF(9), IDCODE, ITR, ITRMAX, ICODE
      COMMON  /INR1/       FSTR(9,11), FKV(9), HF(9), FLMAX(10), FVMAX(10),
     *                     DEST,DESTV,DESTL, BTMS, RFLX,BOIL, PP(50), T(50),
     *                     MU(50), SL(50), SV(50), FL(50), FLL(50,10),
     *                     FV(50), FVV(50,10), ZCONVT, ZCONVF
      COMMON  /INR2/       DFK(10,21), HL(50), HLL(50,10), CL(50), HHE(50),
     *                     DEXH(50,11), HV(50), HVV(50,10), CV(50)
      COMMON  /VLE/        XFK(10), GAM(10), X(10), Y(10), VP(10), FUG(10)
C
      DO 7 I=1,NST
    7 HL(I)=HL(I)+FL(I)*HHE(I)
C
      GO TO (11,15,15), KUNITS
   11 TDEG=(T(1)-273.16)*1.8+32.0
      C1=453.59
      C2=252.16*1.0E-3
      GO TO 17
   15 TDEG=T(1)
      C1=1.0
      C2=1.0
C
   17 ISTR=1
      OUT(1,1)=1
      OUT(2,1)=TDEG
      OUT(3,1)=0.0
      OUT(4,1)=HL(1)/C2
      DO 18 J=1,NK
   18 OUT(J+4,1)=FLL(1,J)/C1
      OUT(NK1+4,1)=FL(1)/C1
C
      DO 60 I=1,NST
      IF (SL(I)+SV(I) .EQ. 0.0) GO TO 60
      GO TO (22,23,23), KUNITS
   22 TDEG=(T(I)-273.16)*1.8+32.0
      GO TO 25
   23 TDEG=T(I)
   25 IF (SL(I).EQ.0.) GO TO 40
      ISTR=ISTR+1
      DO 30 J=1,NK
   30 PROD(J)=FLL(I,J)*SL(I)/FL(I)
      H=HL(I)/FL(I)*SL(I)/C2
   35 OUT(1,ISTR)=I
      OUT(2,ISTR)=TDEG
      OUT(3,ISTR)=0.0
      OUT(4,ISTR)=H
```

```
      DO 39 J=1,NK
   39 OUT(J+4,ISTR)=PROD(J)/C1
      OUT(NK1+4,ISTR)=SL(I)/C1
   40 IF (SV(I).EQ.0.) GO TO 60
      ISTR=ISTR+1
      DO 50 J=1,NK
   50 PROD(J)=FVV(I,J)*SV(I)/FV(I)
      H=HV(I)/FV(I)*SV(I)/C2
   55 OUT(1,ISTR)=I
      OUT(2,ISTR)=TDEG
      OUT(3,ISTR)=1.0
      OUT(4,ISTR)=H
      DO 59 J=1,NK
   59 OUT(J+4,ISTR)=PROD(J)/C1
      OUT(NK1+4,ISTR)=SV(I)/C1
   60 CONTINUE
C
      GO TO (61,62,62), KUNITS
   61 TDEG=(T(NST)-273.16)*1.8+32.0
      GO TO 65
   62 TDEG=T(NST)
C
   65 ISTR=ISTR+1
      OUT(1,ISTR)=NST
      OUT(2,ISTR)=TDEG
      OUT(3,ISTR)=1.0
      IF (IDCODE.NE.0) OUT(3,ISTR)=0.0
      OUT(4,ISTR)=HV(NST)/C2
      DO 66 J=1,NK
   66 OUT(J+4,ISTR)=FVV(NST,J)/C1
      OUT(NK1+4,ISTR)=FV(NST)/C1
C
   70 IF (NCASE.EQ.1) GO TO 90
      IF (IDCODE.NE.0) GO TO 71
      QC=HV(NSTM1)-HL(NST)*(1.0+SL(NST)/FL(NST))-HV(NST)
      GO TO 72
   71 QC=HV(NSTM1)-HL(NST)/FL(NST)*(FL(NST)+DEST)
   72 QR=HV(1)+HL(1)-HL(2)
C
      QC=QC/C2
      QR=QR/C2
C
   79 WRITE (NPRT,84) QR
      WRITE (NPRT,86) QC
   84 FORMAT ('0REBOILER DUTY    =',1PE14.6)
   86 FORMAT ('0CONDENSER DUTY   =',1PE14.6)
C
   90 WRITE (NPRT,100)
  100 FORMAT ('0PRODUCT STREAMS:')
      WRITE (NPRT,101) (OUT(1,I),I=1,ISTR)
  101 FORMAT (' STAGE', 15X, 10F12.0)
      WRITE (NPRT,102) (OUT(2,I),I=1,ISTR)
  102 FORMAT (' TEMP ', 15X, 10F12.2)
      WRITE (NPRT,103) (OUT(3,I),I=1,ISTR)
  103 FORMAT (' FRACV', 15X, 10F12.4)
      WRITE (NPRT,104) (OUT(4,I),I=1,ISTR)
```

```
      104 FORMAT (' H     ', 15X, 1P10E12.4)
          DO 105 J=1,NK
      105 WRITE (NPRT,106) J, (NAME(K,J),K=1,2),(OUT(J+4,I),I=1,ISTR)
      106 FORMAT (' COMP', I2, 2X,2A4,5X, F11.3, 9F12.3)
          WRITE (NPRT,107) (OUT(NK1+4,I),I=1,ISTR)
      107 FORMAT (' TOTAL', 15X, 10F12.3)
C
          WRITE (NPRT,200)
      200 FORMAT ('0FINAL COLUMN PROFILES:'/
         * ' STAGE     TEMP          PRES         EFF(%)      LIQUID(MOLS)   VAPOR
         *(MOLS)')
          DO 210 I=1,NST
C
          GO TO (201,202,202), KUNITS
      201 TDEG=(T(I)-273.15)*1.8+32.0
          PRES=PP(I)*14.696
          GO TO 205
      202 TDEG=T(I)
          PRES=PP(I)
C
      205 FLZ=FL(I)/C1
          FVZ=FV(I)/C1
          IF (IDCODE.NE.0.AND.I.EQ.NST) FVZ=0
          WRITE (NPRT,206) I,TDEG,PRES,MU(I),FLZ,FVZ
      206 FORMAT (I5,F10.2,F12.3,2PF12.2,0PF15.3,F14.3)
      210 CONTINUE
C
          DO 310 J1=1,NK,5
          J2=J1+4
          IF (J2.GT.NK) J2=NK
          WRITE (NPRT,301) ((NAME(K,J),K=1,2),J=J1,J2)
      301 FORMAT ('0FINAL VAPOR COMPOSITION PROFILE (MOLE%):'/
         *  ' STAGE', 3X,2A4,4(5X,2A4))
          DO 303 I=1,NST
          DO 302 J=J1,J2
          Y(J)=FVV(I,J)/FV(I)
          IF(IDCODE.NE.0.AND.I.EQ.NST) Y(J)=0
      302 CONTINUE
      303 WRITE (NPRT,304) I, (Y(J),J=J1,J2)
      304 FORMAT (I5,2P5F13.5)
      310 CONTINUE
C
          DO 410 J1=1,NK,5
          J2=J1+4
          IF (J2.GT.NK) J2=NK
          WRITE (NPRT,401) ((NAME(K,J),K=1,2),J=J1,J2)
      401 FORMAT ('0FINAL LIQUID COMPOSITION PROFILE (MOLE%):'/
         *  ' STAGE', 3X,2A4,4(5X,2A4))
          DO 403 I=1,NST
          DO 402 J=J1,J2
      402 X(J)=FLL(I,J)/FL(I)
      403 WRITE (NPRT,304) I, (X(J),J=J1,J2)
      410 CONTINUE
C
          DO 429 J1=1,NK,5
          J2=J1+4
```

```
      IF (J2.GT.NK) J2=NK
      WRITE (NPRT,421) ((NAME(K,J),K=1,2),J=J1,J2)
  421 FORMAT ('0FINAL VAPOR COMPOSITION PROFILE (MOLES):'/
     *  ' STAGE', 3X,2A4,4(5X,2A4))
      DO 423 I=1,NST
      DO 422 J=J1,J2
      Y(J)=FVV(I,J)/C1
      IF(IDCOOF.NE.0.AND.I.EQ.NST) Y(J)=0.0
  422 CONTINUE
  423 WRITE (NPRT,424) I, (Y(J),J=J1,J2)
  424 FORMAT (I5,5F13.3)
  429 CONTINUE
C
      DO 439 J1=1,NK,5
      J2=J1+4
      IF (J2.GT.NK) J2=NK
      WRITE (NPRT,431) ((NAME(K,J),K=1,2),J=J1,J2)
  431 FORMAT ('0FINAL LIQUID COMPOSITION PROFILE (MOLES):'/
     *  ' STAGE', 3X,2A4,4(5X,2A4))
      DO 433 I=1,NST
      DO 432 J=J1,J2
  432 X(J)=FLL(I,J)/C1
  433 WRITE (NPRT,424) I, (X(J),J=J1,J2)
  439 CONTINUE
C
C     IF (NK.GT.0) GO TO 700
      DO 550 I=1,NST
      CALL KFAC1(I)
C     TDEG=(T(I)-273.16)*1.8+32.0
C     PRES=PP(I)*14.696
      TDEG=T(I)
      PRES=PP(I)
      WRITE (NPRT,501) I,TDEG,PRES
  501 FORMAT ('0STAGE #', I5/
     *         ' TEMP, DEG K', F10.3/
     *         ' PRES, MMHG ', F10.4)
      WRITE (NPRT,502)
  502 FORMAT ('  #',2X,'NAME',4X,2X,6X,'K',14X,
     *         'VP',13X,'FUG',12X,'GAM')
      DO 510 J=1,NK
  510 WRITE (NPRT,520) J,(NAME(K,J),K=1,2),XFK(J),
     *                  VP(J),FUG(J),GAM(J)
  520 FORMAT (I3,2X,2A4,2X,1P6G15.5)
  550 CONTINUE
C
  700 RETURN
      END
```

```
      SUBROUTINE KFAC(I)
C
      IMPLICIT REAL     (M)
      INTEGER           COMPNT
      REAL              XX(10), GAMX(10), YY(10), FIX(10), XFKX(10),
     *                  VSAVE(10)
C
      COMMON  /CTRL/    NCR, NPRT, NSTART, TITLE(20)
      COMMON  /NJIT0/   NC, NCM1, IDLL, IDLV, IDH, LDBUG, ISW,
     *                  NAME(4,10), L(10), NDIM, COMPNT(10)
      COMMON  /NJIT1/   CPL(10,4), CPV(10,4), ENP(10,10), ANT(6,10),
     *                  W(10)
      COMMON  /INR0/    NST, NSTM1, NK1, NK2, NK11, NK21, NCASE, KUNITS,
     *                  NFEED, LF(9), IDCODE, ITR, ITRMAX, ICODE
      COMMON  /INR1/    FSTR(9,11), FKV(9), HF(9), FLMAX(10), FVMAX(10),
     *                  DEST,DESTV,DESTL, BTMS, RFLX,BOIL, PP(50), T(50),
     *                  MU(50), SL(50), SV(50), FL(50), FLL(50,10),
     *                  FV(50), FVV(50,10), ZCONVT, ZCONVF
      COMMON  /INR2/    DFK(10,21), HL(50), HLL(50,10), CL(50), HHE(50),
     *                  DEXH(50,11), HV(50), HVV(50,10), CV(50)
      COMMON  /VLE/     XFK(10), GAM(10), X(10), Y(10), VP(10), FUG(10)
      COMMON  /KNST/    XFKNST(10)
C
      DATA              SMALL /0.0/
C
      HL(I)=0.0
      HV(I)=0.0
      CL(I)=0.0
      CV(I)=0.0
      DHV=0.0
      HHE(I)=0.0
      DO 1 J=1,NC
      DO 1 K=1,NK2
    1 DFK(J,K)=0.0
      DO 2 J=1,NK1
    2 DEXH(I,J)=0.0
C
      TT=T(I)
      T5=TT+5.0
      P=PP(I)
      XT=FL(I)
      YT=FV(I)
      DO 3 J=1,NC
      Y(J)=FVV(I,J)/YT
    3 X(J)=FLL(I,J)/XT
C
      IF (I.NE.NST) GO TO 8
      IF (IDCODE.EQ.0) GO TO 8
      VSAVE(NK1)=FV(NST)
      YT=0.0
      DO 5 J=1,NC
      Y(J)=XFKNST(J)*X(J)
    5 YT=YT+Y(J)
      DO 6 J=1,NC
      Y(J)=Y(J)/YT
      VSAVE(J)=FVV(NST,J)
```

```
        6 FVV(NST,J)=Y(J)*DEST
          YT=DEST
          FV(NST)=DEST
    C
        8 DO 9 J=1,NC
          FIX(J)=1.0
          FUG(J)=1.0
          GAM(J)=1.0
          HLL(I,J)=(((ENP(J,5)*TT+ENP(J,4))*TT+ENP(J,3))*TT+ENP(J,2))*
         *          TT+ENP(J,1)
          HVV(I,J)=(((ENP(J,10)*TT+ENP(J,9))*TT+ENP(J,8))*TT+
         *          ENP(J,7))*TT+ENP(J,6)
          HL(I)=HL(I)+HLL(I,J)*FLL(I,J)
          HV(I)=HV(I)+HVV(I,J)*FVV(I,J)
          CL(I)=CL(I)+FLL(I,J)*(((CPL(J,4)*TT+CPL(J,3))*TT+CPL(J,2))*TT+
         *       CPL(J,1))
          CV(I)=CV(I)+FVV(I,J)*(((CPV(J,4)*TT+CPV(J,3))*TT+CPV(J,2))*TT+
         *       CPV(J,1))
          VP(J)=EXP(ANT(1,J)+ANT(2,J)/(ANT(3,J)+TT)+ANT(4,J)*TT+ANT(5,J)*
         *       TT*TT+ANT(6,J)*ALOG(TT))
        9 CONTINUE
    C
       10 IF (NDIM.EQ.0) GO TO 11
          CALL QUEDI (P,TT,Y(NDIM),AKA,ZDIM,ZNODIM)
          VP(NDIM)=(SQRT(1.0+4.0*AKA*VP(NDIM))-1.0)/2.0/AKA
    C
       11 IF (IDLL.EQ.0) GO TO 20
          ISW=0
          CALL ACTVTY (TT,X,GAM)
    C
       20 IF (IDLV.EQ.0) GO TO 40
          CALL FUGCTY (TT,P,Y,VP,FUG,DHV)
          IF (IDH.EQ.2) GO TO 35
          HV(I)=HV(I)+DHV*FV(I)
          DO 30J=1,NC
       30 HVV(I,J)=HVV(I,J)+DHV
       35 IF (IDLV.EQ.4) GO TO 60
    C
       40 DO 50 J=1,NC
       50 XFK(J)=VP(J)/P*GAM(J)*FUG(J)
    C
    C     CALCULATION OF THE DERIVATIVE OF THE SEPARATION FACTOR
    C     WITH RESPECT TO COMPONENT FLOW IN THE LIQUID PHASE.
    C
       60 IF (IDLL.EQ.0) GO TO 110
          ISW=1
          DO 105 K=1,NC
          IF (L(K).EQ.0 .OR. X(K).LT.SMALL) GO TO 105
          FLOWK=FLL(I,K)*0.01
          DO 70 J=1,NC
       70 XX(J)=FLL(I,J)/(XT+FLOWK)
          XX(K)=(FLL(I,K)+FLOWK)/(XT+FLOWK)
       91 CALL ACTVTY (TT,XX,GAMX)
       99 DO 100 J=1,NC
      100 DFK(J,K)=VP(J)/P*FUG(J)*(GAMX(J)-GAM(J))/FLOWK
      105 CONTINUE
```

```
C
C      CALCULATION OF THE DERIVATIVE OF THE SEPARATION FACTOR
C      WITH RESPECT TO COMPONENT FLOW IN THE VAPOR PHASE.
C
  110 IF (IDLV.EQ.0.0) GO TO 140
      DO 135 K=1,NC
      IF (L(K).EQ.-1 .OR. Y(K).LT.SMALL) GO TO 135
      FLOWK=FVV(I,K)*0.01
  120 YY(J)=FVV(I,J)/(YT+FLOWK)
      YY(K)=(FVV(I,K)+FLOWK)/(YT+FLOWK)
      CALL FUGCTY (TT,P,YY,VP,FIX,DHVFK)
      IF (IDH.EQ.2) GO TO 125
      HVV(I,K)=HVV(I,K)+(DHVFK-DHV)/FLOWK*FV(I)
  125 DO 130 J=1,NC
  130 DFK(J,K+NK1)=VP(J)/P*GAM(J)*(FIX(J)-FUG(J))/FLOWK
  135 CONTINUE
C
C      CALCULATION OF THE DERIVATIVE OF THE SEPARATION FACTOR
C      WITH RESPECT TO TEMPERATURE.
C
  140 DO 152 J=1,NC
  152 DFK(J,NK1)=XFK(J)*(-ANT(2,J)/(TT+ANT(3,J))**2+ANT(4,J)+
     *              2.0*ANT(5,J)*TT+ANT(6,J)/TT)
C
C      CALCULATION OF THE DERIVATIVE OF THE SEPARATION FACTOR
C      WITH RESPECT TO TEMPERATURE FOR A DIMERIZING COMPONENT.
C
  160 IF (NDIM.EQ.0) GO TO 161
      CALL ONEDI (P,T5,Y(NDIM),AKAS,ZDIMM,ZNO)
      VPNDIM=EXP(ANT(1,NDIM)+ANT(2,NDIM)/(ANT(3,NDIM)+T5)+
     *              ANT(4,NDIM)*T5+ANT(5,NDIM)*T5*T5+ANT(6,NDIM)*ALOG(T5))
      VPNDIM=(SQRT(1.0+4.0*AKAS*VPNDIM)-1.0)/2.0/AKAS
      DFK(NDIM,NK1)=(VPNDIM-VP(NDIM))/5.0/P*GAM(NDIM)*FUG(NDIM)
C
  161 IF (IDLV.EQ.0) GO TO 180
      CALL FUGCTY (T5,P,Y,VP,FIX,DHVT)
      IF (IDH.EQ.2) GO TO 165
      CV(I)=CV(I)+(DHVT-DHV)/5.0*FV(I)
  165 DO 170 J=1,NC
  170 DFK(J,NK1)=DFK(J,NK1)+VP(J)/P*GAM(J)*(FIX(J)-FUG(J))/5.0
C
  180 IF (IDLL.EQ.0) GO TO 200
      ISW=0
      CALL ACTVTY (T5,X,GAMX)
      DO 190 J=1,NC
  190 DFK(J,NK1)=DFK(J,NK1)+VP(J)/P*FUG(J)*(GAMX(J)-GAM(J))/5.0
C
  200 IF (IDLL.EQ.0) GO TO 230
      IF (IDH.GT.0) GO TO 230
C     ISW=0
      CALL XSHLIQ (TT,X,HHE(I))
      ISW=1
      DO 220 K=1,NC
      IF (L(K).EQ.0 .OR. X(K).LT.SMALL) GO TO 220
      FLOWK=FLL(I,K)*0.10
```

```
          DO 210 J=1,NC
      210 XX(J)=FLL(I,J)/(XT+FLOWK)
          XX(K)=(FLL(I,K)+FLOWK)/(XT+FLOWK)
          CALL XSHLIQ (TT,XX,XSH)
          DEXH(I,K)=(XSH-HHE(I))/FLOWK
      220 CONTINUE
          ISW=0
          CALL XSHLIQ (TT+20.0,X,XSH)
          DEXH(I,NK1)=(XSH-HHE(I))/20.0
C
      230 IF (I.NE.NST) GO TO 250
          IF (IDCODE.EQ.0) GO TO 250
          FV(NST)=VSAVE(NK1)
          DO 240 J=1,NC
          XFKNST(J)=XFK(J)
      240 FVV(NST,J)=VSAVE(J)
C
      250 RETURN
          END
```

```
      SUBROUTINE FUGCTY (T,P,Y,VP,F,DH)
C
      REAL              Y(1), VP(1), F(1)
      INTEGER           COMPNT
C
      COMMON  /NJITO/   NC, NCM1, IDLL, IDLV, IDH, LDBUG, ISW,
     *                  NAME(4,10), L(10), NDIM, COMPNT(10)
C
      GO TO (10,20), IDLV
   10 CALL RKFUG (T,P,Y,VP,F,DH)
      GO TO 99
   20 CALL VIRFUG (T,P,Y,VP,F,DH)
C
   99 RETURN
      END
```

```
001               SUBROUTINE ACTVTY (T,X,G)
            C
002               REAL                X(1), G(1)
003               INTEGER             COMPNT
            C
004               COMMON  /NJITO/  NC, NCM1, IDLL, IDLV, IDH, LDBUG, ISw,
                 *                 NAME(4,10), L(10), NDIM, COMPNT(10)
            C
005               GO TO (10,20,30), IDLL
006            10 CALL RENON (T,X,G)
007               GO TO 99
008            20 CALL WILSON (T,X,G)
009               GO TO 99
010            30 CALL UNIQAC (T,X,G)
            C
011            99 RETURN
012               END
```

```
0001                SUBROUTINE XSHLIQ (T,X,XSH)
          C
0002                REAL                X(1)
0003                INTEGER             COMPNT
          C
0004                COMMON  /NJITO/  NC, NCM1, IDL, IDLV, IDH, LDBUG, ISW,
                  *                  NAME(4,10), L(10), NDIM, COMPNT(10)
          C
0005                GO TO (10,20,30), IDLL
0006             10 CALL XSHREN (T,X,XSH)
0007                GO TO 99
0008             20 CALL XSHWIL (T,X,XSH)
0009                GO TO 99
0010             30 CALL XSHUNQ (T,X,XSH)
          C
0011             99 RETURN
0012                END
```

```
      SUBROUTINE RKFUG (T,P,Y,VP,FUG,DHV)
C
      INTEGER            COMPNT
      REAL               Y(1), VP(1), FUG(1), A(10), B(10)
C
      COMMON  /NJIT0/  NC, NCM1, IDLL, IDLV, IDH, LDBUG, ISW,
     *                 NAME(4,10), L(10), NDIM, COMPNT(10)
      COMMON  /NJIT2/  C(180), ALPHA(45), VC(10), VOL(10), TC(10),
     *                 PC(10), OA(10), OB(10), QQ(10,10), Q(10,10)
C
C     P = ATM
C     T = DEG K
C     VOL = MOLAR VOLUME (CC/G-MOL)
C     OA AND OB = R-K PARAMETERS
C
      D=T**1.25
      AA=0.0
      BB=0.0
      DO 30 J=1,NC
      IF (Y(J).EQ.0.0) GO TO 30
      Z=J
      A(J)=OA(J)/D
      B(J)=OB(J)/T
      AA=AA+A(J)*Y(J)
      BB=BB+B(J)*Y(J)
      IF (L(J)-1) 30,20,10
   10 FUG(J)=EXP(VOL(J)*P/(82.05*T))
      GO TO 30
   20 CALL ZCALC (A(J),B(J),VP(J),Z)
      FUG(J)=EXP(VOL(J)*(P-VP(J))/(82.05*T))
      FUG(J)=EXP(Z-1.0)/((Z-B(J)*VP(J))*((1.0+B(J)*VP(J)/Z)**
     *         (A(J)*A(J)/B(J))))*FUG(J)
   30 CONTINUE
C
      Z=NC+1
      CALL ZCALC (AA,BB,P,Z)
      ZMIX=Z
      FN=(Z-1.0)/BB
      DF=ALOG(Z-BB*P)
      DZ=(AA*AA/BB)*ALOG(1.0+BB*P/Z)
      DHV=1.9872*T*(Z-1.0-1.5*DZ)
      DO 50 J=1,NC
      IF (Y(J).EQ.0.0) GO TO 50
      IF (L(J).LE.0) GO TO 50
   40 FUG(J)=FUG(J)/EXP(FN*B(J)-DF-DZ*(2.0*A(J)/AA-B(J)/BB))
   50 CONTINUE
C
      IF (NDIM.EQ.0) GO TO 70
      CALL ONEDI (P,TE,Y(NDIM),AK,ZDIM,ZNOD)
      DO 60 J=1,NC
   60 FUG(J)=FUG(J)/ZNOD
      FUG(NDIM)=1.0/ZDIM
C
   70 RETURN
      END
```

```
      SUBROUTINE ZCALC (A,B,P,Z)
C
      INTEGER          COMPNT
C
      COMMON  /CTRL/   NCR, NPRT, NSTART, TITLE(20)
      COMMON  /NJITO/  NC, NCM1, IDLL, IDLV, IDH, LDBUG, ISW,
     *                 NAME(4,10), L(10), NDIM, COMPNT(10)
C
      K=7
C
      J=0
      D=(A*A-B-B*B*P)*P
      Z=1.0
   10 FN=Z**3-Z*Z+D*Z-A*A*P*P*B
      DF=3.0*Z*Z-Z-Z+D
      DZ=-FN/DF
      J=J+1
      IF (J.GT.50) GO TO 30
      IF (ABS(DZ)/Z.LT.0.0001) GO TO 50
      DZ=SIGN(AMIN1(ABS(DZ),0.1*Z,0.1),DZ)
      Z=Z+DZ
      GO TO 10
C
   30 Z=AMAX1(Z,0.3)
C
   50 IF (LDBUG.EQ.2) WRITE (NPRT,60) K,A,B,P,J,Z
   60 FORMAT (' ** ZCALC ** K,A,B,P,J,&Z:', I5,3G15.6,I5,G15.6)
C
      RETURN
      END
```

```
      SUBROUTINE XSHREN (T,X,XSH)
C
      INTEGER            COMPNT
      REAL               X(1)
C
      COMMON  /NJIT0/  NC, NCM1, IDLL, IDLV, IDH, LDBUG, ISW,
     *                 NAME(4,10), L(10), NDIM, COMPNT(10)
      COMMON  /NJIT2/  C(180), ALPHA(45), VC(10), VOL(10), TC(10),
     *                 PC(10), OA(10), OB(10), A(10,10), G(10,10),
     *                 THETA(10), THS(10), HFAC(10), HHFA(10), HM(10),
     *                 W(10),R(10),XL(10),PHI(10),DUMMY(10)
C
      IF (ISW.NE.0) GO TO 20
C
      RT=1.9872*T
      K=0
      DO 15 I=1,NCM1
      IF (X(I).NE.0.0) GO TO 5
      K=K+NC-I
      GO TO 15
    5 IJ=I+1
      DO 10 J=IJ,NC
      K=K+1
      IF (X(J).EQ.0.0) GO TO 10
      II=4*K
      S=(C(II-3)+C(II-2)*T)/RT
      A(I,J)=S
      G(I,J)=EXP(-S*ALPHA(K))
      S=(C(II-1)+C(II)*T)/RT
      A(J,I)=S
      G(J,I)=EXP(-S*ALPHA(K))
   10 CONTINUE
   15 CONTINUE
C
   20 XSH=0.0
      DO 70 I=1,NC
      IF (X(I).EQ.0.0) GO TO 70
      SA=0.0
      SB=0.0
      SC=0.0
      SD=0.0
      DO 60 J=1,NC
      IF (X(J).EQ.0.0) GO TO 60
      S=G(J,I)*X(J)
      SB=SB+S
      SC=SC+S*A(J,I)
      IF (I-J)30,60,40
   30 K=NC*(I-1)+J-I*(I+1)/2
      IJ=4*K-1
      GO TO 50
   40 K=NC*(J-1)+I-J*(J+1)/2
      IJ=4*K-3
   50 SA=SA+(1.0-ALPHA(K)*A(J,I))*C(IJ)*S
      SD=SD+ALPHA(K)*C(IJ)*S
   60 CONTINUE
      XSH=XSH+X(I)*(SC*SD/SB+SA)/SB
```

```
)048            70 CONTINUE
           C
)049               RETURN
)050               END
```

```
      SUBROUTINE RENON (T,X,GAM)
C
      INTEGER           COMPNT
      REAL              X(1), GAM(1)
C
      COMMON   /NJIT0/  NC, NCM1, IDLL, IDLV, IDH, LDBUG, ISW,
     *                  NAME(4,10), L(10), NDIM, COMPNT(10)
      COMMON   /NJIT2/  C(180), ALPHA(45), VC(10), VDL(10), TC(10),
     *                  PC(10), OA(10), OB(10), A(10,10), G(10,10),
     *                  THETA(10), THS(10), HFAC(10), HHFA(10), HM(10),
     *                  Q(10),R(10),XL(10),PHI(10),DUMMY(10)
C
      IF (ISW.NE.0) GO TO 20
C
      RT=1.9872*T
      K=0
      DO 15 I=1,NCM1
      IF (X(I).NE.0.0) GO TO 5
      K=K+NC-I
      GO TO 15
    5 IJ=I+1
      DO 10 J=IJ,NC
      K=K+1
      IF (X(J).EQ.0.0) GO TO 10
      II=4*K
      S=(C(II-3)+C(II-2)*T)/RT
      A(I,J)=S
      G(I,J)=EXP(-S*ALPHA(K))
      S=(C(II-1)+C(II)*T)/RT
      A(J,I)=S
      G(J,I)=EXP(-S*ALPHA(K))
   10 CONTINUE
   15 CONTINUE
C
   20 DO 50 I=1,NC
      IF (X(I).EQ.0.0) GO TO 50
      S=0.0
      SA=0.0
      SB=0.0
      DO 40 J=1,NC
      IF (X(J).EQ.0.0) GO TO 40
      SC=0.0
      SD=0.0
      DO 30 K=1,NC
      IF (X(K).EQ.0.0) GO TO 30
      SE=G(K,J)*X(K)
      SC=SC+SE
      SD=SD+SE*A(K,J)
   30 CONTINUE
      SE=G(J,I)*X(J)
      SB=SB+G(I,J)*X(J)*(A(I,J)-SD/SC)/SC
      SA=SA+SE
      S=S+SE*A(J,I)
   40 CONTINUE
      GAM(I)=EXP(S/SA+SB)
   50 CONTINUE
```

```
              C
)048                    RETURN
)049                    END
```

```
      SUBROUTINE XSHWIL (TE,X,XSH)
C
      INTEGER          COMPNT
      REAL             X(1)
C
      COMMON  /NJIT0/  NC, NCM1, IDLL, IDLV, IDH, LDBUG, ISW,
     *                 NAME(4,10), L(10), NDIM, COMPNT(10)
      COMMON  /NJIT2/  C(180), ALPHA(45), VC(10), VOL(10), TC(10),
     *                 PC(10), OA(10), OB(10), A(10,10), G(10,10)
C
      IF (ISW.NE.0) GO TO 20
C     RT=1.9872*TE
      K=0
      DO 10 I=1,NCM1
      IJ=I+1
      DO 10 J=IJ,NC
      K=K+4
      S=VOL(I)/VOL(J)
      G(I,J)=EXP(-(C(K-3)+C(K-2)*TE)/RT)*S
      G(J,I)=EXP(-(C(K-1)+C(K)*TE)/RT)/S
   10 CONTINUE
C
   20 XSH=0.0
      DO 70 I=1,NC
      IF (X(I).EQ.0.0) GO TO 70
      SA=0.0
      SB=0.0
      DO 60 J=1,NC
      IF (X(J).EQ.0.0) GO TO 60
      S=G(J,I)*X(J)
      SB=SB+S
      IF (I-J) 30,60,40
   30 K=NC*(I-1)+J-I*(I+1)/2
      IJ=4*K-1
      GO TO 50
   40 K=NC*(J-1)+I-J*(J+1)/2
      IJ=4*K-3
   50 SA=SA+C(IJ)*S
   60 CONTINUE
      SB=1.0/SB
      XSH=XSH+X(I)*SA*SB
   70 CONTINUE
C
      RETURN
      END
```

```
      SUBROUTINE WILSON (TE,X,GAM)
C
      INTEGER           COMPNT
      REAL              X(1), GAM(1)
C
      COMMON  /NJITO/   NC, NCM1, IDLL, IDLV, IDH, LDBUG, ISW,
     *                  NAME(4,10), L(10), NDIM, COMPNT(10)
      COMMON  /NJIT2/   C(180), ALPHA(45), VC(10), VOL(10), TC(10),
C    *                  PC(10), OA(10), OB(10), A(10,10), G(10,10)
      IF (ISW.NE.0) GO TO 20
C
      RT=1.9872*TE
      K=0
      DO 10 I=1,NCM1
      IJ=I+1
      DO 10 J=IJ,NC
      K=K+4
      S=VOL(I)/VOL(J)
      G(I,J)=EXP(-(C(K-3)+C(K-2)*TE)/RT)*S
      G(J,I)=EXP(-(C(K-1)+C(K)*TE)/RT)/S
   10 CONTINUE
C
   20 DO 60 I=1,NC
      S=0.0
      SA=0.0
      DO 50 J=1,NC
      IF (X(J).EQ.0.0) GO TO 50
   30 SB=0.0
      DO 40 K=1,NC
      IF (X(K).EQ.0.0) GO TO 40
      SB=G(K,J)*X(K)+SB
   40 CONTINUE
      S=S+X(J)*G(J,I)
      SA=SA+X(J)*G(I,J)/SB
   50 CONTINUE
      GAM(I)=EXP(1.0-SA)/S
   60 CONTINUE
C
      RETURN
      END
```

```
      SUBROUTINE UNIQAC (TE,X,GAM)
C
      INTEGER             COMPNT
      REAL                X(1), GAM(1)
C
      COMMON  /NJIT0/     NC, NCM1, IDLL, IDLV, IDH, LDBUG, ISW,
     *                    NAME(4,10), L(10), NDIM, COMPNT(10)
      COMMON  /NJIT12/    C(180), ALPHA(45), VC(10), VOL(10), TC(10),
     *                    PC(10), OA(10), OB(10), A(10,10), G(10,10),
     *                    THETA(10), THS(10), HFAC(10), HHFA(10), HM(10),
     *                    Q(10),R(10),XL(10),PHI(10),DUMMY(10)
C
      IF (ISW.NE.0) GO TO 20
C
      RT=1.9872*TE
      K=0
      DO 10 I=1,NCM1
      IJ=I+1
      DO 10 J=IJ,NC
      K=K+4
      G(I,J)=EXP(-(C(K-3)+C(K-2)*TE)/RT)
      G(J,I)=EXP(-(C(K-1)+C(K)*TE)/RT)
   10 CONTINUE
C
   20 THETS=0.0
      PHS=0.0
      XLS=0.0
      DO 30 I=1,NC
      THETS=THETS+Q(I)*X(I)
      PHS=PHS+R(I)*X(I)
   30 XLS=XLS+XL(I)*X(I)
      DO 40 I=1,NC
      THETA(I)=Q(I)*X(I)/THETS
   40 PHI(I)=X(I)*R(I)/PHS
      DO 50 I=1,NC
      THS(I)=0.0
      DO 50 J=1,NC
   50 THS(I)=THS(I)+THETA(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)
      GA=GA+XL(I)-R(I)/PHS*XLS
      GB=1.0-ALOG(THS(I))
      DO 60 J=1,NC
   60 GB=GB-THETA(J)*G(I,J)/THS(J)
   70 GAM(I)=EXP(GA+Q(I)*GB)
C
      RETURN
      END
```

```
C     SUBROUTINE XSHUNQ (TE,X,XSH)
      INTEGER            COMPNT
      REAL               X(1)
C
      COMMON   /NJIT0/   NC, NCM1, IDLL, IDLV, IDH, LDBUG, ISW,
     *                   NAME(4,10), L(10), NDIM, COMPNT(10)
      COMMON   /NJIT2/   C(180), ALPHA(45), VC(10), VOL(10), TC(10),
     *                   PC(10), OA(10), OB(10), A(10,10), G(10,10),
     *                   THETA(10), THS(10), HFAC(10), HHFA(10), HM(10),
     *                   Q(10),R(10),XL(10),PHI(10),DUMMY(10)
C
      IF (ISW.NE.0) GO TO 20
C
      RT=1.9872*TE
      K=0
      DO 10 I=1,NCM1
      IJ=I+1
      DO 10J=IJ,NC
      K=K+4
      G(I,J)=EXP(-(C(K-3)+C(K-2)*TE)/RT)
      G(J,I)=EXP(-(C(K-1)+C(K)*TE)/RT)
   10 CONTINUE
   20 XSH=0.0
      THETS=0.0
      DO 30 I=1,NC
   30 THETS=THETS+Q(I)*X(I)
      DO 40 J=1,NC
   40 THETA(J)=Q(J)*X(J)/THETS
      DO 50 I=1,NC
      HFAC(I)=0.0
      HHFA(I)=0.0
      DO 50 J=1,NC
      ARG=G(J,I)
      HFAC(I)=HFAC(I)+THETA(J)*ARG*ALOG(ARG)
   50 HHFA(I)=HHFA(I)+THETA(J)*ARG
      DO 60 I=1,NC
   60 HM(I)=Q(I)*X(I)*HFAC(I)/HHFA(I)
      DO 70 I=1,NC
   70 XSH=XSH-1.9872*TE*HM(I)
C
      RETURN
      END
```

```
      SUBROUTINE        VIRFUG (T,P,Y,VP,FUG,DHV)
C
      REAL              Y(1),VP(1),FUG(1)
C
      COMMON  /NJIT0/   NC, NCM1, IDLL, IDLV, IDH, LDBUG, ISW, NDIM,
     *                  NAME(4,10), L(10)
      COMMON  /NJIT2/   C(180), ALPHA(45), VC(10), VOL(10), TC(10),
     *                  PC(10), QA(10), QB(10), AA(10,10), G(10,10)
      COMMON  /NJIT3/   TTC(10,10),PPC(10,10),VVC(10,10),ZZC(10,10),
     *                  AK(10,10), AVALUE(10,10), BVALUE(10,10),
     *                  BCROSS(10,10), OMEGA(10), DIPOLE(10), B(10,10)
      P=P/760.0
C
C
C     SUBROUTINE TSONOP GENERATES B(I,J) FOR VIRGUG
      CALL TSONOP(T,P,MARK)
C
      RT=82.057*T
      PORT=P/RT
      SUMY=0.0
      BMIX=0.0
      DO 15 I=1,NC
      VP(I)=VP(I)/760.0
      SUMY=SUMY+Y(I)
      DO 10 J=1,NC
      BMIX=BMIX+Y(I)*Y(J)*B(I,J)
   10 CONTINUE
   15 CONTINUE
      BMIX=BMIX /SUMY**2
      IF (MARK) 20,20,22
   20 SQARG=0.25 + BMIX*PORT
C
C   IF BMIX*P/RT IS MORE NEGATIVE THAN 0.25, THE PRESSURE SERIES VIRIAL
C   EQ. MUST BE USED. THE ARGUMENT MARK IS USED TO COMUNICATE THIS
C   TO THE MAIN PROGRAM
C
      IF (SQARG) 22,25,25
   22 VMIX=BMIX +1. /PORT
      ZMIX=PORT*VMIX
      DO 24 I=1,NC
      SUMB=0.0
      DO 23 J=1,NC
      SUMB =SUMB +Y(J)*B(I,J)
   23 CONTINUE
       SUMB=SUMB / SUMY
      PHI=EXP ((2.0*SUMB-BMIX)*PORT)
      PHIS=EXP (B(I,I)*VP(I)/RT)
      FACTOR=(P-VP(I))*VOL(I)
      PONTY= EXP(FACTOR/RT)
      FUG(I) = PHIS*PONTY/PHI
C     PRINT 300,I,PHIS,PONTY,PHI,FUG(I),Y(I),VP(I)
  24  CONTINUE
      MARK=MARK+1
      GO TO 50
   25 VMIX=(0.5+SQRT (SQARG))/PORT
      ZMIX=PORT*VMIX
```

```
C
C   CALCULATION OF FUGACITY COEFFICIENTS
C
      DO 40 I=1,NC
      SUMB=0.0
      DO 30 J=1,NC
      SUMB=SUMB + Y(J)*B(I,J)
   30 CONTINUE
      SUMB=SUMB /SUMY
      PHI=EXP (2.0*SUMB/VMIX)/ZMIX
      PHIS = EXP((B(I,I)*VP(I))/RT)
      FACTOR=(P-VP(I))*VOL(I)
      PONTY= EXP(FACTOR/RT)
      FUG(I) = PHIS*PONTY/PHI
C     PRINT 300,I,PHIS,PONTY,PHI,FUG(I),Y(I),VP(I)
  300 FORMAT(I5,6G15.6)
   40 CONTINUE
   50 DHV=1.9872*T*(ZMIX-1.0)
C     PRINT 400,DHV,T,P
  400 FORMAT(5X,'DHV=',G15.6,'TEMP=',G15.6,'PRESS=',G15.6)
C     DO 51 I=1,NC
C     DO 51 J=1,NC
C 51  WRITE(6,401) I,J,B(I,J)
  401 FORMAT(5X,'B(',I2,',',I2,')=',G15.5)
      DO 52 I=1,NC
   52 VP(I)=VP(I)*760.0
      P=P*760.0
      RETURN
      END
```

```
          SUBROUTINE TSONOP(T,P,MARK)
   C
   C      THIS SUBROUTINE CALCULATES SECOND VIRIAL COEFFICIENTS FOR THE
   C      TRUNCATED VIRIAL EQUATION OF STATE BY USE OF TSONOPOULOS'
   C      CORRELATION; AICHE JOURNAL,VOL. 20,NO. 2,P. 263,MARCH 1974
   C
   C
   C
   C      THE INPUT COMMONS PASS ALONG ALL THE INPUTTED INFORMATION
   C
         *COMMON  /NJITT0/  NOMENOM10)IDLK(10)IDLV, IDH, LDBUG, ISW, NDIM,
          COMMON  /NJIT2/   C(180), ALPHA(45), VC(10), VOL(10), TC(10),
         *                  PC(10), OA(10), OB(10), AA(10,10), G(10,10)
          COMMON  /NJIT3/   TTC(10,10),PPC(10,10),VVC(10,10),ZZC(10,10),
         *                  AK(10,10), AVALUE(10,10), BVALUE(10,10),
         *                  BCROSS(10,10), OMEGA(10), DTPOLE(10), B(10,10)
   C      THE OUTPT COMMONS PASS ALONG MOST OF THE CALCULATED INFORMATION
   C
   C
   C
          FTS0(TR)=0.1445-(0.330+0.1385/TR)/TR-(0.0121+0.000607
         1 /TR**5)/TR**3
          FTS1(TR)=0.0637+(0.331-0.423/TR-0.008/TR**6)/TR**2
          FTS2(TR,AAA,BBB)=(AAA-BBB/TR**2)/TR**6
   C
   C      CALL VIRMIX
          MARK=-1
          R=82.055
          DO 101 I=1,NC
          TR=T/TTC(I,I)
   101    B(I,I)=(FTS0(TR)+OMEGA(I)*FTS1(TR)+FTS2(TR,AVALUE(I,I),
         1BVALUE(I,I)))*R/PPC(I,I)*TTC(I,I)
   C
          DO 121 J=2,NC
          KMAX=I-1
          DO 122 K=1,KMAX
          TR=T/TTC(J,K)
          W=(OMEGA(J)+OMEGA(K))/2.0
          B(J,K)=(FTS0(TR)+W*FTS1(TR)+FTS2(TR,AVALUE(J,K),BVALUE(J,K)))*R
         1/PPC(J,K)*TTC(J,K)
          B(K,J)=B(J,K)
    122   CONTINUE
   121    CONTINUE
          RETURN
          END
```

```
      SUBROUTINE VIRMIX
      COMMON  /NJIT0/  NC, NCM1, IDLL, IDLV, IDH, LDBUG, ISW, NDIM,
     *                 NAME(4,10),L(10)
      COMMON  /NJIT3/  TTC(10,10),PPC(10,10),VVC(10,10),ZZC(10,10),
     *                 AK(10,10), AVALUE(10,10), BVALUE(10,10),
     *                 BCROSS(10,10), OMEGA(10), DIPOLE(10), B(10,10)
      COMMON  /NJIT2/  C(180), ALPHA(45), VC(10), VOL(10), TC(10),
     *                 PC(10), OA(10), OB(10), AA(10,10), G(10,10)
C
C
C     THIS SUBRUTINE CALCULATES THE MIXING BINARY PROPERTIES
C
      RCONST=82.057
      EXPN = 1.0/3.0
C
C   CALCULATE CRITICAL PROPERTIES FOR BINARY INTERACTIONS
C
      DO 100 I=2,NC
      JMAX=I-1
      DO 100 J=1,JMAX
      TTC(I,J) = SQRT (TTC(I,I) * TTC(J,J))
       TTC(I,J)=TTC(I,J)*(1.-AK(I,J))
      PPC(I,J) = 4.0 * TTC(I,J) * (PPC(I,I) * VC(I) / TTC(I
     1,I)+PPC(J,J) * VC(J) / TTC(J,J)) / (VC(I)**EXPN +
     2 VC(J)**EXPN)**3
      BVALUE(I,J) = (BVALUE(I,I) + BVALUE(J,J))/2.
      AVALUE(I,J) = (AVALUE(I,I) +AVALUE(J,J))/2.
      BVALUE(J,I) = BVALUE(I,J)
      AVALUE(J,I) = AVALUE(I,J)
      VVC(J,I)=VVC(I,J)
      TTC(J,I)=TTC(I,J)
      PPC(J,I)=PPC(I,J)
  100 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE ONEDI (P,ATEM,Y,AKA,ZDI,ZNODI)
C
C     ATEM IN DEGREE K
C
C     THIS SUBROUTINE CALCULATES THE VAPORPHASE DIMERIZATION CORRECTIONS
C     WHEN NO MORE THAN ONE COMPONENT DIMERIZES.
C     FOR THE DIMERIZATING COMPONENT, THE FUGACITY COEFFICIENT IS MODI-
C     FIED BY THE FACTOR ZDI. FOR ALL THE OTHER COMPONENTS, THE FUGACITY
C     COEFFICIENTS ARE MODIFIED BY THE FACTOR ZNODI.
C
      COMMON  /DATA3/  BI1(10,10), BI2(10,10), T1, T2, A, BX
C
      IF (Y-0.0001)20,20,10
   10 AKA=EXP((2.880814-A+BX/ATEM)*2.3025851)
      AKOR=4.0*AKA*P*Y*(2.0-Y)
      ZDI=(SQRT(1.0+AKOR)-1.0)*2.0/AKOR
      ZNODI=2.0*(1.0-Y+SQRT(1.0+AKOR))/(2.0-Y)/(1.0+SQRT(1.0+AKOR))
      GO TO 30
   20 ZDI=1.0
      ZNODI=1.0
   30 CONTINUE
C
      RETURN
      END
```

```
      SUBROUTINE KFAC1(I)
C
      IMPLICIT REAL     (M)
      INTEGER           COMPNT
      REAL              XX(10), GAMX(10), YY(10), FIX(10), XFKX(10),
     *                  VSAVE(10)
C
      COMMON  /CTRL/    NCR, NPRT, NSTART, TITLE(20)
      COMMON  /NJIT0/   NC, NCM1, IDLL, IDLV, IDH, LDBUG, ISW,
     *                  NAME(4,10), L(10), NDIM, COMPNT(10)
      COMMON  /NJIT1/   CPL(10,4), CPV(10,4), ENP(10,10), ANT(6,10),
     *                  W(10)
      COMMON  /INR0/    NST, NSTM1, NK1, NK2, NK11, NK21, NCASE, KUNITS,
     *                  NFEED, LF(9), IDCODE, ITR, ITRMAX, ICODE
      COMMON  /INR1/    FSTR(9,11), FKV(9), HF(9), FLMAX(10), FVMAX(10),
     *                  DEST,DESTV,DESTL, BTMS, RFLX,BOIL, PP(50), T(50),
     *                  MU(50), SL(50), SV(50), FL(50), FLL(50,10),
     *                  FV(50), FVV(50,10), ZCONVT, ZCONVF
      COMMON  /INR2/    DFK(10,21), HL(50), HLL(50,10), CL(50), HHE(50),
     *                  DEXH(50,11), HV(50), HVV(50,10), CV(50)
      COMMON  /VLE/     XFK(10), GAM(10), X(10), Y(10), VP(10), FUG(10)
      COMMON  /KNST/    XFKNST(10)
C
      DATA              SMALL /0.0/
C
      HL(I)=0.0
      HV(I)=0.0
      CL(I)=0.0
      CV(I)=0.0
      DHV=0.0
      HHE(I)=0.0
      DO 1 J=1,NC
      DO 1 K=1,NK2
    1 DFK(J,K)=0.0
      DO 2 J=1,NK1
    2 DEXH(I,J)=0.0
C
      TT=T(I)
      T5=TT+5.0
      P=PP(I)
      XT=FL(I)
      YT=FV(I)
      DO 3 J=1,NC
      Y(J)=FVV(I,J)/YT
    3 X(J)=FLL(I,J)/XT
C
      IF (I.NE.NST) GO TO 8
      IF (IDCODE.EQ.0) GO TO 8
      VSAVE(NK1)=FV(NST)
      YT=0.0
      DO 5 J=1,NC
      Y(J)=XFKNST(J)*X(J)
    5 YT=YT+Y(J)
      DO 6 J=1,NC
      Y(J)=Y(J)/YT
      VSAVE(J)=FVV(NST,J)
```

```
    6 FVV(NST,J)=Y(J)*DEST
      YT=DEST
      FV(NST)=DEST
C
    8 DO 9 J=1,NC
      FIX(J)=1.0
      FUG(J)=1.0
      GAM(J)=1.0
      HLL(I,J)=(((ENP(J,5)*TT+ENP(J,4))*TT+ENP(J,3))*TT+ENP(J,2))*
     *         TT+ENP(J,1)
      HVV(I,J)=(((ENP(J,10)*TT+ENP(J,9))*TT+ENP(J,8))*TT+
     *         ENP(J,7))*TT+ENP(J,6)
      HL(I)=HL(I)+HLL(I,J)*FLL(I,J)
      HV(I)=HV(I)+HVV(I,J)*FVV(I,J)
      CL(I)=CL(I)+FLL(I,J)*(((CPL(J,4)*TT+CPL(J,3))*TT+CPL(J,2))*TT+
     *       CPL(J,1))
      CV(I)=CV(I)+FVV(I,J)*(((CPV(J,4)*TT+CPV(J,3))*TT+CPV(J,2))*TT+
     *       CPV(J,1))
      VP(J)=EXP(ANT(1,J)+ANT(2,J)/(ANT(3,J)+TT)+ANT(4,J)*TT+ANT(5,J)*
     *       TT*TT+ANT(6,J)*ALOG(TT))
C   9 CONTINUE
   10 IF (NDIM.EQ.0) GO TO 11
      CALL ONEDI (P,TT,Y(NDIM),AKA,ZDIM,ZNODIM)
      VP(NDIM)=(SQRT(1.0+4.0*AKA*VP(NDIM))-1.0)/2.0/AKA
C
   11 IF (IDLL.EQ.0) GO TO 20
      ISW=0
      CALL ACTVTY (TT,X,GAM)
C
   20 IF (IDLV.EQ.0) GO TO 40
      CALL FUGCTY (TT,P,Y,VP,FUG,DHV)
      IF (IDH.EQ.2) GO TO 35
      HV(I)=HV(I)+DHV*FV(I)
      DO 30J=1,NC
   30 HVV(I,J)=HVV(I,J)+DHV
   35 IF (IDLV.EQ.4) GO TO 60
C
   40 DO 50 J=1,NC
   50 XFK(J)=VP(J)/P*GAM(J)*FUG(J)
C
C     CALCULATION OF THE DERIVATIVE OF THE SEPARATION FACTOR
C     WITH RESPECT TO COMPONENT FLOW IN THE LIQUID PHASE.
C
   60 IF (IDLL.EQ.0) GO TO 110
      ISW=1
      DO 105 K=1,NC
      IF (L(K).EQ.0 .OR. X(K).LT.SMALL) GO TO 105
      FLOWK=FLL(I,K)*0.01
      DO 70 J=1,NC
   70 XX(J)=FLL(I,J)/(XT+FLOWK)
      XX(K)=(FLL(I,K)+FLOWK)/(XT+FLOWK)
   91 CALL ACTVTY (TT,XX,GAMX)
   99 DO 100 J=1,NC
  100 DFK(J,K)=VP(J)/P*FUG(J)*(GAMX(J)-GAM(J))/FLOWK
  105 CONTINUE
```

```
C
C       CALCULATION OF THE DERIVATIVE OF THE SEPARATION FACTOR
C       WITH RESPECT TO COMPONENT FLOW IN THE VAPOR PHASE.
C
  110 IF (IDLV.EQ.0.0) GO TO 140
      DO 135 K=1,NC
      IF (L(K).EQ.-1 .OR. Y(K).LT.SMALL) GO TO 135
      FLOWK=FVV(I,K)*0.01
      DO 120 J=1,NC
  120 YY(J)=FVV(I,J)/(YT+FLOWK)
      YY(K)=(FVV(I,K)+FLOWK)/(YT+FLOWK)
      CALL FUGCTY (TT,P,YY,VP,FIX,DHVFK)
      IF (IDH.EQ.2) GO TO 125
      HVV(I,K)=HVV(I,K)+(DHVFK-DHV)/FLOWK*FV(I)
  125 DO 130 J=1,NC
  130 DFK(J,K+NK1)=VP(J)/P*GAM(J)*(FIX(J)-FUG(J))/FLOWK
  135 CONTINUE
C
C       CALCULATION OF THE DERIVATIVE OF THE SEPARATION FACTOR
C       WITH RESPECT TO TEMPERATURE.
C
  140 DO 152 J=1,NC
  152 DFK(J,NK1)=XFK(J)*(-ANT(2,J)/(TT+ANT(3,J))**2+ANT(4,J)+
     *              2.0*ANT(5,J)*TT+ANT(6,J)/TT)
C
C       CALCULATION OF THE DERIVATIVE OF THE SEPARATION FACTOR
C       WITH RESPECT TO TEMPERATURE FOR A DIMERIZING COMPONENT.
C
  160 IF (NDIM.EQ.0) GO TO 161
      CALL ONEDI (P,T5,Y(NDIM),AKAS,ZDIMM,ZNO)
      VPNDIM=EXP(ANT(1,NDIM)+ANT(2,NDIM)/(ANT(3,NDIM)+T5)+
     *          ANT(4,NDIM)*T5+ANT(5,NDIM)*T5*T5+ANT(6,NDIM)*ALOG(T5))
      VPNDIM=(SQRT(1.0+4.0*AKAS*VPNDIM)-1.0)/2.0/AKAS
      DFK(NDIM,NK1)=(VPNDIM-VP(NDIM))/5.0/P*GAM(NDIM)*FUG(NDIM)
C
  161 IF (IDLV.EQ.0) GO TO 180
      CALL FUGCTY (T5,P,Y,VP,FIX,DHVT)
      IF (IDH.EQ.2) GO TO 165
      CV(I)=CV(I)+(DHVT-DHV)/5.0*FV(I)
  165 DO 170 J=1,NC
  170 DFK(J,NK1)=DFK(J,NK1)+VP(J)/P*GAM(J)*(FIX(J)-FUG(J))/5.0
C
  180 IF (IDLL.EQ.0) GO TO 200
      ISW=0
      CALL ACTVTY (T5,X,GAMX)
      DO 190 J=1,NC
  190 DFK(J,NK1)=DFK(J,NK1)+VP(J)/P*FUG(J)*(GAMX(J)-GAM(J))/5.0
C
  200 IF (IDLL.EQ.0) GO TO 230
      IF (IDH.GT.0) GO TO 230
C     ISW=0
      CALL XSHLIN (TT,X,HHE(I))
      ISW=1
      DO 220 K=1,NC
      IF (L(K).EQ.0 .OR. X(K).LT.SMALL) GO TO 220
      FLOWK=FLL(I,K)*0.10
```

```
      DO 210 J=1,NC
  210 XX(J)=FLL(I,J)/(XT+FLOWK)
      XX(K)=(FLL(I,K)+FLOWK)/(XT+FLOWK)
      CALL XSHLIQ (TT,XX,XSH)
      DEXH(I,K)=(XSH-HHE(I))/FLOWK
  220 CONTINUE
      ISW=0
      CALL XSHLIQ (TT+20.0,X,XSH)
      DEXH(I,NK1)=(XSH-HHE(I))/20.0
C
  230 IF (I.NE.NST) GO TO 250
      IF (IDCODE.EQ.0) GO TO 250
      FV(NST)=VSAVE(NK1)
      DO 240 J=1,NC
      XFKNST(J)=XFK(J)
  240 FVV(NST,J)=VSAVE(J)
C
  250 RETURN
      END
```

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