AN IMPROVED MODEL FOR PACKED COLUMN DISTILLATION

By

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Durgapur, India

1989

Submitted to the Faculty of the
Graduate College of the
Oklahoma State University
in partial fulfillment of
the requirements for
the degree of
MASTER OF SCIENCE
July, 1991

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ACKNOWLEDGMENTS

I wish to express my gratitude to all those who have influenced, inspired and encouraged this work.

My sincere gratitude is extended to Dr. Ruth C. Erbar, thesis adviser, whose encouragement, enthusiasm and support has made this study possible. I am indebted to her for providing me with the opportunity to pursue graduate studies.

Special thanks to Dr. Arland Johannes for his help and advice. Thanks also to Dr. David A. Tree, member of the advisory committee, for his valuable comments and suggestions.

I appreciate all that I have learned through my association with such fine friends as Edgardo and Gloria Lopez, Guohai Liu and Hong Jin Yoo.

To my parents, Prithwish and Aditi Roy, and my brother Prabal Roy, I will always be indebted for their love, encouragement and belief in me.

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LIST OF SYMBOLS

A_{ij}	coefficient matrix of first derivatives of orthogonal polynomials
C_{fl}	packing parameter
D'	lesser of column diameter in ft or 2
F	packing constant
G'	vapor mass flux
G	vapor mole flux
H	enthalpy of vapor
H_g	HTU in ft.
H_l	liquid holdup
H_l	HTU in ft.
H_{og}	height of an overall transfer unit, ft.
H_p	height of packed bed in ft.
K_i	equilibrium constant
K_{og}	overall gas phase mass transfer coefficient
L	liquid flowrate (lbmole/hr)
L'	liquid mass flux
N	number of theoretical stages
R	external reflux ratio
S	tower cross sectional area
Sc_l	Schmidt no. for liquid = $\mu_l/p_l D_l$
Sc_v	Schmidt no. for vapor = $\mu_v/p_v D_v$
T_v	bulk temperature of vapor (K)

T_l	bulk temperature of liquid (K)
T_i	interface temperature (K)
V	vapor flowrate (lbmole/hr)
W	bottoms product from the column
W_l	weight mass flux of liquid $lb/s.ft^2$
Z_i	feed mole fraction
a	packing surface area
b1	1.24 (rings) or 1.11 (saddles)
b2	0.6 (rings) or 0.5 (saddles)
g_c	acceleration due to gravity
h	enthalpy of liquid
h_v	heat transfer coefficient for vapor phase
m	slope of the equilibrium curve
t	time
x_k	mole fraction of liquid
y_k	mole fraction of vapor
z	height of column
α	packing constants
β	packing constants
Ω	packing parameter
ϕ	packing parameter
μ_l	viscosity of liquid
μ_w	viscosity of water
μ_v	viscosity of vapor
ρ_l	density of liquid
ρ_w	density of water

ρ_v	density of vapor
σ_l	surface tension of liquid
σ_w	surface tension of water
ΔP	pressure drop (inches of water/ft of packing)

CHAPTER I

INTRODUCTION

Distillation is a method of separation based on the difference in composition between a liquid mixture and the vapor formed from it. The composition difference is due to differing effective vapor pressures, or volatilities, of the components of the liquid. A distillation column may be described as a series of flash separators in which liquid from one flash is fed to the flash below and the vapor from below flows to the flash above.

The two main types of distillation processes are batch distillation and continuous distillation. If the feed mixture is available as an isolated batch of material, the process is a form of batch distillation and the compositions of the collected vapor and residual liquid are thus time dependent. When operated with a continuous feed mixture and continuous removal of product fractions, the process is continuous distillation.

Most distillations conducted commercially operate continuously, with a more volatile fraction recovered as distillate and a less volatile fraction remaining as residue or bottoms. The apparatus in which the enrichment occurs is usually a vertical, cylindrical vessel called a still or distillation column. This apparatus normally contains internal devices for effecting vapor-liquid contact, the devices may be trays or packings.

The packed column is widely used as a vapor/liquid contacting device for mass transfer in distillation, absorption and stripping. For many years it was confined largely to corrosive applications where ceramic packings were advantageous, or to small-diameter columns where it was inconvenient to install trays. In recent years, however, the use of packings has been extended to large-scale vapor/liquid operations of all types, thanks to their economic and performance advantages, e.g.low pressure drop. Indeed, today, the packed column should be regarded as a serious candidate for any application of distillation, absorption and stripping.

There are essentially two kinds of packings, random and structured. Random packings which are basically dumped into the tower come in many types, materials and sizes. The most common types in commercial installations are slotted rings (some variants include Ballast rings, Pall rings, Flexirings and Trimer rings) and saddles. Structured type packings have been used for decades and improved designs offer particularly high performance. Structured packings are broadly classified as knitted or nonknitted type. Either style can be assembled in a segmented or spiral form.

There have been relatively few attempts at modeling packed distillation columns; equilibrium stage methods and HETP/stage efficiency have been exclusively used in packed distillation column design. The modeling of packed columns as a continuous contacting device has mainly been confined to studying problems at constant molal overflow or total reflux.

Our work is two fold, one involves using literature correlations to model the HETP method which will be subsequently used as a reference model. The other approach models the packed column as a continuous unit using the two film theory of heat and mass transfer. The resulting nonequilibrium model is expressed as a set of partial differential equations. The numerical technique used is a polynomial approximation method called orthogonal collocation which is especially suited to modeling continuous systems.

The results of the simulation will be compared to the data available from the literature. This work also intends to emphasize the use of personal computers to carry out such simulations while minimizing the computation time.

CHAPTER II

LITERATURE SURVEY

Introduction

Within the past decade several significant developments have occurred in distillation technology applied to petroleum refining and chemical processing. These can be grouped into three general categories:

* New design practices
* New contacting devices and new applications for existing contacting devices
* New troubleshooting techniques

There are essentially two kinds of problems that one encounters in the literature on packed column modeling and simulation, design problems and operating or rating problems. Design calculations involve the estimation of the height of a packed column needed to achieve a desired degree of separation. Operating problems involve predicting the performance of a column of a given configuration (packed height, feed location and so on).

Staged Modeling

Basically, two approaches have been proposed for modeling packed columns. In the first approach, the continuous contact device is divided into sections and each section is treated more or less as though it were a stage in a tray tower (e.g. Holland, 1975). The other approach is to write differential mass and energy balances for a small element of packing and solve them by a numerical integration scheme (Treybal, 1969; Fientuch and Treybal, 1978; Kelly et al., 1984; Serwinski and Gorak, 1983; Srivastava and Joseph,1984).

Rigorous simulation of multistage processes such as distillation or absorption is, more often than not, based upon the equilibrium stage model (e.g. King 1971;Holland 1975, 1981; Henley and Seader, 1981). Briefly, the model includes the assumption that the streams leaving any particular stage are in equilibrium with each other. In actual operation, stages rarely ever operate at equilibrium. The usual way of dealing with deviations from equilibrium is by incorporating a stage efficiency into the equilibrium relations. There are several problems associated with this. The first problem is that there are several different definitions of stage efficiency: Murphree (1925), Hausen (1953), generalized Hausen (Standart, 1966), vaporization (Holland, 1975) and others. There is no consensus on which definition is best and various arguments have been presented by Standart (1966, 1979), Holland (1975), Holland and McMohan (1970) as cited by

Krishnamurthy (1985), King (1971) etc.. Moreover in case of multicomponent systems the individual component efficiencies are assumed equal which is rarely true.

Phenomena such as reverse diffusion or osmotic diffusion occur in multicomponent systems and these affect the tray efficiencies. Models of mass transfer that are able to account for interaction effects are available now (e.g.Krishna and Standart 1976). These models have been used as a basis for developing methods for calculating efficiencies in multicomponent systems (Toor and Burchard, 1960, as cited by Krishnamurthy (1985); Toor, 1964; Diener and Gerster, 1968; Krishna, 1977; Medina et al., 1979; Vogelpohl, 1979). R. Krishnamurthy and R. Taylor (1985 and 1987) contend that arbitrary and ambiguous multicomponent stage efficiency adds unnecessary complexity to separation process modeling and suggest a sequence of nonequilibrium stages for which the solution of the conservation equations for each phase is used directly. Computations of quantities such as HETP and HTU are completely avoided in their paper (Krishnamurthy and Taylor, 1985). However the accuracy of the model predictions is limited by the accuracy of the correlations used to calculate the mass transfer coefficients. Other nonequilibrium models of staged equipment in the same class are Waggoner and Loud (1977), Waggoner and Burkhart (1978) and Ricker et al. (1981). Another sophisticated two-phase model is that of

Billingsley and Chirachavalla (1981), as cited by Krishnamurthy (1985).

In contrast to the nonequilibrium staged models which are effective for steady-state simulation Hitch, Rousseau and Ferrell (1987), as cited by Krishnamurthy (1985), developed an algorithm for the unsteady-state simulation of multicomponent adiabatic absorption in packed columns. The accuracy of the predictions of transient behavior depended strongly on the correlations used. Other proponents of the sectional approach include Holland and co-workers (1975). Their model accounts for mass transfer effects by using vaporization efficiencies. These efficiencies must be fitted by experimental data for any given system. This is a serious flaw because it means that their model cannot be used to simulate or design a new process.

Continuous Modeling

The other approach to modeling packed columns which is also more common involves writing differential mass and energy balances for a small element of packing. Sherwood and Pigford (Sherwood et al., 1975) developed a simple model for adiabatic packed absorbers based on this approach. They made several assumptions which have limited the usefulness of their model (e.g. liquid phase resistances to heat and mass transfer were neglected and liquid and gas flows were assumed constant through the tower). A more general model for single solute systems that included heat and mass transfer resistances in both phases was developed by Treybal (1969). Raal and Khurana (1973) verified this model by using it to successfully simulate their experiments on ammonia absorption in water. Treybal's model was extended to multicomponent systems by Feintuch and Treybal (1978). A computer program implementing this generalized model is given by Feintuch. Kelly et al., (1984) used this program to simulate their own experiments involving the absorption of acid gases using refrigerated methanol as solvent; good agreement between measurement and model prediction was obtained. In all of these models mass transfer rates were calculated using effective diffusivity methods sometimes with the flux correction factors set to unity and the convective term ignored. Equilibrium was assumed to exist at the interface.

There have been relatively few attempts at modeling packed distillation columns; equilibrium stage methods and HETP/stage efficiency have been exclusively used in packed distillation column design. Von Rosenberg and Hadi (1980) have presented a simplified differential model of a packed distillation column. Simple expressions for the mass transfer rates were used in which all species were assigned the same value for the overall mass transfer coefficient.

The consequence of this assumption is equimolar overflow which, in turn, means that the energy balance can be ignored. Serwinski and Gorak (1983) have presented a somewhat more sophisticated differential model of a packed distillation column operating at total reflux (Equimolar overflow was assumed). Some simulation results are discussed by Gorak (1983). Gorak and Vogelpohl (1985) conducted distillation experiments in a packed column using the ternary systems methanol, 2-propanol and water and acetone, ethanol and benzene. They simulated their experiments with the method of Serwinski and Gorak (1983). Their calculations show that while models based on solutions of the Maxwell-Stefan equations do very well, the HETP approach is too conservative and inaccurate, the discrepancy for the HETP methods becoming greater when the driving forces are large.

It is seen that the nonequilibrium stage model is in a sense, a more general version of the absorber model of Feintuch and Treybal (1978) and the distillation models of Gorak and co-workers. The most important differences between the various approaches are, therefore, in how the model equations are solved.

Numerical Techniques

Equation tearing and simultaneous correction procedures are some methods for solving nonlinear algebraic equations which arise in staged models. Feintuch and

Treybal (1978) solved their differential equations using the simple Euler method. This however, involved no less than five levels of nested iteration loops (Kelly et al., 1981) resulting in fairly large computation times. Serwinski and Gorak (1983) used the Runge-Kutta method of integration to solve their differential equations. Von Rosenberg and Hadi (1980) approximated derivatives by finite difference equations. Cho and Joseph (1983) achieved drastic reduction in the number of equations to be solved by using orthogonal collocation for discretization in the spatial direction. This was found to work well for both steady state and dynamic simulation of relatively ideal systems but not for nonlinear equilibrium relationships. In such cases the steady state solution was obtained as the asymptote of the transient response. Srivastava and Joseph (1984) suggested solving the steady state equations directly by Newton's method. This method was used by Taylor and Krishnamurthy (1985) to solve their nonequilibrium stage model equations.

Orthogonal Collocation

Orthogonal collocation is a polynomial approximation method used to solve systems of ODE's and PDE's. Analytical solutions to PDE's are difficult to obtain except in very simple cases. Numerical solutions are possible by discretization in the space and time variables.

Discretization in the spatial variable is achieved by the method of orthogonal collocation. The method attempts to minimize the residuals in the differential equations at selected points in the column. It has been shown (Michelson et al., 1978) that a very efficient collocation method results when the collocation points are chosen as zeros of certain orthogonal polynomials, the so called Jacobi polynomials.

There are three main differences in the collocation method: the trial function is taken as a series of orthogonal polynomials, the collocation points are taken as the roots of one of those polynomials (N roots of $Pn(x)=0$) and the dependent variables are the solution values at the collocation points rather than the coefficients in the expansion (perturbation theory).

The collocation approximation is obtained as follows. The variables y and z are expressed in terms of polynomials $l_k(z)$, $k=1,2....n+2$

$$y(z,t) = \sum_{k=1}^{n+2} l_k(z).y_k(t) \tag{2.1}$$

where $y_k(t)$ = value of y evaluated at collocation point $z = z_k$

The collocation points are chosen as the zeros of orthogonal Jacobi polynomials $P_n^{ab}(z)$ defined by

$$\int_0^1 z^b(1-z)^a z^j P_n^{ab}(z)dz = 0 \qquad j=0,1...n-1 \tag{2.2}$$

Differentiating eqn. 2.2 we have:

$$\left.\frac{\delta y}{\delta z}\right|_{z=z_j} = \sum_{k=1}^{n+2} \left.\frac{dl_k}{dz}\right|_{z=z_j} y_k(t) \qquad (2.3)$$

$$= \sum_{k=1}^{n+2} A_{jk} y_k(t)$$

where:

$$A_{jk} = \left.\frac{dl_k}{dz}\right|_{z=z_j}$$

The discretization involving orthogonal collocation introduces some approximations. It is important that overall mass and heat balances are met by the new approximated set of equations. It has been shown (Cho et al., 1980) to be true in this case. Note that we have included both the boundary points in the equations given above. This is because the boundary conditions are given at both end points of the boundary.

All roots of the orthogonal polynomials lie between zero and one. There have been comparative studies carried out to determine the optimum number of collocation points required to approximate a system such as ours (Srivastava et al., 1984). It was suggested that three point collocation yielded solutions of sufficient accuracy. As per the suggestion, all our simulations were carried out using three point collocation.

While increasing the number of collocation points may improve the solution marginally, the computation time will increase tremendously due to the much larger number of equations to be solved. Therefore three point collocation is the best simulation solution. The roots of the Jacobi polynomial are obtained at weighting function W, equal to one.

Recommendations

In evaluating the various models suggested in the literature the foremost concern is one of reliability. The reliability of a packed column design model can be defined by the standard deviation of the logarithmic-ratio objective function obtained by execution of the model against a comprehensive data bank (Fair and Bolles,1982). The reliabilities of competing models can be compared on the basis of the safety factor (Fs) required for reasonable (95%) confidence of success.

Keeping in mind the present status of packed column models it may be recommended that future engineering research be devoted to further attempts to improve the reliability of models for prediction of packed-column capacity, mass-transfer efficiency and pressure drop.

Research should be focussed on exploring more efficient numerical techniques, reducing simulation time and improving thermodynamic property prediction methods.

CHAPTER III

STAGED MODELING

Even though a packed tower has continuous instead of discontinuous contact of liquid and vapor, it can be analyzed like a staged tower. We assume that the packed section of the column can be divided into a number of segments of equal height. Each segment acts as an equilibrium stage, and liquid and vapor leaving the segment are in equilibrium. This staged model is not an accurate physical description of the process but it can be used for design. Equilibrium stage methods and HETP/stage efficiency have been used extensively in packed distillation column design.

Height Equivalent of Theoretical Plate

There are a number of correlations in the literature to predict the mass transfer coefficients or the HTU values. We will use the correlation of Bolles and Fair (1982) which is an improvement of the previous correlation of Cornell et. al. (1960).

H_{og} can be calculated as follows :

$$H_g = \frac{\Omega (D')^{b1} (Hp/10)^{1/3} (Sc_v)^{1/2}}{[(3600) W_l (\mu_l/\mu_w)^{0.16} \ (\rho_l/\rho_w)^{-1.25} \ (\sigma_l/\sigma_w)^{-0.8}]^{b2}} \qquad (3.1)$$

$$H_l' = \phi C_{fl}(H_p/10)^{0.15}(Sc_l)^{1/2} \tag{3.2}$$

$$H_{og} = H_g + \theta H_l' \tag{3.3}$$

where: $\theta = mV/L$

The calculated H_g and H_l values can vary from location to location in the column. When this occurs, an integrated mean value should be used. Even if H_g and H_l are constant, Hog will vary owing to the curvature of the equilibrium curve. The HETP may now be calculated using the following equation:

$$\text{HETP} = H_{og}\ln(\theta)/(\theta-1) \tag{3.4}$$

Notice that the calculation of HETP requires that the packed height be supplied as input. For our simulation this height is determined by solving the differential equation model of the packed column. Once the HETP is calculated the following relationship is used to find the number of theoretical plates

$$\text{HETP} = \frac{\text{height of packing (Hp)}}{\text{number of theoretical stages (N)}} \tag{3.5}$$

The number of theoretical plates calculated from the equation given above is rounded of to the next highest whole number. The calculated packed height is then

$$Hp = \text{HETP}*N \tag{3.6}$$

Diameter of Column

Another input required for the HETP calculation is column diameter. The column is sized to operate at 65 to 90% of flooding or to have a given pressure drop per foot of packing.

Given the pressure drop the following equation is recommended by P.C.Wankat (1988):

$$p = \alpha(10^{\beta L'})(G'^2/\rho_g) \qquad (3.7)$$

α, β = const. for packing ; $L' = G'*L*MWl/(V*MWv)$

G' can be found from this equation by successive substitution and the area will then be:

$$\text{area} = V*MWv/G' \qquad (3.8)$$

The diameter can thus be found.

Alternately, G'_{flood} can be estimated from:

$$\log(G^2 F \mu^{0.2} \psi/\rho_g \rho_l g_c) = -1.6678-1.085\log(F_{lv})-0.29655(\log(F_{lv})) \qquad (3.9)$$

where: $F_{lv} = L'/G'*(\rho_g/\rho_l)^{1/2}$

then $G'_{actual} = 0.7*G'_{flood}$ (for 70% of flood)

the area and diameter may be calculated as before.

Simulation

The computer program has been designed to calculate the diameter and HETP of the packed column. In order to do this the properties of the vapor and liquid at any one point in the column have to be determined. Typically, the user fixes a point in the column and carries out a vapor liquid equilibrium calculation. This is followed by the calculation of vapor and liquid densities, diffusivities, viscosities and surface tension. A brief description of each phase of this calculation is given below.

Vapor Liquid Equilibrium

This is carried out by a series of subroutines. The user can carry out flash, bubble and dew point calculations by specifying the appropriate "id" numbers displayed on the screen. Pure fluid properties are read from a data file (DFILE.DAT). Figures 12-19 (appendix B) contain the flowcharts for some subroutines presented here.

Subroutine VLE carries out vapor liquid equilibrium calculations. If any VLE operation such as flash, bubble point or dew point is to be carried out this subroutine calls up the appropriate subroutines to perform the task. It is used to control and track the convergence to a solution.

Subroutine MIXING contains the mixing rules for the equations of state that are to be used (Soave Redlich Kwong (SRK) & Peng Robinson (PR)).

Subroutine EOS contains the equations of state that the user may choose. The Soave-Redlich-Kwong and the Peng Robinson equations of state are included in this subroutine.

Subroutine VAPPR has the vapor pressure method programed into this subroutine. The equation used is the Wagner equation for vapor pressures.

Subroutine FUGACITY is used to estimate the fugacities and fugacity coefficients which will then be used to calculate the k-values.

Subroutine FLASH carries out VLE flash calculation. There is a check for the two phase region and then the function

$$F = \Sigma Z_i(1-K_i)/(\alpha+(1-\alpha)K_i) = 0 \qquad \alpha = L/F$$

is estimated. If the function is within a tolerance limit the control returns to the VLE subroutine. Otherwise the L/F ratio is updated using a form of the Newton-Raphson method.

In subroutine BUBBLE bubble point temperature/pressure is estimated using the algorithm suggested by Erbar and Maddox in 'Gas Conditioning and Processing - Vol. 3'.

Subroutine DEW is designed on the basis of the recommendations of Erbar and Maddox like the bubble point subroutine. Subroutines TEMP or PRESSURE are called to update the temperature or pressure as required.

Subroutine TEMP is used to adjust the temperature estimates for the bubble and dew point calculations. This is based on the suggestions of Erbar and Maddox.

A similar subroutine PRESSURE (as TEMP) to adjust the pressure is programed here. The algorithm essentially uses the Secant method to adjust the pressure at each iteration.

The initial estimates of the K-values for flash, bubble and dew point are provided by subroutine INITIAL.

Liquid and Vapor Density

The vapor density is calculated from the equation of state (Peng Robinson and SRK). The vapor pressure method should not be used to calculate the vapor densities. This calculation is carried out in the VLE subroutine.

The liquid densities (both pure and mixture) are calculated using the Hankinson Thompson method. The subroutine HANKTHM is called from VLE.

Diffusion Coefficients

The diffusion coefficient for the vapor is calculated by first calculating the binary diffusion coefficients for each combination in the mixture using the Wilke-Lee equation and then using the simplified Stefan-Maxwell equation to calculate the mixture diffusivity.

The liquid mixture diffusivity is calculated using the modified Wilke-Chang equation as recommended by Reid et.al. The subroutine DIFF carries out both types of calculation.

Viscosity

The viscosity of the vapor and liquid may be calculated using the series of subroutines in the file

VIS.FOR. This is the model of Ely and Hanley and is based on the corresponding states principle and the conformal, one fluid concept. The reference fluid used is methane. If the viscosity is to be calculated near the two phase region, it is suggested that the following guidelines be followed :

1) Bubble point : increase the pressure, decrease the temperature (20K).

2) Dew point : decrease the pressure, increase the temperature.

This is required because the program assumes that the mixture is single phased resulting in convergence to the wrong solution.

Surface Tension

The surface tension of water and the liquid mixture is required to estimate the HETP. The surface tension of water is calculated using a correlation suggested by Jasper. The pure fluid surface tension is calculated using the corresponding states correlation of Brock and Bird. The mixture surface tension is calculated as per the recommendations of Reid et al. All calculations are carried out in the subroutine SRFTN.

Diameter and Hetp

The subroutine DIA calculates the diameter of the column based on percentage flood or specified pressure drop once the properties of the liquid and vapor are known. The packing factors are read from a file (PACKF.DAT).

The diameter of the column is required, to estimate the HETP therefore, the subroutine HETP is always called after DIA. The coefficients ø and Ω are represented as curve fit polynomials. The coefficients of these polynomials are placed under block data and subroutine PARAM is used to estimate these parameters. A table containing the types of packings which can be used for simulation is presented in appendix, A.

CHAPTER IV

CONTINUOUS MODELING

Two Film Theory

Our model is based on the two film theory of heat and mass transfer. Consider figure 1. given below.

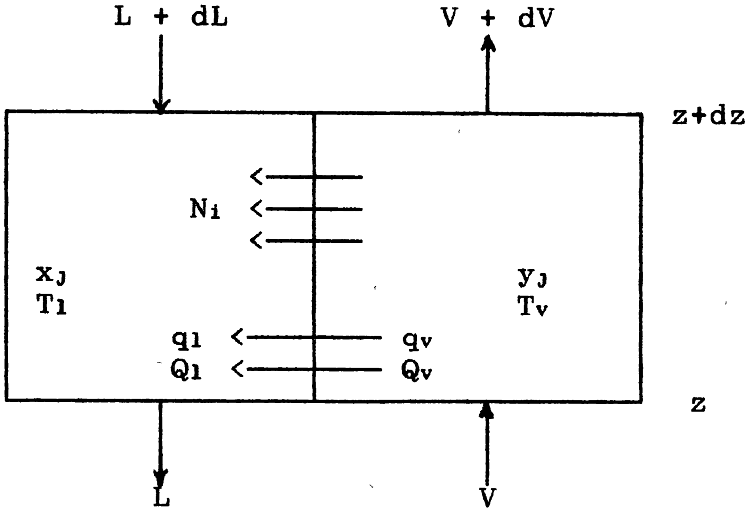

Figure 1. Liquid vapor film

We can write the following partial differential equations over an element dz of the packing based on the following assumptions:

1) the pressure drop through the bed is negligible.

2) the accumulation of mass in the vapor phase is small in comparison with the liquid phase.

Overall mass balance:

$$\frac{\delta H_l}{\delta t} = \frac{\delta L}{\delta z} - \frac{\delta V}{\delta z} \tag{4.1}$$

Overall heat balance:

$$\frac{\delta (H_l h)}{\delta t} = \frac{\delta (Lh)}{\delta z} - \frac{\delta (VH)}{\delta z} \tag{4.2}$$

Overall component balance:

$$\frac{\delta (H_l x_k)}{\delta t} = \frac{\delta (L x_k)}{\delta z} - \frac{\delta (V y_k)}{\delta z} \tag{4.3}$$

$k=1,2 - - c$

for the vapor phase: (neglecting vapor phase holdup)

a) mass balance :

$$0 = - \frac{\delta V}{\delta z} - \sum_{k=1}^{c} N_k \tag{4.4}$$

b) component balance:

$$0 = - \frac{\delta (V y_k)}{\delta z} - N_k \tag{4.5}$$

$k=1,2 - - c$

c) heat balance:

$$0 = - \frac{\delta (VH)}{\delta z} - h_v a_h S (T_v - T_l) - \sum_{j=1}^{c} N_j H_j \tag{4.6}$$

assuming the liquid and vapor phases are ideal mixtures we have:

$$N_k = K_{og}a(y-y^*)(S)$$

It is seen that the two film theory of mass transfer yields 2C+5 equations in 2C+5 unknowns (L, V, T^v, T^l, T^i, x and y).

These equations can be used to model both the enriching and stripping sections of the packed distillation column.

Model I

We will make certain simplifying assumptions in order to reduce these equations to ones which will facilitate reasonable computation times on a personal computer without losing practical significance.

The assumptions are:

1) Molar latent heats of vaporization for the components in the system are equal, so that molar vapor and liquid flow rates are constant in the column.
2) Liquid and vapor streams are assumed to be at bubble and dew temperatures respectively. Consequently, no enthalpy balance is needed.
3) The gas phase overall mass transfer coefficient is used for defining the mass transfer rates. The resistance to heat and mass transfer on the liquid side is neglected.

Based on the above mentioned assumptions, model equations can be simplified as:

Overall component balance:

$$H_l \frac{\delta(x_k)}{\delta t} = L \frac{\delta(x_k)}{\delta z} - V \frac{\delta(y_k)}{\delta z} \qquad (4.7)$$

$$k=1,2 - - c$$

Vapor phase component balance:

$$0 = - V \frac{\delta(y_k)}{\delta z} - N_k \qquad (4.8)$$

$$k=1,2 - - c$$

where:

$$N_k = K_{og} a(y-y^*)(S)$$

Enriching Section

The equations in our model are applicable to the enriching as well as the stripping sections.

The differences in the two sections lie in the boundary conditions and the mass transfer coefficients. Since a total condenser is used, the boundary condition at the top is

$$y = x \quad \text{at} \quad z = z_t$$

the mass transfer coefficient (Brown et al.) in the enriching section is

$$K_{og} a = 0.74*(G)^{1.175}*(R/R+1)^{1.175} \qquad (4.9)$$

We can now write the normalized collocation equations in the enriching section as follows:

$$H_l \frac{dx_{ik}}{dt} = L \sum_{j=1}^{n+1} A_{ij} x_{kj} - V \sum_{j=2}^{n+1} A_{ij} y_{kj} - V A_{i1} y_{k1}$$

$$+ A_{in+2} y_{kn+2} (L-V)$$

$$k=1,2.. c \; ; \; i=1,2...n+1 \qquad (4.10)$$

$$0 = -V\sum_{j=2}^{n+2} A_{ij}y_{kj} - VA_{i1}y_{k1} - K_{og}aSH_p(y_{ki}-y^*_{ki})$$

$$k=1,2,..c \; ; \quad i=2,...n+2 \qquad (4.11)$$

Stripping Section

The boundary condition at the reboiler is obtained from material balances around the reboiler and the equilibrium relation between the vapor entering the column and the liquid bottom product. This is

$$y = [\, L_m \,/\, (V + Wx_w/y^*)]x \qquad \text{at} \quad z = 0$$

the mass transfer coefficient (Brown et al.) is a function of the vapor rate.

$$K_{og}a = 0.5\ (G)^{1.29} \qquad (4.12)$$

where G may be estimated from the flooding relation:

$$G_f = 13.3 - 1.8\ (L/V) \qquad (4.13)$$

the collocation equations in the stripping section may be written as:

$$H_l \frac{dx_{ik}}{dt} = L\sum_{j=2}^{n+1} A_{ij}x_{kj} - V\sum_{j=1}^{n+1} A_{ij}y_{kj} + LA_{i1}x_{k1}$$

$$-VA_{in+2}y_{kn+2} + LA_{in+2}x_{kn+2}$$

$$k=1,2..\ c \; ; \quad i=1,2...n+1 \qquad (4.14)$$

$$0 = -V\sum_{j=1}^{n+1} A_{ij}y_{kj} - VA_{in+2}y_{kn+2} - K_{og}aSH_p(y_{k1}-y^*_{ki})$$

$$k=1,2,..c \; ; \quad i=2,...n+2 \qquad (4.15)$$

where:

$$y_{kn+2} = [\, L_m \,/\, (V + Wx_{kw}/y^*_k)]\ x_{kn+2}$$

In the continuous system, the feed is introduced at the point where the mole fraction of the heavy key in the liquid stream is the same as that in the feed.

Model II

Model I is extended here by eliminating the assumption of equimolar counter diffusion and saturated liquid and vapor streams. Simultaneous heat and mass transfer is considered.

The assumption made here involves the gas phase overall mass transfer coefficient used for defining the mass transfer rates.

The equations may now be written as follows:

Overall mass balance:

$$\frac{\delta H_l}{\delta t} = \frac{\delta L}{\delta z} - \frac{\delta V}{\delta z} \qquad (4.16)$$

Overall heat balance:

$$\frac{\delta(H_l h)}{\delta t} = \frac{\delta(Lh)}{\delta z} - \frac{\delta(VH)}{\delta z} \qquad (4.17)$$

Overall component balance:

$$\frac{\delta(H_l x_k)}{\delta t} = \frac{\delta(Lx_k)}{\delta z} - \frac{\delta(Vy_k)}{\delta z} \qquad k=1,2 - - c \qquad (4.18)$$

Vapor phase component balance:

$$0 = -\frac{\delta(Vy_k)}{\delta z} - N_k \qquad k=1,2 - - c \qquad (4.19)$$

where:

$$N_k = K_{og}a(y-y^*)(S)$$

The above is a system of 3C+3 equations in 3C+3 unknowns (namely L, V, T, x, y and y*)

<u>Enriching Section</u>

The boundary condition for the total condenser is as given in model I :

$$y = x \qquad \text{at} \qquad z = z_t$$

the mass transfer coefficient (Brown) is

$$K_{og}a = 0.74*(G)^{1.175}*(R/R+1)^{1.175} \qquad (4.20)$$

the normalized collocation equations for the enriching section may be written as follows:

$$\frac{d(H_{li})}{dt} = \sum_{j=1}^{n+1} A_{ij}L_j - \sum_{j=1}^{n+1} A_{ij}V_j + A_{in+2}(L_{n+2}-V_{n+2})$$

$$i=1,\ldots.n+1 \qquad (4.21)$$

$$\frac{d(H_{li}x_{ik})}{dt} = \sum_{j=1}^{n+1} A_{ij}L_jx_{kj} - \sum_{j=2}^{n+1} A_{ij}V_jy_{kj} - A_{i1}V_1y_{k1} + A_{in+2}y_{kn+2}(L_{n+2}-V_{n+2})$$

$$k=1,2.. \ c \ ; \ i=1,2...n+1 \qquad (4.22)$$

$$0 = -\sum_{j=2}^{n+1} A_{ij} V_j y_{kj} - A_{i1} V_1 y_{k1} - K_{og} aSH_p (y_{ki} - y^*_{ki}) - A_{i\,n+2}\, y_{k\,n+2} V_{n+2}$$

$$k=1,2,..c \;;\; i=2,...n+2 \qquad (4.23)$$

$$\frac{d(H_{li} h_i)}{dt} = \sum_{j=1}^{n+1} A_{ij} L_j h_j - \sum_{j=1}^{n+1} A_{ij} V_j H_j - A_{i\,n+2} V_{n+2} H_{n+2} + A_{i\,n+2} h_{n+2} L_{n+2}$$

$$i=1,...n+1 \qquad (4.24)$$

The liquid and vapor rates at the top of the column (L_{n+2} , V_{n+2}) may be determined from the external reflux ratio (known) and the distillate rate (known).

Stripping Section.

The boundary condition for a partial reboiler is given by the following equation:

$$y = [\, L_{n+2} \,/\, (V_{n+2} + Wx_w/y^*)]x \qquad \text{at} \quad z = 0$$

The mass transfer coefficient (Brown et al.) is a function of the vapor rate in the stripping section.

$$K_{og} a = 0.5\ (G)^{1.29} \qquad (4.25)$$

The normalized collocation equations for the stripping section are:

$$\frac{d(H_{li})}{dt} = \sum_{j=2}^{n+2} A_{ij} L_j - \sum_{j=2}^{n+2} A_{ij} V_j + A_{i1} (L_1 - V_1)$$

$$i=1,....n+1 \qquad (4.26)$$

$$\frac{d(H_{li}x_{ik})}{dt} = \sum_{j=2}^{n+1} A_{ij}L_jx_{kj} - \sum_{j=2}^{n+1} A_{ij}V_jy_{kj} - A_{i1}V_1y_{k1}$$

$$+ A_{in+2}x_{kn+2}L_{n+2} - A_{in+2}y_{kn+2}V_{n+2} + A_{i1}L_1x_{k1}$$

$$k=1,2..\ c\ ;\ i=1,2...n+1 \qquad (4.27)$$

$$0 = -\sum_{j=2}^{n+1} A_{ij}V_jy_{kj} - A_{i1}V_1y_{k1} - K_{og}aSH_p(y_{ki}-y^*_{ki})$$

$$- A_{in+2}y_{kn+2}V_{n+2}$$

$$k=1,2,..c\ ;\ i=2,...n+2 \qquad (4.28)$$

$$\frac{d(H_{li}h_i)}{dt} = \sum_{j=2}^{n+2} A_{ij}L_jh_j - \sum_{j=2}^{n+2} A_{ij}V_jH_j - A_{i1}V_1H_1$$

$$+ A_{i1}h_1L_1$$

$$i=1,...n+1 \qquad (4.29)$$

where:

$$y_{kn+2} = [\ L_{n+2}\ /\ (V_{n+2} + Wx_{kw}/y^*_k)]\ x_{kn+2}$$

The program solves the enriching section before solving the stripping section. Therefore, the liquid and vapor rates at the top of the stripping section may be estimated using the simple feed addition model. This also gives the liquid composition at the top of the stripping section.

Simulation

The program is designed to simulate a distillation column under steady state operation using 3 point collocation. The collocation equations are converted to a set of nonlinear simultaneous equations by setting the time derivatives to zero.

The solution scheme used is the Levenberg-Marquardt algorithm which is a variation of Newton's method. The jacobian is approximated by the finite difference method. The user has a choice of carrying out the equilibrium calculations using bubble point temperature estimates or constant relative volatility assumptions.

The column is simulated using the following set of subroutines:

Subroutine DIST is called after the input subroutine and is used to control the column simulation. The collocation points and first derivatives are calculated by calling PLANAR. A data file is opened and the initial guesses are read. It then calls subroutine DNEQNF to solve the nonlinear equations. Once the results are obtained, DSTOUT is called to print the results in an output file.

Subroutine DNEQNF is the IMSL routine used to solve the nonlinear equations. It is called with the initial guesses, number of equations, maximum error and maximum iterations. Its output is the roots of the equations and the norms of the function.

Subroutine FCN contains the collocation equations for both the enriching and the stripping section. A counter is used to switch between the enriching and stripping sections. This subroutine is called by DNEQNF. This subroutine calls a number of functions. These are described as follows :

In function GOK the overall gas phase mass transfer coefficient is calculated at each collocation point as a function of the liquid/vapor rate at that point.

In function ENLV the enthalpy of liquid and vapor at each collocation point is estimated. Subroutine ENTHALPY is called and ideal gas/liquid enthalpies are calculated.

Function YSTAR calculates the equilibrium mole fraction of vapor at each collocation point. This is done by calling subroutine VLE and carrying out a bubble point temperature calculation. The equation of state used is SRK but any other EOS could be used (Peng Robinson or Vapor pressure) by changing IEOS.

Function YSTAR1 contains an alternate method of estimating the equilibrium mole fractions by assuming constant relative volatilities.

Function XBOT1 uses constant relative volatilities to estimate the mole fraction of vapor entering the column at the bottom.

The function XBOT uses bubble point temperature calculations to estimate the mole fraction of vapor entering the column at the bottom.

In Subroutine JACOBI the roots of the orthogonal polynomial are calculated. Newton's method is used to find the roots. These roots are the collocation points in each element.

The matrices without symmetry are calculated in the subroutine PLANAR. The result is a N+2 by N+2 matrix, A, which is a matrix of the first derivatives of the orthogonal polynomials. PLANAR is called by DIST. PLANAR calls JACOBI for the roots of the polynomials.

Subroutine DSTOUT: The results of the simulation are printed in an output file (ROOT.DAT). The results include the composition profiles, temperatures, pressures and flowrates.

CHAPTER V

RESULTS AND DISCUSSION

The Rosenberg Problem

Using this simulator we have studied the distillation problem solved by D. U. Von Rosenberg et al., (1980). The system is briefly described in the following tables

TABLE 1

DISTILLATION DATA

Component	x_f	Spec. x_d	Spec. x_w
Methyl cyclohexane	0.25		
Toluene	0.25		0.01
Para-xylene	0.25	0.02	
Meta-xylene	0.25		

TABLE 2

COLUMN SPECIFICATION

Parameter	Type
Type of packing	1" Raschig Rings

TABLE 2 (Continued)

Parameter	Type
Type of Condenser	Total Condenser
Feed	at bubble point
Column Pressure	1 atm

Case I

Using model I the simulation has been carried out to determine the composition profiles, temperature profiles and the height of the column.

Von Rosenberg et al., (1980) have solved this problem using a finite difference scheme and constant relative volatilities. This approach did not allow an estimate of the temperature profiles.

Our simulation was carried out using both constant relative volatilities and bubble point temperature estimates. The latter is used to produce a temperature profile (as shown in figure 2.). Figures 3 and 4 show the composition profiles obtained by simulation. The composition profiles match Rosenberg's solution very well.

In addition the optimum height of the column was found by repeated simulation using different heights until the

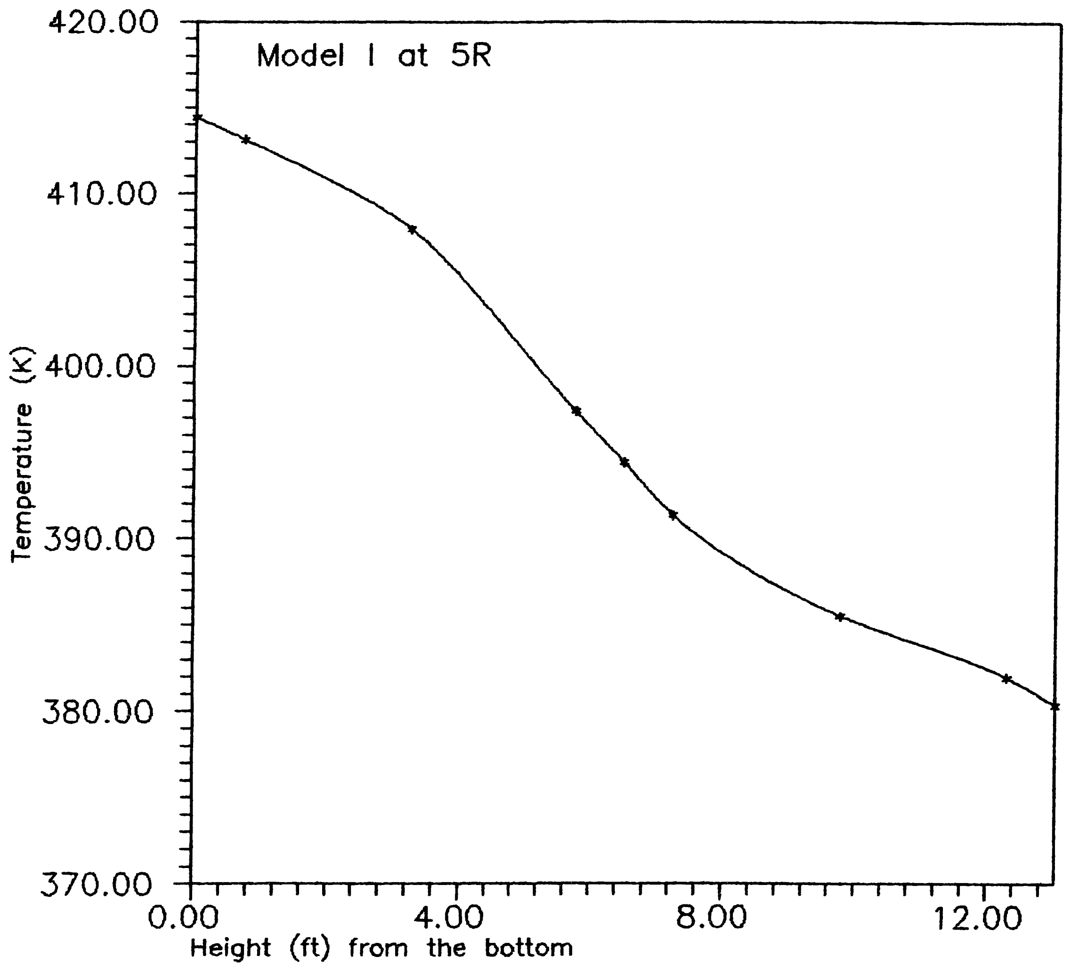

Figure 2. Temperature Profile

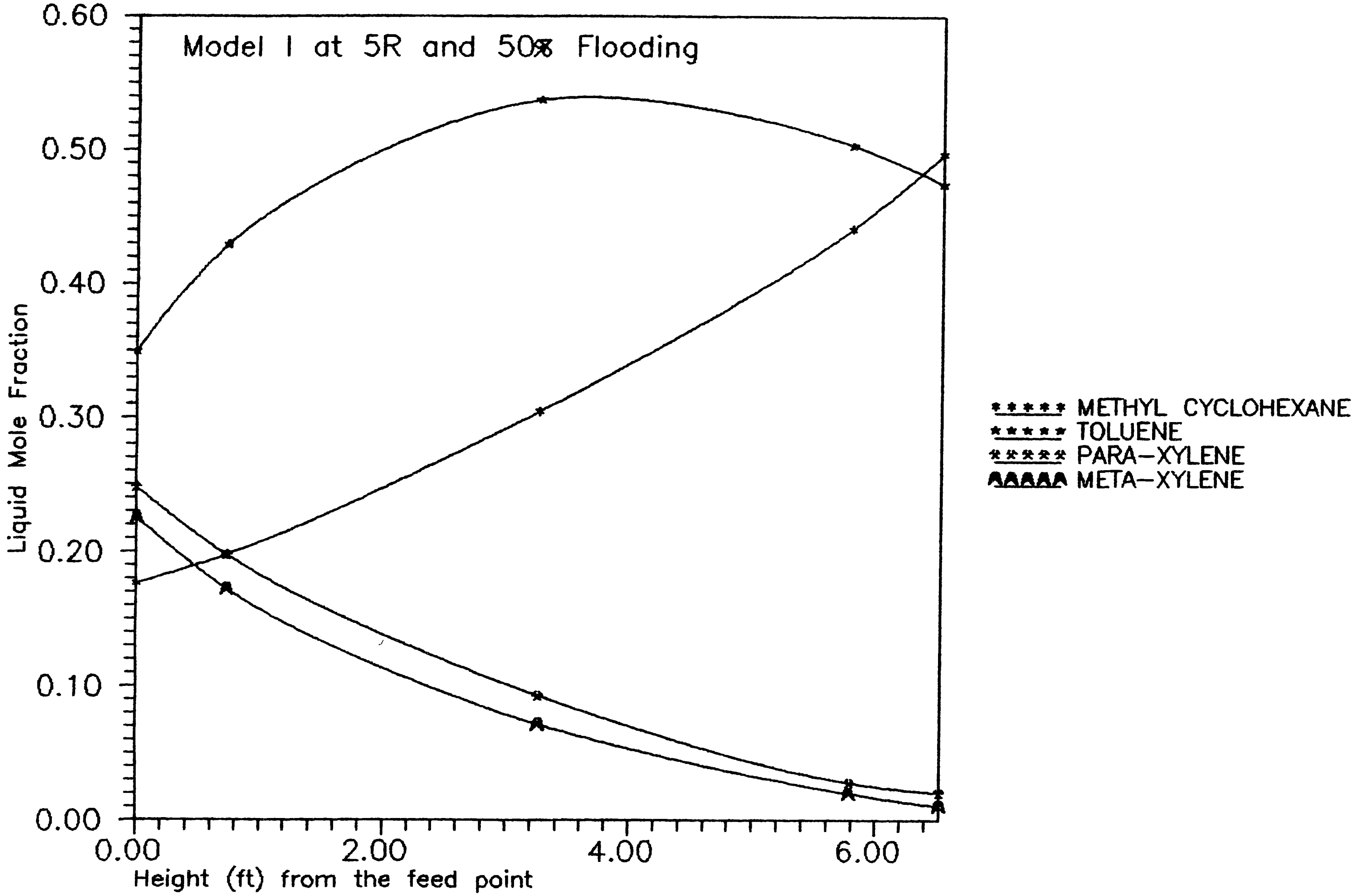

Figure 3. Liquid Composition Profile
(Enriching Section)

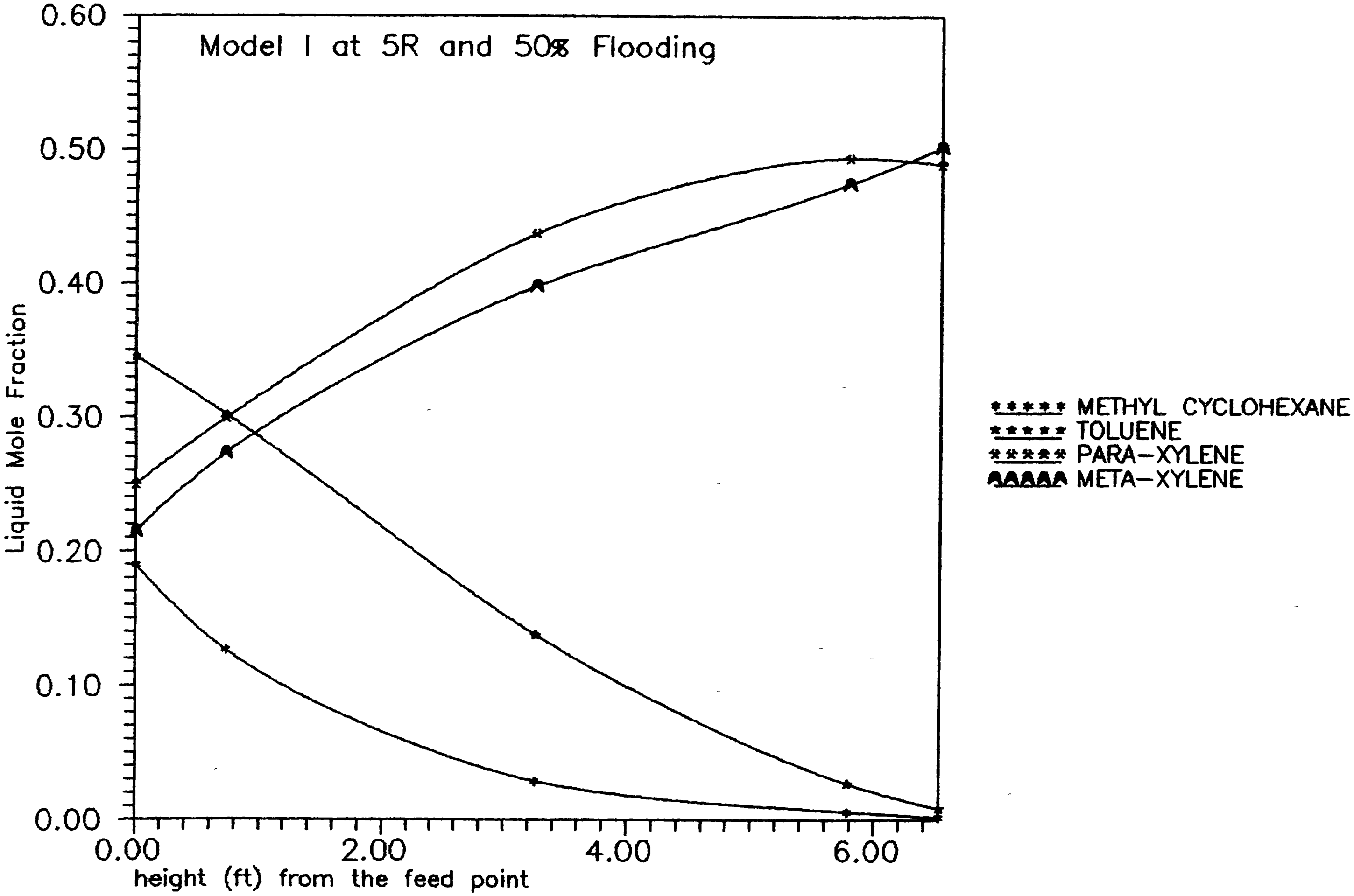

Figure 4. Liquid Composition Profile in the Stripping Section

key component compositions matched the specifications. The result for 50% flooding and a reflux ratio of 5 is as shown in the table below:

TABLE 3

CASE 1 RESULTS

Method	Height (ft.)
Finite difference (Rosenberg)	12.90
Analog (Brown)	13.50
Collocation (our simulation)	13.04
HETP (our simulation)	13.60
HETP (Brown)	13.90

Case II

The distillation problem was solved using MAXISIM. Short cut distillation was carried out to determine minimum reflux/stages. A more detailed tray by tray calculation was also performed and the results are included.

A look at the liquid and vapor flowrates indicate that the assumption of constant molal overflow was quite good for this problem (as shown in figure 5.). However, since this situation will not apply to all systems a more general

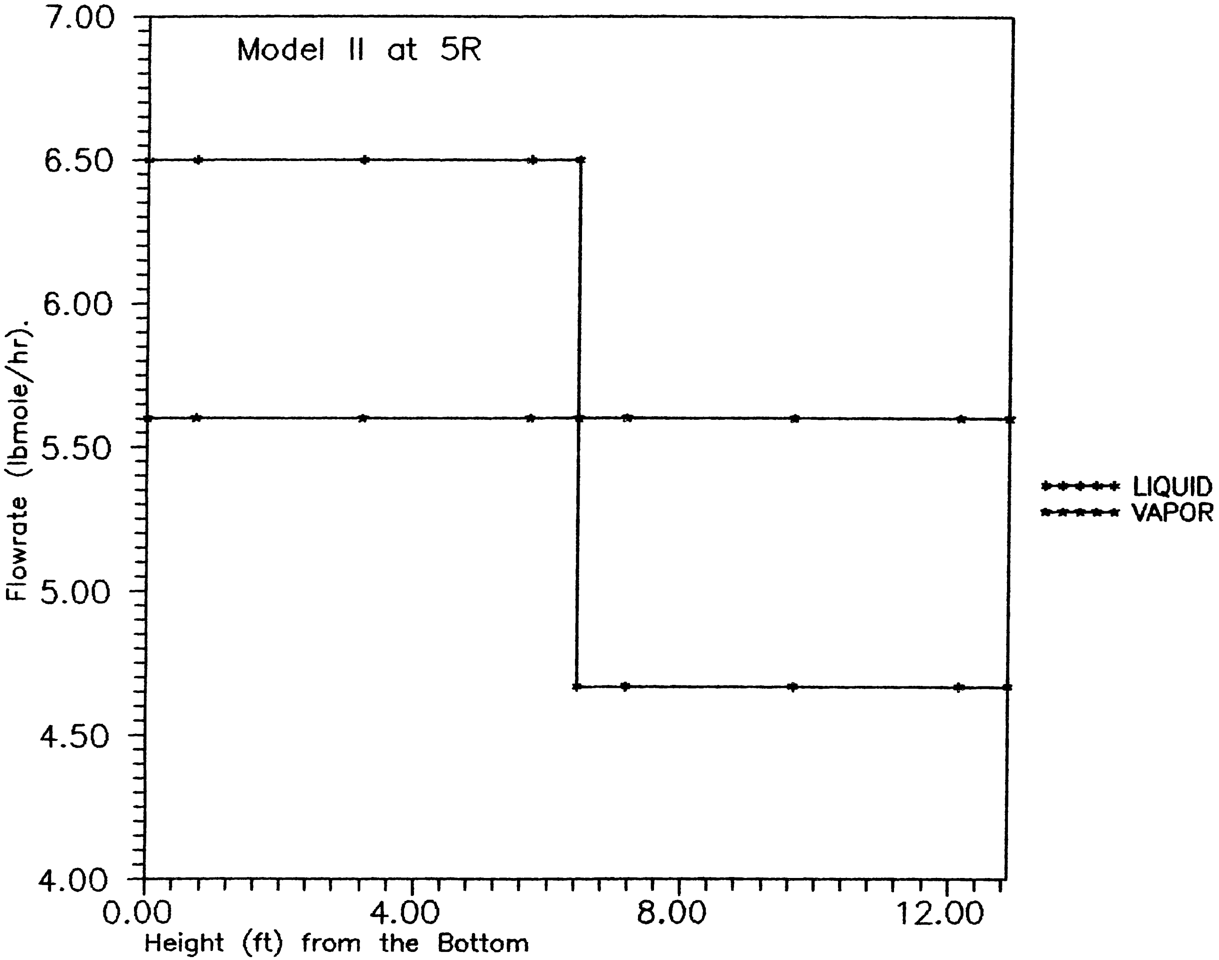

Figure 5. Liquid and Vapor Flowrates

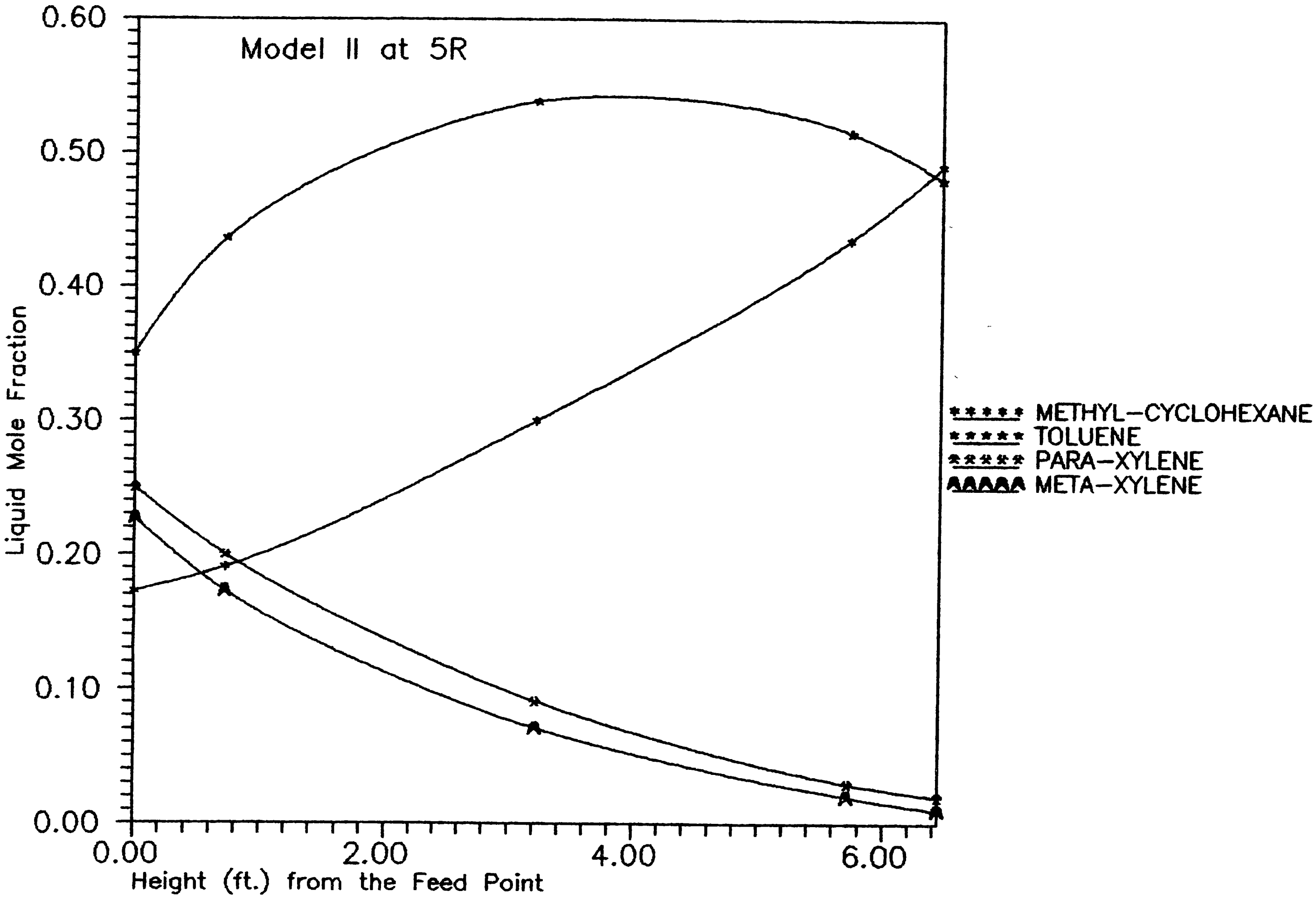

Figure 6. Liquid Composition Profile
(Enriching Section)

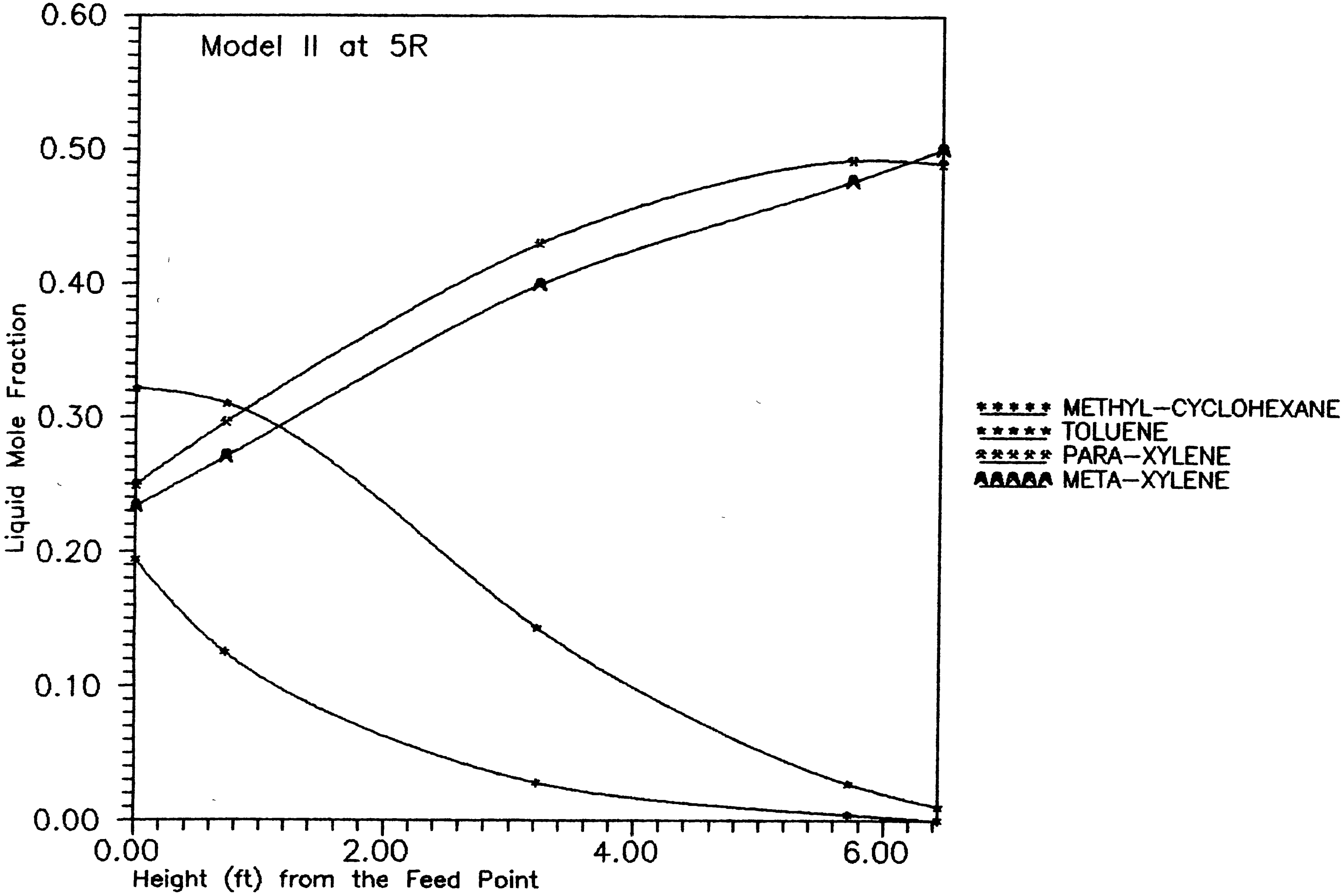

Figure 7. Liquid Composition Profile
(Stripping Section)

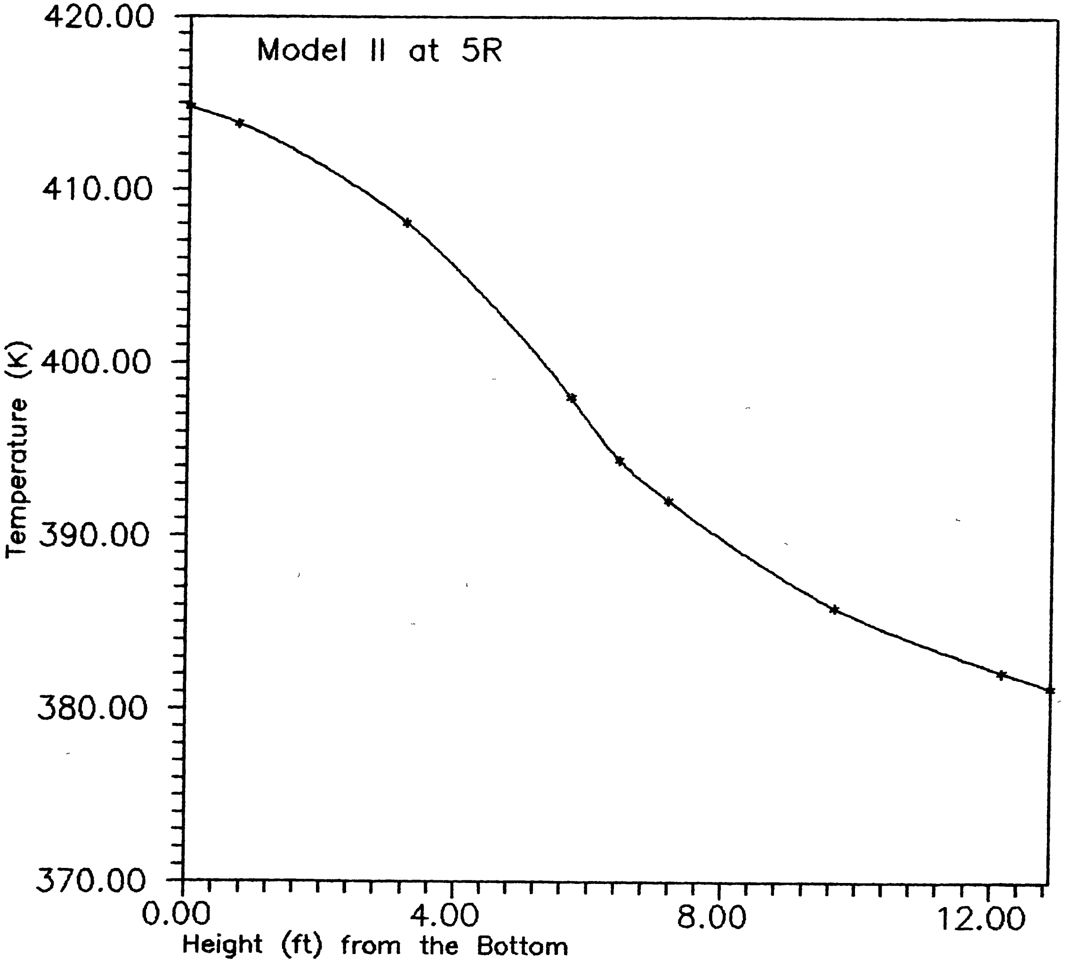

Figure 8. Temperature Profile

model (such as model II) is required.

Model II was able to simulate the behavior of the distillation column accurately. The liquid and vapor composition profiles (as shown by figures 6 and 7) cannot be compared directly because the packed column is a continuous contacting device as opposed to the staged approach of tray by tray distillation. It is clear however that the profiles are similar. The temperature profile (see figure 8) predicted by the two simulators differ slightly and this may be attributed to differences in data, equations of state and convergence techniques.

We have been able to improve our simulation (at 50% flooding) results, these are as shown below:

TABLE 4

CASE II RESULTS

Method	Height (ft.)
Finite difference (Rosenberg)	12.90
Collocation (our simulation)	12.88

Case III

The same system was studied at a reflux ratio of two. The system was first simulated using MAXISIM for short cut and tray by tray distillation. These results are included in appendix C.

The liquid composition profiles (see figure 9) in the stripping section agree with Rosenberg's very well. The enriching section profiles deviate by approximately 10% (see figure 10) from Rosenberg's solution. The height of the column was found to be shorter than Rosenberg's by 0.52 ft. HETP estimates were very good. The liquid and vapor flowrates in the two sections agree with the MAXISIM results when approximated to the first decimal place. The flowrates in the enriching section (see figure 11) vary at the second and third decimal places. This may be attributed to numerical errors or convergence to the wrong root.

Results from case III prove that Newton's method can sometimes yield ambiguous results especially when simulating a system of isomers (which are difficult to simulate). Case III results were obtained under assumptions of constant relative volatilities.

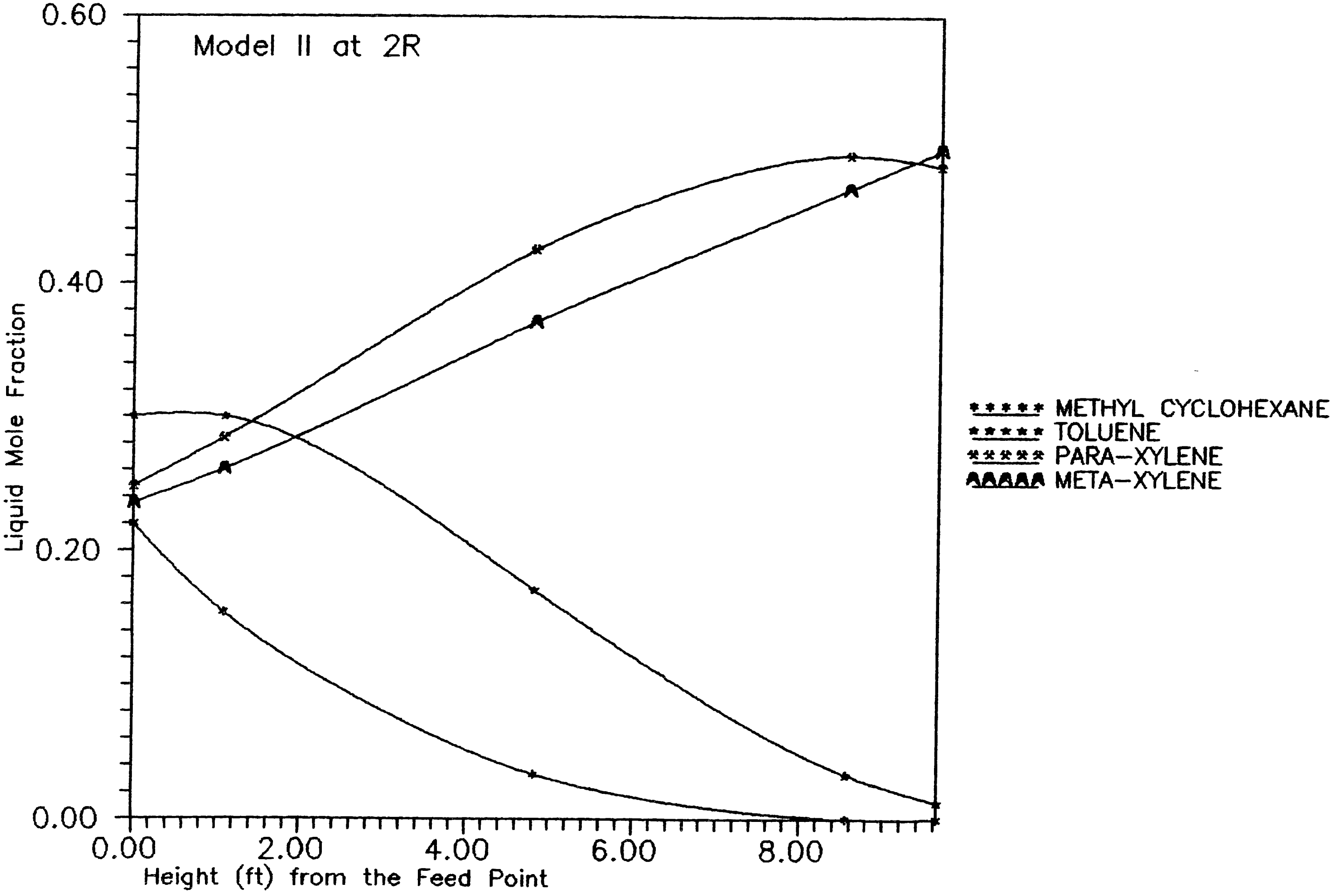

Figure 9. Liquid Composition Profile in the Stripping Section

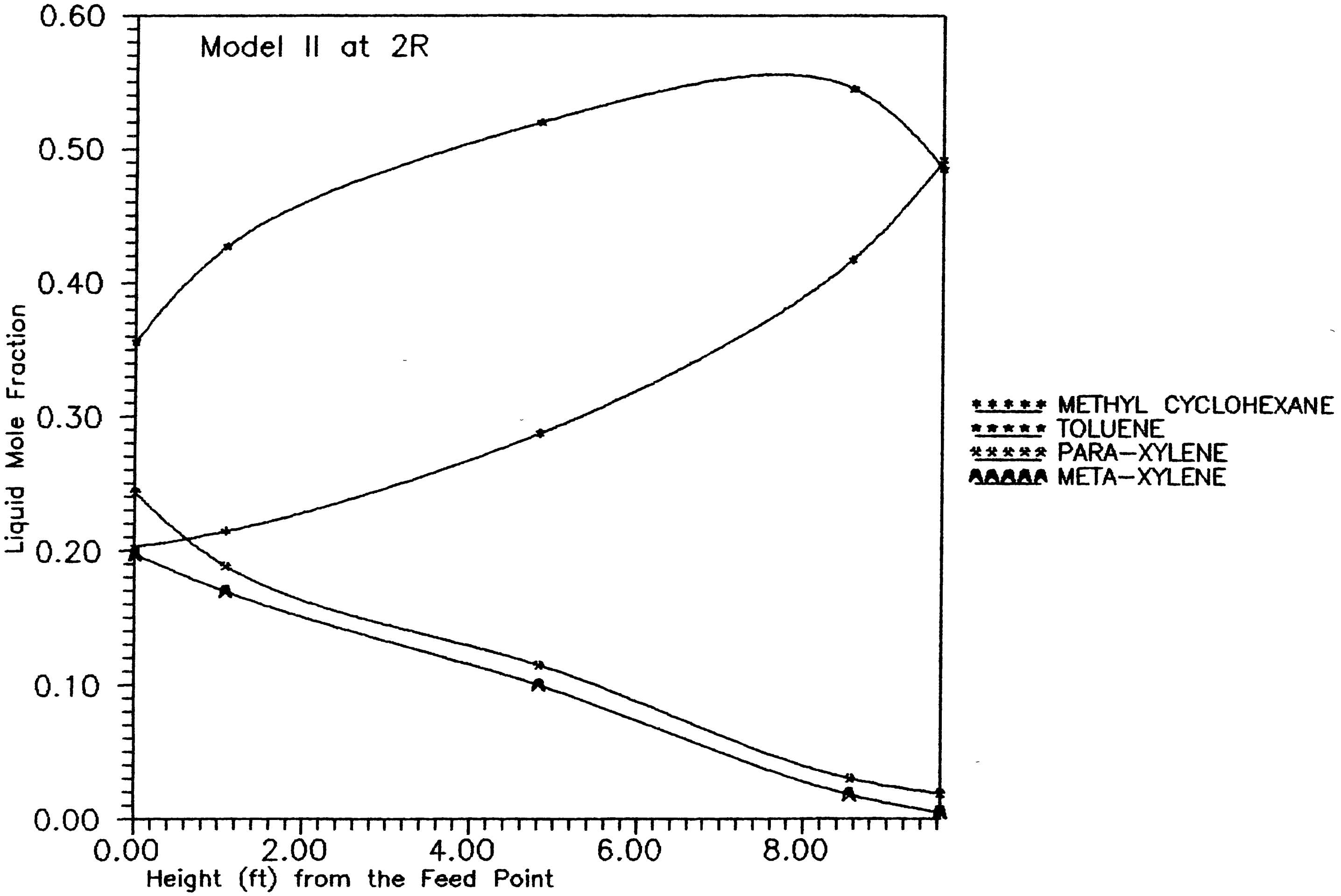

Figure 10. Liquid Composition Profile in the Enriching Section

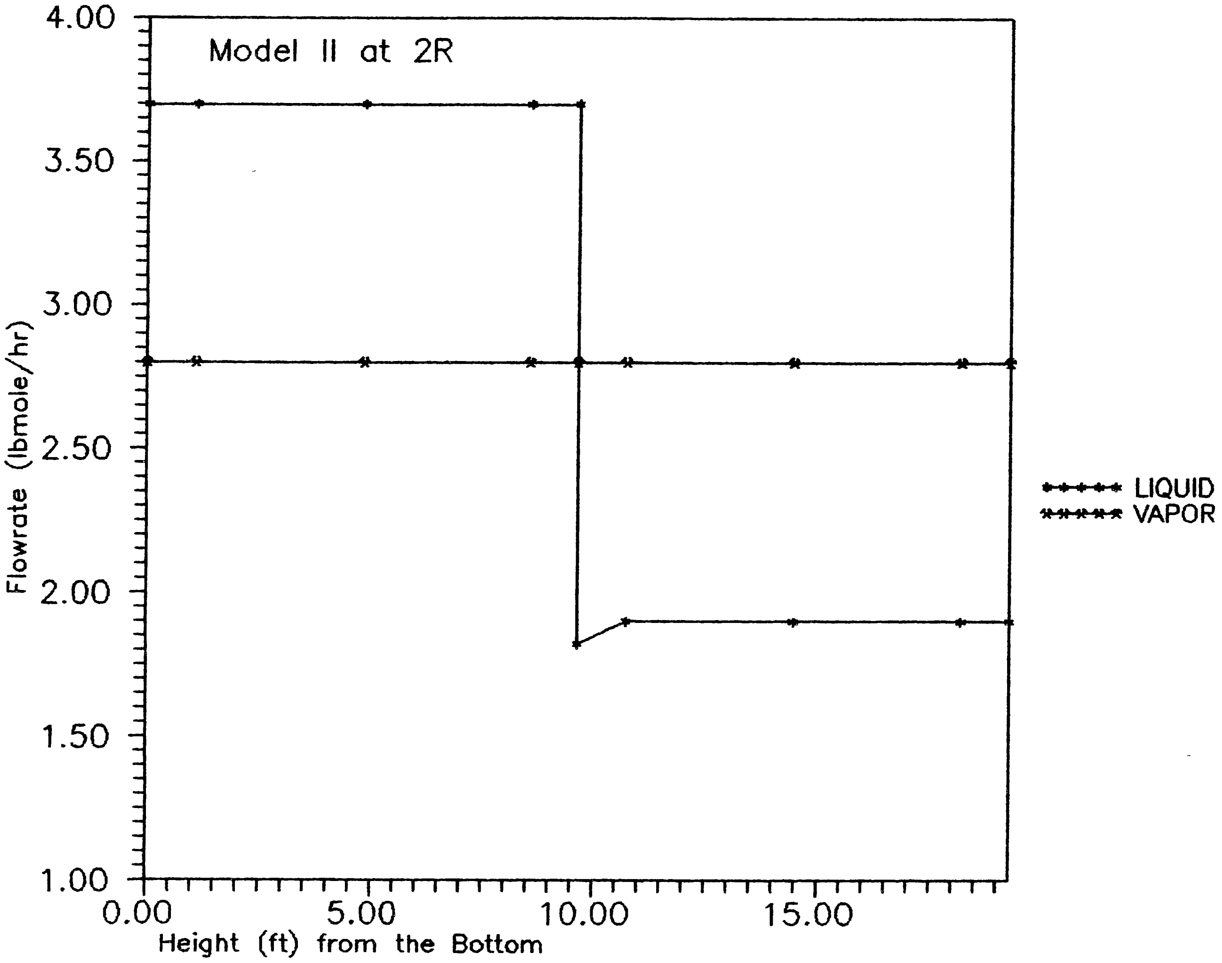

Figure 11. Liquid and Vapor Flowrates

TABLE 5

CASE III RESULTS

Method	Height (ft)
Finite Difference (Rosenberg)	19.80
Analog (Brown)	20.30
HETP (Brown)	21.80
HETP (Our Simulation)	20.52
Collocation (Our Simulation)	19.28

Convergence Techniques

The collocation method reduces the set of PDE's to nonlinear algebraic equations under steady state assumption. The numerical technique applied to solve this problem is the Levenberg-Marquardt algorithm which is a variation of Newton's method. This algorithm, although quite robust, shares many of the disadvantages associated with the Newton's method. Convergence to the right solution may require many simulations and a lot of patience.

The number of nonlinear algebraic equations to be solved for a four component distillation problem using three point collocation are eighty. When simulated under assumptions of constant relative volatilities the time required is 30 seconds for each section. When the VLE is carried out using bubble point temperature calculations the simulation time is eight minutes for the enriching section and ten minutes for the stripping section. The finite difference method used by Rosenberg and Hadi (1980) requires 50 grid points and 8 minutes of CPU time on a DEC 20 machine to simulate the same system under the assumption of constant relative volatilities.

The initial guesses are critical in determining a successful simulation. It is quite possible to converge to a wrong solution if there is a slight change in some initial guesses.

Again, the suggestions for a successful simulation are a good knowledge of the behavior of the system, accurate data and a lot of patience.

CHAPTER VI

CONCLUSION AND RECOMMENDATION

The simulation program developed for this study carries out both HETP calculation and solves the column as a continuous contacting device. The kind of problem handled is essentially a design problem which requires the determination of height and diameter.

The height equivalent of a theoretical plate may be calculated for those types of packings which are presented in appendix A. The HETP is calculated at various points along the column. The success of the simulation depends heavily on the accuracy of the thermodynamic correlations being used. We have made every attempt to use the best correlations available in the literature. It is true however that these correlations are not always accurate.

The prediction of water density from the Ely and Hanley correlation is not reliable. This may be expected since the reference fluid used is methane and the behavior of non hydrocarbons cannot be effectively predicted. An estimate of the water density may be input if the results are suspect. The viscosity prediction has its own pitfalls. The determination of viscosity near the two phase region is unreliable. The instructions provided in chapter 3 must be followed.

The vapor liquid equilibrium calculations are generally reliable but convergence is not always guaranteed because the algorithm used is not very robust. This will vary from system to system.

Our results indicate that despite some large errors attributed to the physical properties package (viscosity 10%, diffusivity 10-20% etc.) it is possible to obtain very good (somewhat conservative) estimates of the HETP.

The other part of the simulator involves a very detailed simulation of a packed distillation column modeled as a continuous contacting device. The Levenberg-Marquardt method (a variation of the Newton method) is extremely sensitive to initial guesses. A study of the behavior of the system using MAXISIM is advised before any attempt is made to simulate it . The mass transfer correlation used may be improved by using better correlations from the literature. The simulation should be carried out using constant relative volatilities first, since the computation time is low. There is a possibility that VLE calculations will fail to converge even though the simulation was successful at constant relative volatility. The suggested procedure to achieve a convergence is to experiment with the allowed error limit.

The orthogonal collocation technique is more economical in terms of memory allocation and computation times as compared to the finite difference scheme. This is because the number of collocation points required to approximate a continuous system is much less than the number of grid points required by the finite difference method. The assumptions made in model I are valid for the simulation of a system of isomers since nearly constant molal overflow exists in such systems. Both models have been tested with data from a system of isomers and we have obtained more accurate results with model II. It is recommended that model II be used for simulation of isomeric systems. Model II may be completely validated only after testing it with systems which do not contain isomers. However, at this time lack of data makes it impossible for us to do this.

Based on the problems encountered and lessons learned during the execution of this project the following are a list of recommendations :

1) The improvement of physical properties prediction methods will improve the estimates of HETP.
2) Improved mass transfer correlations should be used to accurately simulate the behavior of the column.
3) The liquid phase resistance to mass transfer must be incorporated into future models.
4) The bulk vapor and liquid temperatures should be predicted instead of just the interface temperatures.

5) A better numerical technique must be researched to avoid the drawbacks associated with Newton's method.

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APPENDIXES

APPENDIX A

PACKING AND COMPONENT ID

TABLE 6

PACKING ID NUMBERS

PACKING ID	PACKING (TYPE, SIZE, WALL)
1	RASCHIG RINGS (METAL,1/32",5/8")
* 2	RASCHIG RINGS (METAL,1/16",1/2")
3	RASCHIG RINGS (METAL,1/16",5/8")
4	RASCHIG RINGS (METAL,1/16",3/4")
* 5	RASCHIG RINGS (METAL,1/16",1")
* 6	RASCHIG RINGS (METAL,1/16",1.5")
* 7	RASCHIG RINGS (METAL,1/16",2")
* 8	RASCHIG RINGS (CERAMIC,1/2")
9	RASCHIG RINGS (CERAMIC,5/8")
10	RASCHIG RINGS (CERAMIC,3/4")
* 11	RASCHIG RINGS (CERAMIC,1")
* 12	RASCHIG RINGS (CERAMIC,1.5")
* 13	RASCHIG RINGS (CERAMIC,2")
14	RASCHIG RINGS (CERAMIC,3")
15	PALL RINGS (PLASTIC,1")
16	PALL RINGS (PLASTIC,2")
17	PALL RINGS (METAL,5/8")
* 18	PALL RINGS (METAL,1")
* 19	PALL RINGS (METAL,1.5")
* 20	PALL RINGS (METAL,2")
* 21	BERL SADDLES (CERAMIC,1/2")

TABLE 6 (Continued)

PACKING ID	PACKING (TYPE, WALL, SIZE)
22	BERL SADDLES (CERAMIC,3/4")
* 23	BERL SADDLES (CERAMIC,1")
* 24	BERL SADDLES (CERAMIC,1.5")
25	BERL SADDLES (CERAMIC,2")
26	INTALOX SADDLES (CERAMIC,1/2’)
27	INTALOX SADDLES (CERAMIC,3/4")
28	INTALOX SADDLES (CERAMIC,1")
29	INTALOX SADDLES (CERAMIC,1.5")
30	INTALOX SADDLES (CERAMIC,2")

* These may be used to calculate HETP.

TABLE 7

COMPONENT ID NUMBERS

COMPONENT ID	COMPONENT NAME
1	Hydrogen
2	Methane
3	Ethane
4	Propane
5	Iso-Butane
6	N-Butane
7	Iso-Pentane
8	N-Pentane
9	Neo-Pentane
10	N-Hexane
11	N-Heptane
12	N-Octane
13	N-Nonane
14	N-Decane
15	N-Undercane
16	N-Dodecane
17	N-Tridecane
18	N-tetradecane
19	N-Pentadecane
20	N-Hexadecane
21	N-Heptadecane
22	Ethylene

TABLE 7 (Continued)

COMPONENT ID	COMPONENT NAME
23	Propylene
24	1-Butene
25	Cis-2-Butene
26	Trans-2-Butene
27	Iso-Butene
28	1,3 Butadiene
29	1-Pentene
30	Cis-2-Pentene
31	Trans-2-Pentene
32	2-Methyl-1-Butene
33	3-Methyl-1-Butene
34	2-Methyl-2-Butene
35	1-Hexene
36	Cyclopentane
37	Methylcyclopentane
38	Cyclohexane
39	Methylcyclohexane
40	Benzene
41	Toluene
42	O-Xylene
43	M-Xylene
44	P-Xylene
45	Ethylbenzene

TABLE 7 (Continued)

COMPONENT ID	COMPONENT NAME
46	Nitrogen
47	Oxygen
48	Carbon Monoxide
49	Carbon Dioxide
50	Hydrogen Sulfide
51	Sulfur Dioxide
52	2-Methyl-Pentane
53	3-Methyl-Pentane
54	2,2 Dimethyl-Butane
55	2,3 Dimethyl-Butane
56	1-Heptene
57	Propadiene
58	1,2 Butadiene
59	Ethylcyclopentane
60	Ethylcyclohexane
61	Water

APPENDIX B

SELECTED FLOWCHARTS

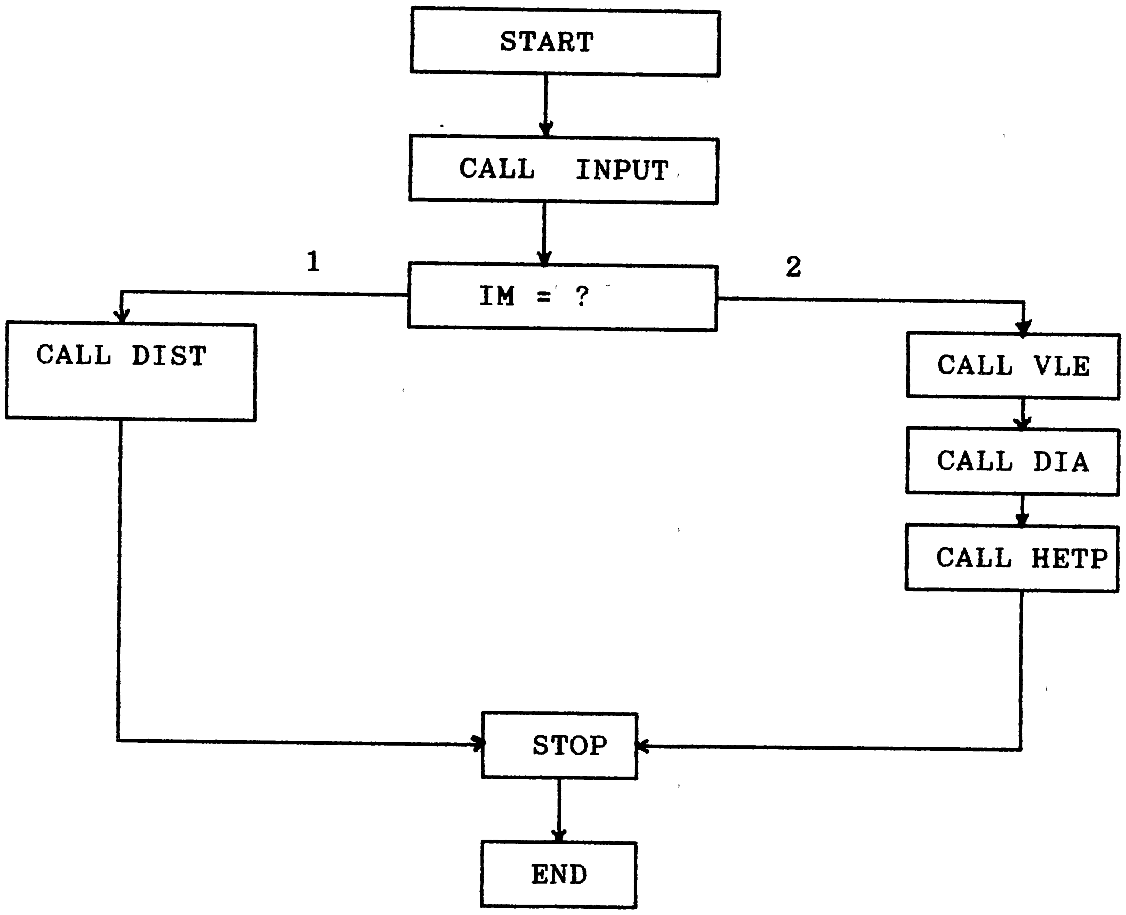

Figure 12. Main program flowchart.

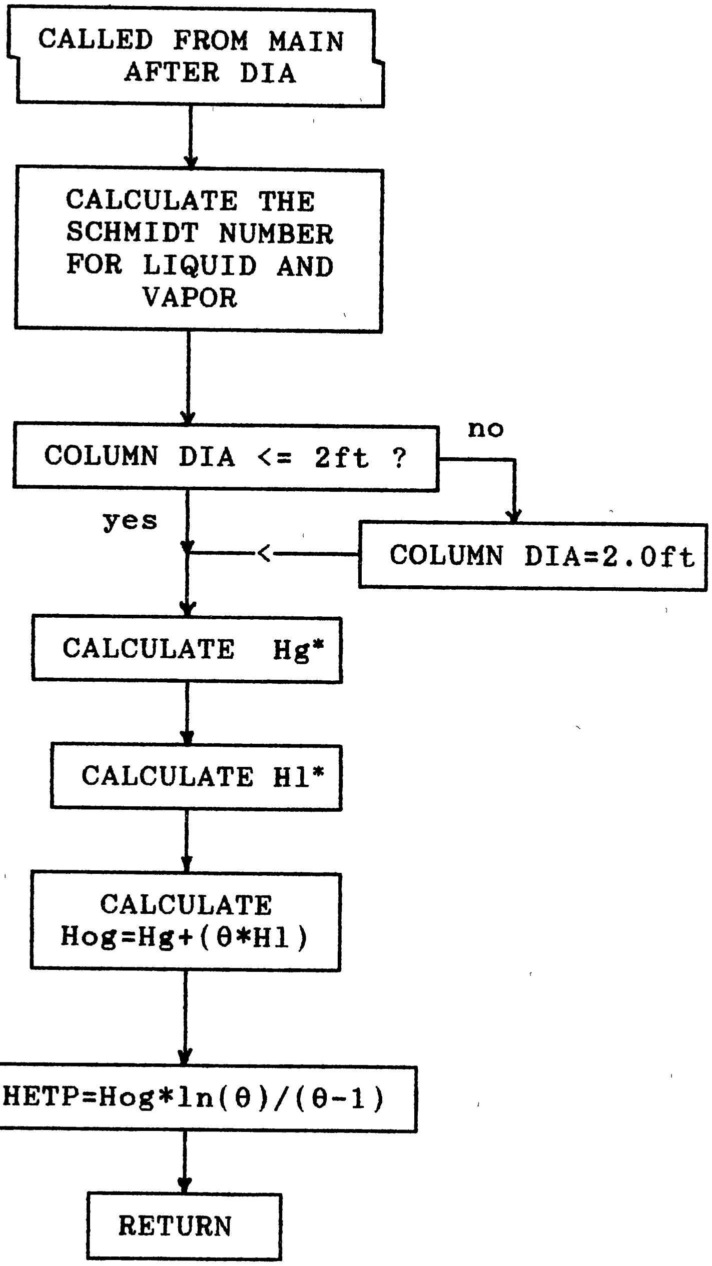

Figure 13. Subroutine HETP.

---

* Correlation of Bolles and Fair.

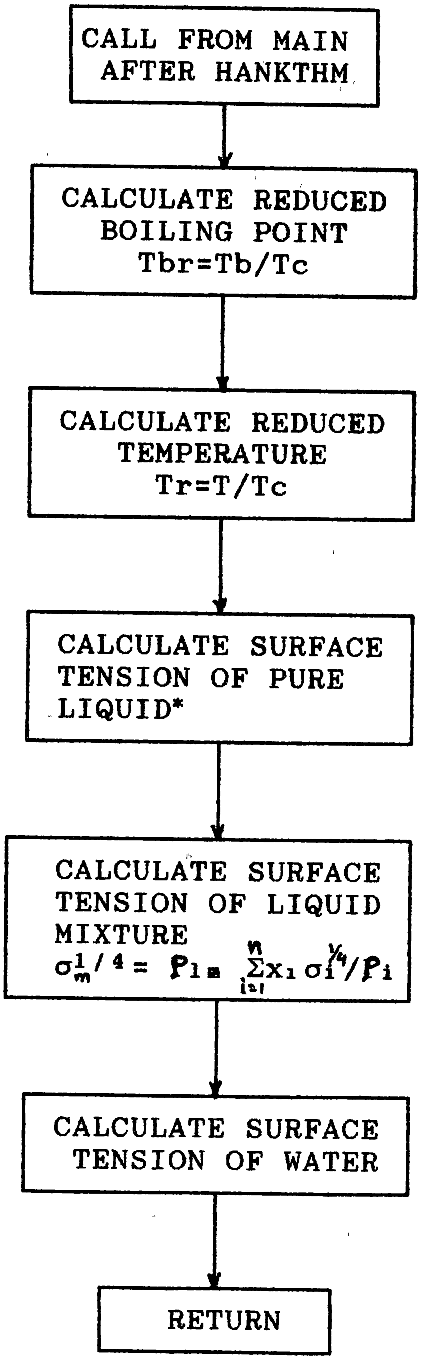

Figure 14. Subroutine SRFTN.

* Correlation of Brock and Bird.

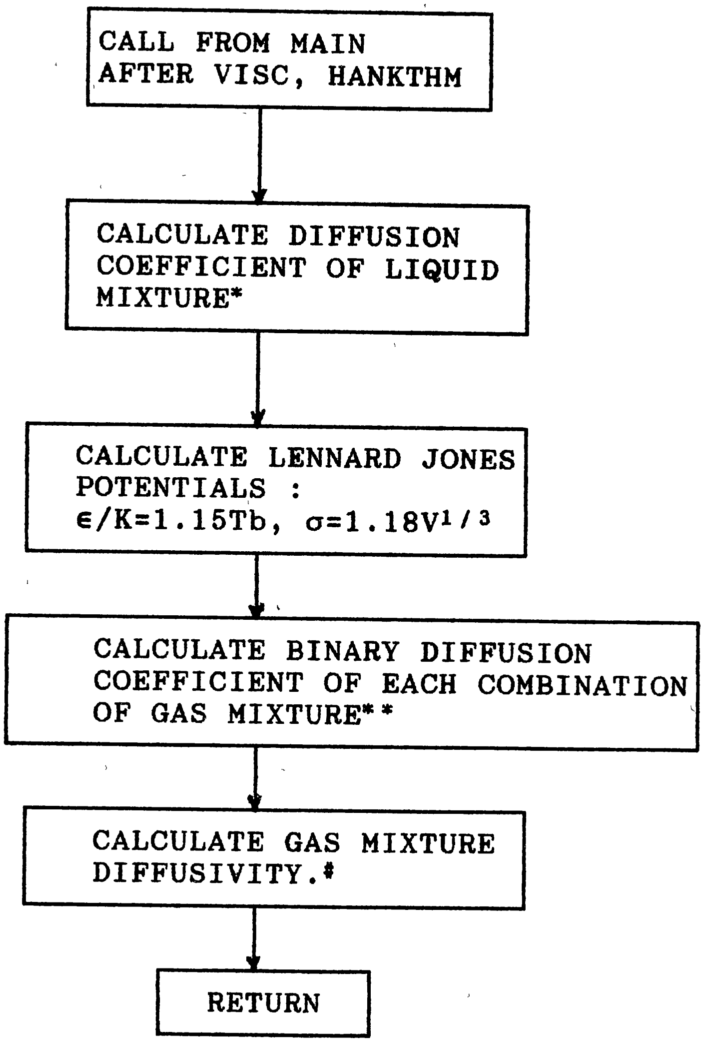

Figure 15. Subroutine DIFF.

* Modified Wilke-Chang equation.
** Wilke-Lee equation for binaries
\# Simplified Stefan-Maxwell equation

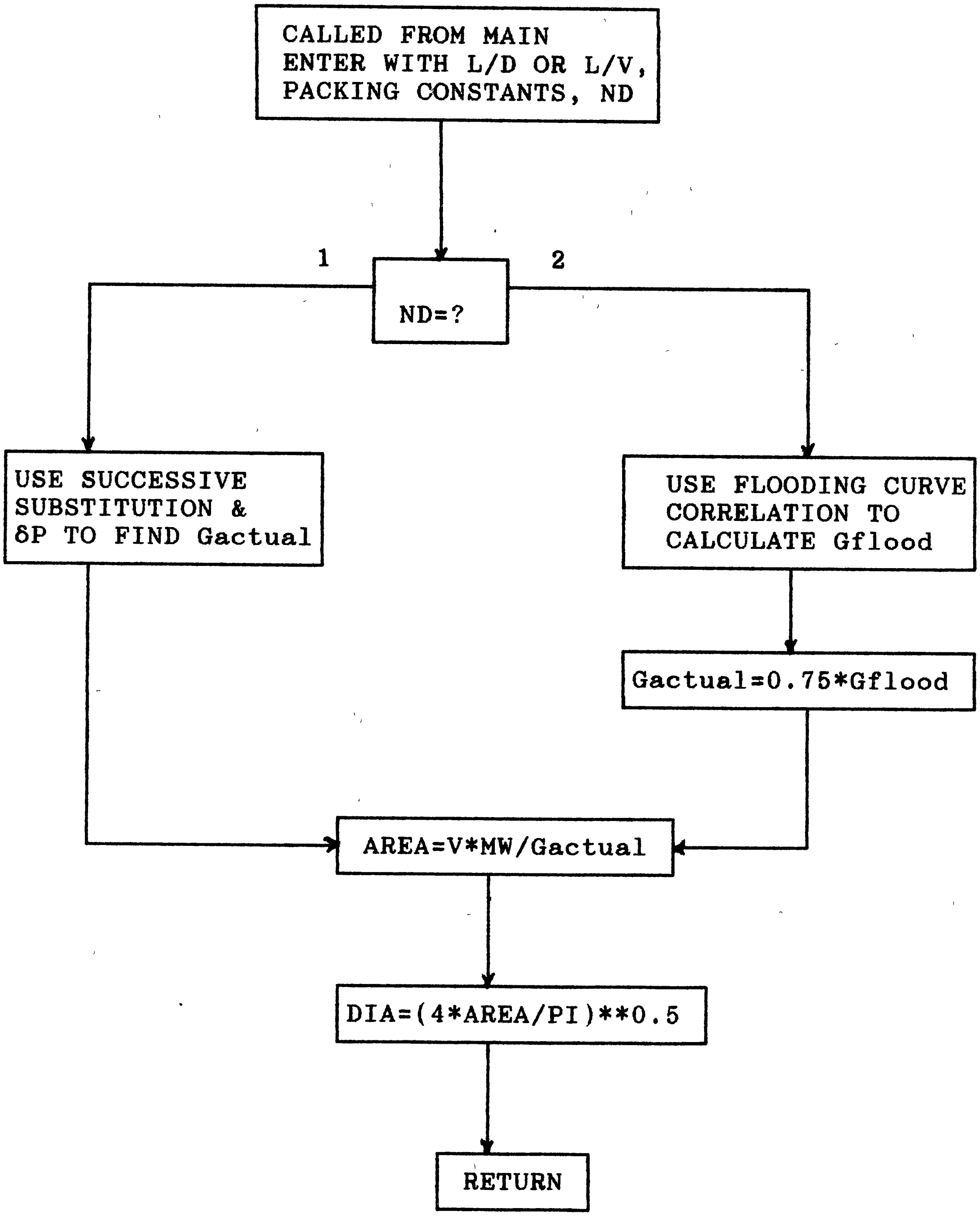

Figure 16. Subroutine DIA.

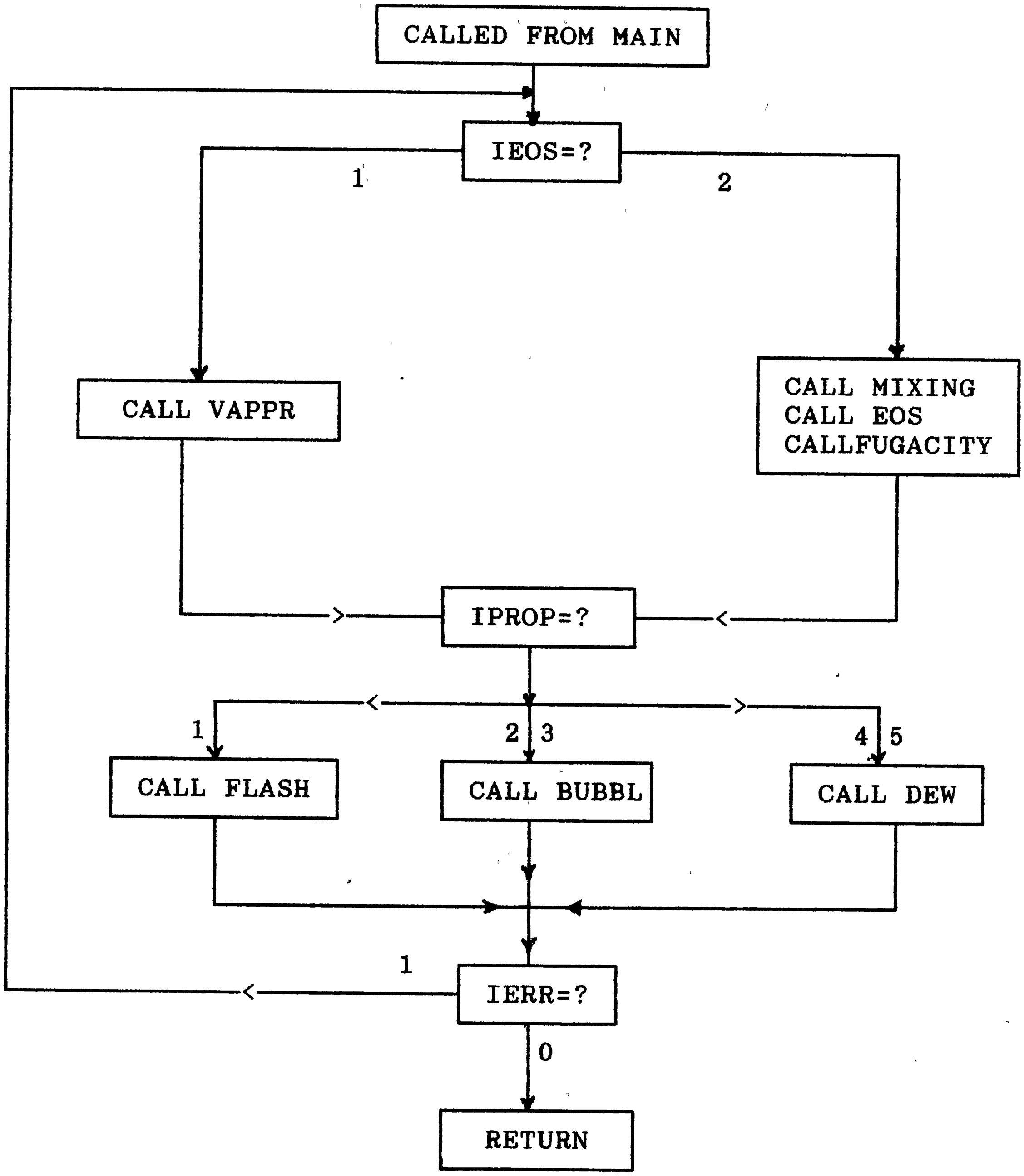

Figure 17. Subroutine VLE.

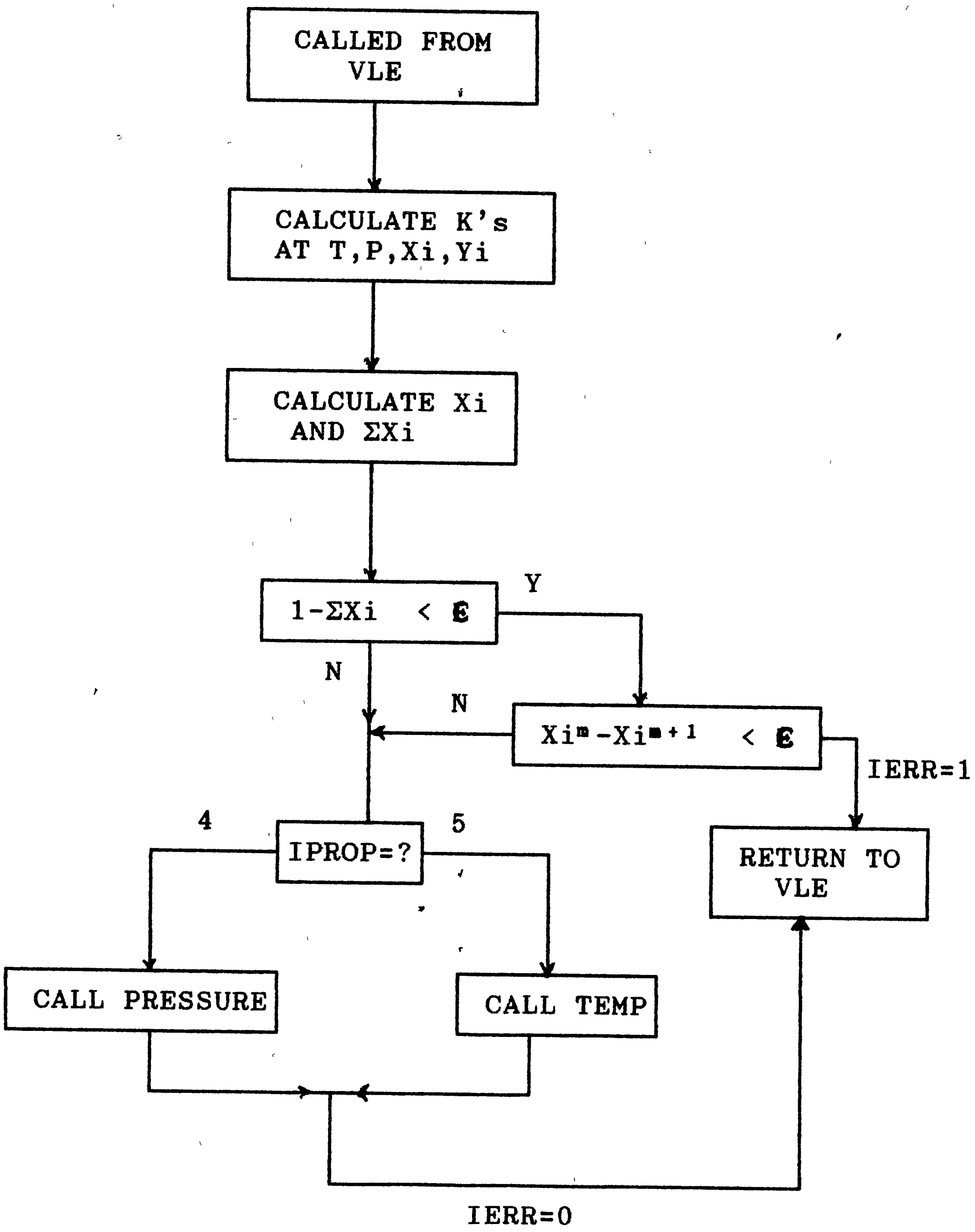

Figure 18. Subroutine DEW.

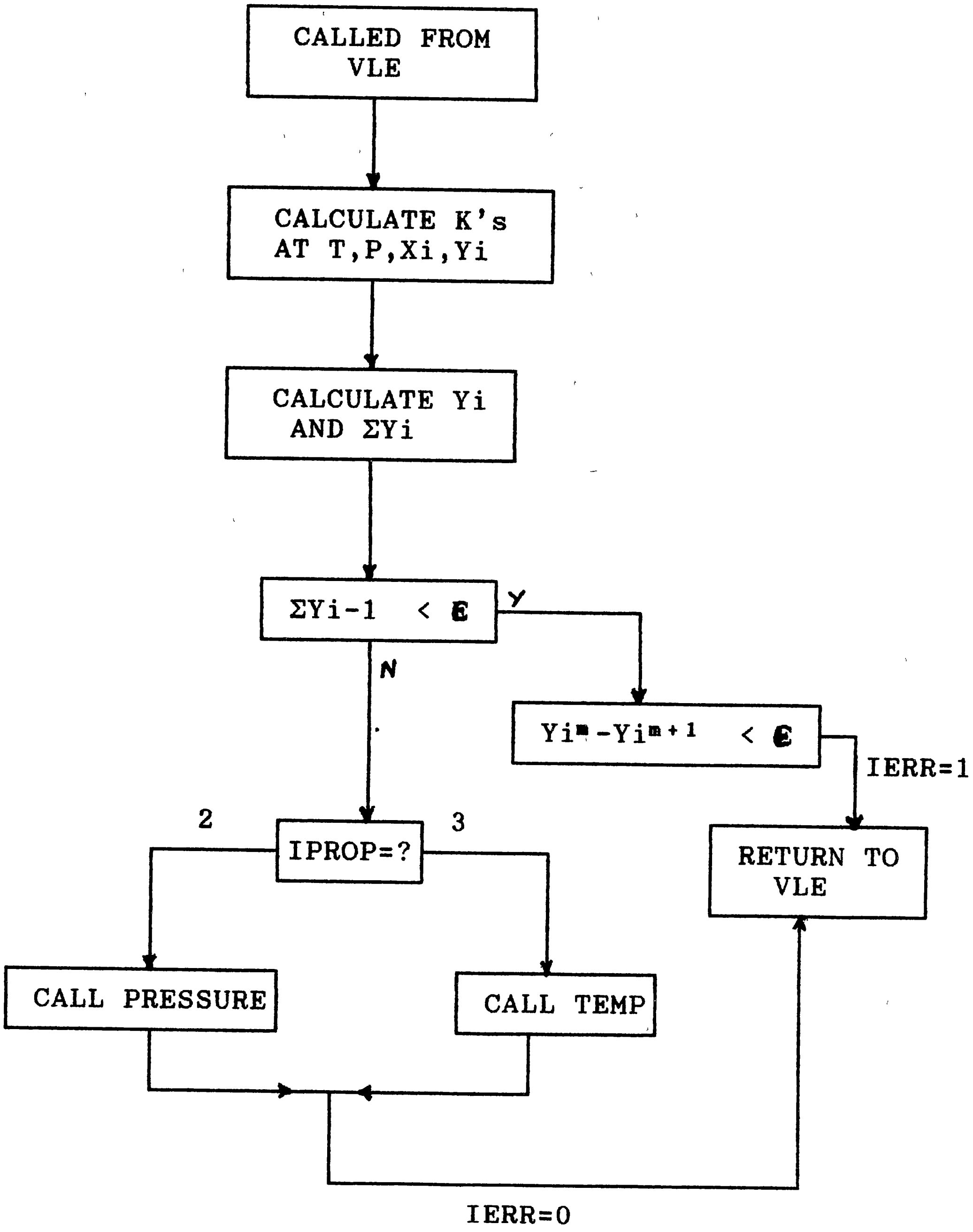

Figure 19. Subroutine BUBBLE.

APPENDIX C

SIMULATION RESULTS

DISTILLATION PROBLEM

COMPONENT	FEED	DISTILLATE	BOTTOMS
MT-CYC	0.4575	0.4574	0.0001
C7H8	0.4575	0.4484	0.0091
P-XYLENE	0.4575	0.0187	0.4388
M-XYLENE	0.4575	0.0092	0.4483
	1.8300	0.9337	0.8963

MODEL I AT 5R

ENRICHING SECTION RESULTS

LIQUID COMPOSITION PROFILE

HT(ft)	MT-CYC	TOLUENE	P-XYLENE	M-XYLENE
.0000	.1764	.3494	.2480	.2258
.7348	.1979	.4289	.1973	.1721
3.2600	.3045	.5370	.0926	.0713
5.7852	.4408	.5031	.0278	.0199
6.5200	.4967	.4743	.0203	.0104

TEMPERATURE(K),PRESSURE(BAR) AND FLOWRATES(lbm/hr)

HT(ft)	TEMP	PRESS	LIQUID	VAPOR
.0000	394.4000	1.0300	4.6685	5.6022
.7348	391.3402	1.0300	4.6685	5.6022
3.2600	385.5131	1.0300	4.6685	5.6022
5.7852	381.9526	1.0300	4.6685	5.6022
6.5200	380.3433	1.0300	4.6685	5.6022

MODEL II AT 5R

ENRICHING SECTION RESULTS

LIQUID COMPOSITION PROFILE

HT(ft)	MT-CYC	TOLUENE	P-XYLENE	M-XYLENE
.0000	.1727	.3501	.2500	.2273
.7258	.1910	.4360	.2001	.1730
3.2200	.2999	.5381	.0910	.0711
5.7142	.4350	.5152	.0298	.0201
6.4400	.4899	.4802	.0199	.0099

TEMPERATURE(K),PRESSURE(BAR) AND FLOWRATES(lbm/hr)

HT(ft)	TEMP	PRESS	LIQUID	VAPOR
.0000	394.4000	1.0300	4.6685	5.6022
.7258	392.0402	1.0300	4.6685	5.6022
3.2200	385.8931	1.0300	4.6685	5.6022
5.7142	382.1726	1.0300	4.6685	5.6022
6.4400	381.2433	1.0300	4.6685	5.6022

MODEL II AT 5R

STRIPPING SECTION RESULTS

LIQUID COMPOSITION PROFILE

HT(ft)	MT-CYC	TOLUENE	P-XYLENE	M-XYLENE
.0000	.1945	.3218	.2500	.2337
.7258	.1250	.3103	.2966	.2708
3.2200	.0281	.1436	.4296	.3988
5.7142	.0042	.0273	.4921	.4764
6.4400	.0001	.0102	.4896	.5001

TEMPERATURE(K),PRESSURE(BAR) AND FLOWRATES(lbm/hr)

HT(ft)	TEMP	PRESS	LIQUID	VAPOR
.0000	394.4000	1.0300	6.4985	5.6022
.7258	397.9900	1.0300	6.4985	5.6022
3.2200	408.0774	1.0300	6.4985	5.6022
5.7142	413.8100	1.0300	6.4985	5.6022
6.4400	414.7600	1.0300	6.4985	5.6022

MODEL II AT 2R

ENRICHING SECTION RESULTS

LIQUID COMPOSITION PROFILE

HT(ft)	MT-CYC	TOLUENE	P-XYLENE	M-XYLENE
.0000	.2029	.3559	.2437	.1974
1.0864	.2146	.4269	.1885	.1694
4.8200	.2875	.4979	.1148	.0998
8.5536	.4169	.5448	.0197	.0180
9.6400	.4915	.4852	.0189	.0046

TEMPERATURE(K),PRESSURE(BAR) AND FLOWRATES(lbm/hr)

HT(ft)	TEMP	PRESS	LIQUID	VAPOR
.0000	394.4000	1.0300	1.8213	2.7550
1.0864	391.7958	1.0300	1.8689	2.8026
4.8200	387.5215	1.0300	1.9130	2.8467
8.5536	382.3276	1.0300	1.9622	2.8959
9.6400	380.2803	1.0300	1.8674	2.8011

MODEL II AT 2R

STRIPPING SECTION RESULTS

LIQUID COMPOSITION PROFILE

HT(ft)	MT-CYC	TOLUENE	P-XYLENE	M-XYLENE
.0000	.2202	.3005	.2483	.2358
1.0864	.1541	.3002	.2845	.2612
4.8200	.0333	.1708	.4250	.3709
8.5536	.0002	.0333	.4958	.4707
9.6400	.0001	.0125	.4875	.4999

TEMPERATURE(K),PRESSURE(BAR) AND FLOWRATES(lbm/hr)

HT(ft)	TEMP	PRESS	LIQUID	VAPOR
.0000	394.4000	1.0300	3.6974	2.8011
1.0864	397.0757	1.0300	3.6974	2.8011
4.8200	406.8456	1.0300	3.6974	2.8011
8.5536	413.8136	1.0300	3.6974	2.8011
9.6400	414.6676	1.0300	3.6974	2.8011

HETP and DIAMETER at 5R

(ft)	ENRICHING SEC.	STRIPPING SEC.
50% Flood:		
HETP	2.0449	2.0636
Diameter	1.0389	1.1216
P=0.5"H_2O/ft:		
HETP	1.9168	2.4826
Diameter	1.5352	1.5822
P=0.7"H_2O/ft:		
HETP	1.6451	2.0552
Diameter	1.4189	1.4639

HETP and DIAMETER at 2R

(ft)	ENRICHING SEC.	STRIPPING SEC.
50% Flood:		
HETP	1.7200	1.0158
Diameter	0.6442	0.7121
P=0.5"H_2O/ft:		
HETP	1.0727	0.7705
Diameter	0.6889	0.6980
P=0.7"H_2O/ft:		
HETP	0.9559	0.6377
Diameter	0.6366	0.6451

```
SCI MAXI*SIM     JOB ID:333
VERSION #2.2     DATE:  22-JUN-1991
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FENSKE-UNDERWOOD-ERBAR-MADDOX : SHORTCUT DIST.


DIST #  3
  LIGHT KEY IS COMP NO  2 AND (D/B)LK =      49.27
  HEAVY KEY IS COMP NO  3 AND (B/D)HK =      23.47
  CONDENSER TYPE(1=TOT,2=PART) =     1.0
  SPEC CONDENSER PRESSURE      =    14.70 PSIA
  SPEC REBOILER  PRESSURE      =    14.70 PSIA
  ESTM CONDENSER TEMP          =   210.00 DEG F
  ESTM REBOILER  TEMP          =   290.00 DEG F
```

```
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FENSKE-UNDERWOOD-ERBAR-MADDOX : SHORTCUT DIST.


UNIT OPERATION NO  3 IS A DIST UNIT***ROSENBERG

          FEEDS>>>>>>>PRODUCTS>>>>>>>>>>>>>>>
STREAM FLOW RATES ARE LB-MOLS
STREAM NO          1           2           3
  NAME           FEED        DIST        BOTT
COMPONENT
MTCYC-C6          0.4575      0.4566      0.0009
C7H8              0.4575      0.4484      0.0091
P-X               0.4575      0.0187      0.4388
M-X               0.4575      0.0154      0.4421

  TOTAL           1.8300      0.9391      0.8909

T,DEG F         245.58      222.60      280.92
P,PSIA           14.70       14.70       14.70
H,KBTU           -0.50       -0.75        0.87
S,KBTU/R          0.1330      0.0638      0.0679
MOL WEIGHT      100.6655     95.5882    106.0173
D,LB/FT3         46.7058     45.9154     46.9538
L/F(MOLAR)        1.00000     1.00000     1.00000


MINIMUM NUMBER OF STAGES =       9.51
MINIMUM REFLUX RATE      =       1.20 LB-MOLS


 NO STAGES  REFLUX   CONDENSER  REBOILER FEED TRAY
 IN COLUMN   RATE      DUTY       DUTY    REBOILER
 (INC REB)  LB-MOLS  10E3KBTU   10E3KBTU  =TRAY 1
   47.54      1.22     0.031      0.031     27.1
   31.69      1.27     0.031      0.032     18.1
   23.77      1.36     0.033      0.033     13.5
   19.01      1.54     0.035      0.036     10.8
   15.85      1.87     0.040      0.040      9.0
```

```
SCI MAXI*SIM     JOB ID:333
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ROSENBERG TEST DISTILLATION



DTXT #  9
   COUNT PLATES FROM BOTTOM UP
   NUMBER OF PLATES IN COLUMN        11
   NUMBER OF FEED PLATES              1
   NUMBER OF PRODUCTS                 2
   NUMBER OF SIDE COOLERS/HEATERS     0

    FEED    STREAM  FEED
     NO       NO    PLATE
      1        1      6

   PRODUCT STREAM  DRAW    DRAW
     NO      NO    PLATE   RATE
      1       2     12     ******
      2       3      0     ******

   CONDENSER TYPE-TOTL
   REBOILER TYPE -PART

   CONDENSER/DISTILLATE SPECIFICATIONS-
     MOL FRACT   0.02000 FOR P-X

   REBOILER/BOTTOMS SPECIFICATIONS-
     MOL FRACT   0.01000 FOR C7H8

   COLUMN PRESSURES & ESTIMATED TEMPERATURES
                   P(PSIA)   T(DEG F)
     CONDENSER      14.70    223.97
     TOP PLATE      14.70
     REBOILER       14.70    280.92

   CONVERGENCE PARAMETERS
     NO OF ALLOWABLE CONSTANT MOLAL OVERFLOW ITERATIONS    2
     MAX ALLOWABLE ITERATIONS                  25
     MAX DELTA T PER PLATE                 15.000
     MAX FRACTIONAL LIQ CHANGE PER PLATE 0.300

   PLATE SPACING
     TOP SECTION   24.00 IN
     BOT SECTION   24.00 IN

   ESTIMATED LIQ RATE LEAVING TOP PLATE/CONDENSER 2.550 (L/F)
   ESTIMATED BOTTOMS RATE 0.489 (B/F)
```

```
SCI MAXI*SIM     JOB ID:333
VERSION #2.2     DATE:  22-JUN-1991
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ROSENBERG TEST DISTILLATION


UNIT OPERATION NO  9 IS A DTXT UNIT***ROSENBERG

          FEEDS>>>>>>>PRODUCTS>>>>>>>>>>>>>>>
STREAM FLOW RATES ARE LB-MOLS
STREAM NO        1           2           3
  NAME        FEED        DIST        BOTT
COMPONENT
MTCYC-C6        0.4575      0.4564      0.0011
C7H8            0.4575      0.4486      0.0089
P-X             0.4575      0.0165      0.4410
M-X             0.4575      0.0136      0.4439

  TOTAL         1.8300      0.9351      0.8949

T,DEG F        245.58      222.43      280.92
P,PSIA          14.70       14.70       14.70
H,KBTU          -0.50       -0.75        0.87
S,KBTU/R        0.1330      0.0634      0.0682
MOL WEIGHT    100.6655     95.5421    106.0194
D,LB/FT3       46.7058     45.9074     46.9529
L/F(MOLAR)     1.00000     1.00000     1.00000


COLUMN CONDENSER,REBOILER & SIDE HEATER/COOLER DUTIES
  CONDENSER                                       -80.589 KBTU
  REBOILER                                         88.505 KBTU


ESTIMATED COLUMN DIAMETERS
  TOP SECTION        0.50 FT
  BOTTOM SECTION     0.53 FT
 (BASED ON 75% VAPOR FLOOD VELOCITY &)
 (    5 SEC LIQ RESID IN DOWNCOMER    )
```

```
SCI MAXI*SIM     JOB ID:333
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ROSENBERG TEST DISTILLATION


         TEMPERATURE,PRESSURE,LIQUID AND VAPOR PROFILES

TRAY                         STREAMS LEAVING TRAY
                        LIQUID                       VAPOR
 NO   TEMP       PRES    LB-MOL  MOL WT  DENSITY     LB-MOL  MOL WT
      DEG F      PSIA                    LB/FT3
 12   222.43     14.7     4.7     95.5   45.907       0.0      0.0
 11   225.52     14.7     4.7     95.7   46.324       5.6     95.5
 10   230.02     14.7     4.7     96.3   46.692       5.6     95.7
  9   236.36     14.7     4.7     97.6   46.978       5.6     96.2
  8   244.20     14.7     4.7     99.3   47.142       5.6     97.3
  7   252.18     14.7     4.7    101.0   47.185       5.6     98.7
  6   258.79     14.7     6.5    102.3   47.157       5.6    100.1
  5   266.56     14.7     6.5    103.6   47.156       5.6    101.7
  4   272.46     14.7     6.5    104.6   47.104       5.6    103.3
  3   276.37     14.7     6.5    105.3   47.047       5.6    104.4
  2   278.76     14.7     6.5    105.7   47.002       5.6    105.1
  1   280.14     14.7     6.5    105.9   46.972       5.6    105.6
  0   280.92     14.7     0.9    106.0   46.953       5.6    105.9
```

```
SCI MAXI*SIM    JOB ID:333
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ROSENBERG TEST DISTILLATION

                         LIQUID COMPOSITION PROFILE

TRAY                          COMPONENT NUMBER
 NO    1       2       3       4
 12   0.48809 0.47969 0.01764 0.01459
 11   0.40305 0.51799 0.04275 0.03621
 10   0.32177 0.51678 0.08652 0.07493
  9   0.24583 0.46937 0.15109 0.13372
  8   0.18050 0.38609 0.22760 0.20580
  7   0.13138 0.29377 0.29889 0.27596
  6   0.09930 0.21661 0.35222 0.33187
  5   0.05416 0.14983 0.40895 0.38705
  4   0.02743 0.09558 0.44887 0.42811
  3   0.01321 0.05764 0.47322 0.45593
  2   0.00615 0.03339 0.48622 0.47425
  1   0.00277 0.01866 0.49183 0.48673
  0   0.00120 0.00998 0.49282 0.49601
```

```
SCI MAXI*SIM    JOB ID:333
VERSION #2.2    DATE:  22-JUN-1991
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ROSENBERG TEST DISTILLATION


                           VAPOR COMPOSITION PROFILE

TRAY                                 COMPONENT NUMBER
 NO     1       2       3       4
 12   0.56271 0.42481 0.00690 0.00557
 11   0.48809 0.47969 0.01764 0.01459
 10   0.41724 0.51159 0.03856 0.03260
  9   0.34954 0.51059 0.07502 0.06485
  8   0.28627 0.47109 0.12881 0.11383
  7   0.23185 0.40172 0.19255 0.17388
  6   0.19093 0.32481 0.25194 0.23232
  5   0.11497 0.24962 0.32976 0.30565
  4   0.06262 0.17218 0.39555 0.36965
  3   0.03162 0.10926 0.44185 0.41727
  2   0.01513 0.06526 0.47009 0.44952
  1   0.00694 0.03713 0.48516 0.47077
  0   0.00302 0.02005 0.49168 0.48525
```

```
SCI MAXI*SIM     JOB ID:333
VERSION #2.2     DATE:  22-JUN-1991
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ROSENBERG TEST DISTILLATION


DTXT #  9
   COUNT PLATES FROM BOTTOM UP
   NUMBER OF PLATES IN COLUMN      11
   NUMBER OF FEED PLATES            1
   NUMBER OF PRODUCTS               2
   NUMBER OF SIDE COOLERS/HEATERS   0

    FEED   STREAM  FEED
     NO      NO   PLATE
      1       1      6

   PRODUCT STREAM  DRAW    DRAW
     NO      NO   PLATE    RATE
      1       2     12     ******
      2       3      0     ******

   CONDENSER TYPE-TOTL
   REBOILER TYPE -PART

   CONDENSER/DISTILLATE SPECIFICATIONS-
     MOL FRACT   0.02000 FOR P-X

   REBOILER/BOTTOMS SPECIFICATIONS-
     MOL FRACT   0.01000 FOR C7H8

   COLUMN PRESSURES & ESTIMATED TEMPERATURES
                       P(PSIA)   T(DEG F)
     CONDENSER          14.70    225.60
     TOP PLATE          14.70
     REBOILER           14.70    278.89

   CONVERGENCE PARAMETERS
     NO OF ALLOWABLE CONSTANT MOLAL OVERFLOW ITERATIONS    2
     MAX ALLOWABLE ITERATIONS                     25
     MAX DELTA T PER PLATE                      15.000
     MAX FRACTIONAL LIQ CHANGE PER PLATE        0.300

   PLATE SPACING
     TOP SECTION    24.00 IN
     BOT SECTION    24.00 IN

   ESTIMATED LIQ RATE LEAVING TOP PLATE/CONDENSER 1.020 (L/F)
```

```
SCI MAXI*SIM     JOB ID:333
VERSION #2.2     DATE:  22-JUN-1991
PAGE          35  USER:  PR

ROSENBERG TEST DISTILLATION


UNIT OPERATION NO  9 IS A DTXT UNIT***ROSENBERG

          FEEDS>>>>>>>PRODUCTS>>>>>>>>>>>>>>>>
STREAM FLOW RATES ARE LB-MOLS
STREAM NO         1            2            3
  NAME          FEED         DIST         BOTT
COMPONENT
MTCYC-C6          0.4575       0.4524       0.0051
C7H8              0.4575       0.4286       0.0289
P-X               0.4575       0.0290       0.4285
M-X               0.4575       0.0252       0.4323

  TOTAL           1.8300       0.9351       0.8949

T,DEG F         245.58       223.36       278.89
P,PSIA           14.70        14.70        14.70
H,KBTU           -0.50        -0.70         0.76
S,KBTU/R          0.1330       0.0638       0.0681
MOL WEIGHT      100.6655      95.8764     105.6701
D,LB/FT3         46.7058      45.9176      47.0008
L/F(MOLAR)        1.00000      1.00000      1.00000


COLUMN CONDENSER,REBOILER & SIDE HEATER/COOLER DUTIES
  CONDENSER                                      -40.674 KBTU
  REBOILER                                        44.340 KBTU


ESTIMATED COLUMN DIAMETERS
  TOP SECTION        0.35 FT
  BOTTOM SECTION     0.38 FT
 (BASED ON 75% VAPOR FLOOD VELOCITY &)
 (    5 SEC LIQ RESID IN DOWNCOMER    )
```

```
SCI MAXI*SIM     JOB ID:333
VERSION #2.2     DATE:   22-JUN-1991
PAGE         36  USER:   PR

ROSENBERG TEST DISTILLATION


         TEMPERATURE,PRESSURE,LIQUID AND VAPOR PROFILES

TRAY                          STREAMS LEAVING TRAY
                          LIQUID                       VAPOR
 NO    TEMP       PRES    LB-MOL  MOL WT  DENSITY    LB-MOL  MOL WT
       DEG F      PSIA                    LB/FT3
 12   223.36      14.7      1.9    95.9   45.918       0.0     0.0
 11   227.85      14.7      1.9    96.4   46.375       2.8    95.9
 10   233.11      14.7      1.9    97.3   46.695       2.8    96.2
  9   238.78      14.7      1.9    98.5   46.890       2.8    96.8
  8   244.15      14.7      1.9    99.7   46.988       2.8    97.6
  7   248.60      14.7      1.9   100.6   47.024       2.8    98.4
  6   251.88      14.7      3.7   101.3   47.030       2.8    99.0
  5   257.56      14.7      3.7   102.2   47.133       2.8    99.9
  4   263.50      14.7      3.7   103.1   47.166       2.8   101.0
  3   268.94      14.7      3.7   104.0   47.145       2.8   102.3
  2   273.37      14.7      3.7   104.7   47.098       2.8   103.5
  1   276.64      14.7      3.7   105.3   47.046       2.8   104.5
  0   278.89      14.7      0.9   105.7   47.001       2.8   105.2
```

```
SCI MAXI*SIM     JOB ID:333
VERSION #2.2     DATE:   22-JUN-1991
PAGE          37  USER:   PR

ROSENBERG TEST DISTILLATION


                           LIQUID COMPOSITION PROFILE

TRAY                                COMPONENT NUMBER
 NO     1       2       3       4
 12   0.48383 0.45829 0.03097 0.02690
 11   0.38630 0.47749 0.07209 0.06411
 10   0.30932 0.45393 0.12417 0.11259
  9   0.25034 0.40357 0.17991 0.16617
  8   0.20756 0.34570 0.23023 0.21651
  7   0.17847 0.29466 0.26922 0.25765
  6   0.15982 0.25630 0.29587 0.28800
  5   0.11050 0.22235 0.33843 0.32872
  4   0.07050 0.17703 0.38156 0.37091
  3   0.04171 0.12982 0.41926 0.40922
  2   0.02306 0.08829 0.44807 0.44058
  1   0.01192 0.05582 0.46753 0.46473
  0   0.00565 0.03234 0.47888 0.48314
```

```
SCI MAXI*SIM      JOB ID:333
VERSION #2.2      DATE:   22-JUN-1991
PAGE          38  USER:   PR

ROSENBERG TEST DISTILLATION


                                VAPOR COMPOSITION PROFILE

TRAY                                        COMPONENT NUMBER
 NO     1       2       3       4
 12   0.56539 0.41183 0.01233 0.01045
 11   0.48383 0.45829 0.03097 0.02690
 10   0.41885 0.47108 0.05837 0.05170
  9   0.36755 0.45538 0.09307 0.08400
  8   0.32825 0.42183 0.13021 0.11970
  7   0.29974 0.38327 0.16375 0.15324
  6   0.28036 0.34926 0.18973 0.18065
  5   0.20905 0.32782 0.23744 0.22569
  4   0.14398 0.28302 0.29358 0.27941
  3   0.09121 0.22323 0.35048 0.33508
  2   0.05323 0.16094 0.40022 0.38561
  1   0.02862 0.10616 0.43824 0.42699
  0   0.01392 0.06331 0.46391 0.45886
```

APPENDIX D

COMPUTER PROGRAM

```
$DEBUG
C----------------------------------------------------------
C                   PACKED COLUMN SIMULATOR
C                ****************************
C
C   EXISTING PROGRAM:  VAPOR LIQUID EQUILIBRIUM
C                      HANKINSON THOMPSON LIQUID DENSITY
C                      SURFACE TENSION
C                      DIFFUSIVITY
C                      PACKED COLUMN DIAMETER/HETP
C                      VISCOSITY
C                      DISTILLATION USING COLLOCATION
C                      ENTHALPY
C
C         PARTHA  ROY   :      10th MAY, 1991.
C----------------------------------------------------------
C     VLE MAIN PROGRM
      IMPLICIT REAL*8 (A-H,O-Z)
      EXTERNAL VLE,VISELY,DIST
C----
      COMMON/CVLE/ X(20),XMAX(20),XMIN(20),DELTC(20),
     &            DELMN(20),NV,MAXIT,NPTS
      COMMON/V0/ TC(20),PC(20),OMG(20),TB(20),WT(20),
     &          ZRA(20),A1(20),AL(20),B1(20),BL(20)
      COMMON/V1/ RHOL(5),RHOV(5),RHOLC(5),RHOVC(5),WTM(5),
     &          T(5),P(5),PP(5),ALFAS(5)
      COMMON/VE/ XE(5,20),YE(5,20),ZE(5,20),KE(5,20),
     &          C(20,20)
      COMMON/VC/ XC(5,20),YC(5,20),ZZ(5,20),KC(5,20),
     &          D(20,20)
      COMMON/VF/PHL(5,20),PHV(5,20),FUGL(5,20),FUGV(5,20),
     &         KO(5,20)
      COMMON/V2/ LAMB,PHI,OMGM,PCM
      COMMON/V3/ OMGB,GC,OMGM2,OMGM3
      COMMON/V4/ MIX,NPT,IEOS,IN,IO,LP,IP,NC,KY,INPT
      COMMON/V5/ AN(20,5),TITLE(15)
      COMMON/V6/ A,AAL,B,BBL,U,UU,W,WW,ZC,R,TOL,LV,LL,MODE,
     &          KM,IERR,IPR OP
      COMMON/LD/ CVOL(20),HW(20),RHOPL(20)
      COMMON/VP/ PVAP(20),VPB1(20),VPB2(20),VPB3(20),
     &          VPB4(20)
      COMMON/ENRCHI/ STRA,STRH,REFR,YBOT(20),DT,IM
      DOUBLE PRECISION KO,KC,KE
      OPEN (UNIT=10, FILE = 'DFILE.DAT', STATUS =
     &'UNKNOWN')
      OPEN (UNIT=12, FILE = 'PACKF.DAT', STATUS =
     &'UNKNOWN')
      OPEN (UNIT=14, FILE = 'ENRCH.DAT', STATUS =
     &'UNKNOWN')
      OPEN (UNIT=15, FILE = 'ROOT.DAT', STATUS = 'UNKNOWN')
      OPEN (UNIT=16, FILE = 'STRIP.DAT', STATUS =
     &'UNKNOWN')
```

```
C******
      IN=8
      IO=9
      IP=10
      LP=6
C******
      MAXIT=20
      CALL INPUT
        IF (IM.EQ.1) THEN
        CALL DIST
        GOTO 50
        ENDIF
      CALL VLE
      CALL OUTPUT
      CALL DIA
      CALL HETP
      CALL ENTHALPY
  50  STOP
      END
*
*    This is a program for a single feed , total
*     condenser packed column distillation unit
*
*
      SUBROUTINE DIST
C
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON/COLLO1/A(20,20),B(20,20),Q(20,20),XC(20),W(20)
      COMMON/V4/ MIX,NPT,IEOS,IN,IO,LP,IP,NC,KY,INPT
      COMMON/ENRCHI/ STRA,STRH,REFR,YBOT(20),DT,IM
      COMMON/ENRCHC/ TOPL,TOPV,TEMP(5),FT(5)
      COMMON/STRIP1/ STA,SL1,SV1,IS,STH,XTOP(20)
      COMMON/WORKSP/ RWKSP
      REAL RWKSP(5426)

      N=2*NC*4+2*4
C      PARAMETER   (N=2*4*4+2*4)
C
      DOUBLE PRECISION   FCN,FNORM,X(N),XGUESS(N)
      EXTERNAL   FCN,DNEQNF,UMACH
      CALL IWKIN(5426)
C   check section to be solved (enriching/stripping)
        IF(IS.EQ.2) GOTO 10
C  set the liquid and vapor flowrate at the top.
C   in the enriching section.
        TOPL=REFR*DT
        TOPV=(REFR+1)*DT
C
C      data xguess/ 0.1,0.1,0.1 ---
      READ(14,33333) (XGUESS(J),J=1,N),(TEMP(K),K=1,5)
      GOTO 15
C   50% flooding
```

```
C
   10 CONTINUE
C  initial guesses for the stripping section
      READ(16,33333) (XGUESS(J),J=1,N),(TEMP(K),K=1,5)

C  find the collocation points
   15 CALL PLANAR
C  set maximum error and maximum iterations
      WRITE(*,*) 'ERROR LIMIT ?'
      READ(*,*) ERRREL
C      IF(IS.EQ.2) ERRREL=0.03
      ITMAX=100
C find output input number
      CALL UMACH(2,NOUT)
C solve the nonlinear equations
      CALL DNEQNF(FCN,ERRREL,N,ITMAX,XGUESS,X,FNORM)
C
      CALL DSTOUT(X,N)
C
33333
FORMAT(7F8.4,/,7F8.4,/,7F8.4,/,7F8.4,/,7F8.4,/,5F8.4,/,5F8.
2)
      RETURN
      END
*********
*
*  this is the output subroutine for the distillation *
column
*********
      SUBROUTINE DSTOUT(X,N)
C
      IMPLICIT REAL *8 (A-H,O-Z)
      COMMON/COLLO1/A(20,20),B(20,20),Q(20,20),XC(20),W(20)
      COMMON/V4/ MIX,NPT,IEOS,IN,IO,LP,IP,NC,KY,INPT
      COMMON/VE/ XE(5,20),YE(5,20),ZE(5,20),KE(5,20),
      C(20,20)
      COMMON/V1/ RHOL(5),RHOV(5),RHOLC(5),RHOVC(5),WTM(5),
     &          T(5),P(5),PP(5),ALFAS(5)
      COMMON/ENRCHI/ STRA,STRH,REFR,YBOT(20),DT,IM
      COMMON/ENRCHC/ TOPL,TOPV,TEMP(5),FT(5)
      COMMON/STRIP1/ STA,SL1,SV1,IS,STH,XTOP(20)
      DOUBLE PRECISION X(N),XL(5,5),YV(5,5)


      IF(IS.EQ.1) THEN
      DO 25 I=1,8
      M=NC*(I-1)
      DO 25 K=1,NC
      IF (I.LE.4) THEN
      XL(K,I)=X(K+M)
      ELSE
      J=I-3
```

```
      YV(K,J)=X(K+M)
      ENDIF
   25 CONTINUE
      DO 27 J=1,NC
   27 XL(J,5)=YV(J,5)
      ENDIF
C
      IF(IS.EQ.2) THEN
      DO 28 I=2,9
      M=NC*(I-2)
      DO 28 K=1,4
      IF(I.LE.5) THEN
      XL(K,I)=X(K+M)
      ELSE
      J=I-5
      YV(K,J)=X(K+M)
      ENDIF
   28 CONTINUE
      DO 29 J=1,NC
   29 XL(J,1)=XTOP(J)
      ENDIF
C
      DO 31 I=1,5
      DO 30 J=1,NC
      ZE(1,J)=XL(J,I)
   30 CONTINUE
      T(1)=TEMP(I)
      CALL VLE
      FT(I)=T(1)
   31 CONTINUE
C
      DO 35 K=1,N
      WRITE(*,99999) K,X(K)
   35 CONTINUE
      IF(IS.EQ.1) WRITE(15,10000)
      IF(IS.EQ.2) WRITE(15,10101)
      WRITE(15,10199)
      WRITE(15,11111)
      FT(1)=TEMP(1)
      DO 40 I=1,5
      IF(IS.EQ.1) XC(I)=XC(I)*STRH
      IF(IS.EQ.2) XC(I)=XC(I)*STH
      WRITE(15,66666) XC(I),(XL(K,I),K=1,NC)
   40 CONTINUE
      WRITE(15,10500)
      WRITE(15,10700)
*
      IF(IS.EQ.2) WRITE(15,77777) XC(1),FT(1),PP(1),SL1,SV1
*
      DO 50 J=IS,IS+3
      WRITE(15,77777) XC(J),FT(J),PP(1),X(32+1-
      IS+J),X(36+1-IS+J)
```

```
   50 CONTINUE
*
      IF(IS.EQ.1) WRITE(15,77777)XC(5),FT(5),PP(1),TOPL,
      TOPV
10000 FORMAT(/,/,19X,'ENRICHING SECTION RESULTS')
10101 FORMAT(/,/,19X,'STRIPPING SECTION RESULTS')
10199 FORMAT(/,/,19X,'LIQUID COMPOSITION PROFILE')
10500 FORMAT(/,/,12X,'TEMPERATURE(K),PRESSURE(BAR) AND
      FLOWRATES(lbm/hr) ')
10700 FORMAT(/,/,5X,'HT(ft)',7X,' TEMP ',5X,' PRESS ',5X,'
      LIQUID ',
     &5X,' VAPOR  ')
11111 FORMAT(/,/,5X,'HT(ft)',7X,'MT-CYC',5X,'TOLUENE',5X,
      'P-XYLENE', &5X,'M-XYLENE')
66666 FORMAT(4X,F8.4,4X,F8.4,4X,F8.4,4X,F8.4,4X,F8.4)
77777 FORMAT(4X,F8.4,4X,F8.4,4X,F8.4,4X,F8.4,4X,F8.4)
99999 FORMAT(' the solution to the system is X
      ',I2,'=',F8.4)
C
      RETURN
      END
*
*********
*   this subroutine contains the nonlinear algebraic *
equations obtained after applying orthogonal *
collocation on the PDE's of the steady state *
nonequilibrium model of a packed column distillation
*   unit.
*********
      SUBROUTINE FCN(X,F,N)
*
      IMPLICIT REAL *8 (A-H,O-Z)
      COMMON/COLLO1/A(20,20),B(20,20),Q(20,20),XC(20),W(20)
      COMMON/V4/ MIX,NPT,IEOS,IN,IO,LP,IP,NC,KY,INPT
      COMMON/ENRCHI/ STRA,STRH,REFR,YBOT(20),DT,IM
      COMMON/ENRCHC/ TOPL,TOPV,TEMP(5),FT(5)
      COMMON/STRIP1/ STA,SL1,SV1,IS,STH,XTOP(20)
      DOUBLE PRECISION X(N),F(N),FA(5,40),FB(5,40),
      FA1(5,30), FB1(5,30), EL(5),EV(5),BL(5),BV(5)
*  check for section to be solved

C  DEFINE: FL=LIQUID (L)  :  FV=VAPOR (V)  :  GOK=KOG*A*H*S
      LN=NC*4+1
      N2=2*NC*4
      N1=N2/2
C
      WRITE(*,*) X(1),X(5),X(9)
      DO 10 I=1,5
      DO 10 K=1,LN+NC-1
      FA(I,K)=0.0
      FB(I,K)=0.0
      FA1(I,K)=0.0
```

```
      FB1(I,K)=0.0
      BL(I)=0.0
      BV(I)=0.0
      EL(I)=0.0
      EV(I)=0.0
   10 CONTINUE
C
      IF(IS.EQ.2) GOTO 100
C
C    equations for the enriching section
C
      DO 20 I=1,4
      DO 20 K=1,NC
      M=K
      DO 20 J=1,4
      FA(I,K)=A(I,J)*X(M)*X(N2+J)+FA(I,K)
      M=M+NC
   20 CONTINUE
      DO 30 I=1,5
      DO 30 K=LN,LN+NC-1
      M=K
      DO 30 J=2,4
      FB(I,K)=A(I,J)*X(M)*X(N2+4+J)+FB(I,K)
      M=M+NC
   30 CONTINUE
      DO 35 I=1,4
      DO 35 J=1,4
      BL(I)=A(I,J)*X(N2+J)+BL(I)
      EL(I)=A(I,J)*X(N2+J)*ENLV(J,1,X,N)+EL(I)
      BV(I)=A(I,J)*X(N2+4+J)+BV(I)
      EV(I)=A(I,J)*X(N2+4+J)*ENLV(J,2,X,N)+EV(I)
   35 CONTINUE
      J=1
      DO 40 I=1,4
      DO 40 K=1,NC
      F(J)=(FA(I,K))-(FB(I,K+N1))-(A(I,1)*X(N2+5)*YBOT(K))+
      (A(I,5)*X(N2-NC+K)*(TOPL-TOPV))
      J=J+1
   40 CONTINUE
      J=N1+1
      DO 50 I=2,5
      DO 50 K=1,NC
      F(J)= -(1.0/STRH)*(FB(I,K+N1)+A(I,5)*TOPV*X(N2-
      NC+K))-(A(I,1)*X(N2+5)*YBOT(K)/STRH)-
      GOK(I,X,N)*(X(J)-YSTAR(K,I,X,N))
      J=J+1
   50 CONTINUE
      DO 60 I=1,4
      F(N2+I)=BL(I)-BV(I)+(A(I,5)*(TOPL-TOPV))
   60 CONTINUE
      DO 70 I=1,4
      F(N2+4+I)=EL(I)-EV(I)+(A(I,5)*TOPL*ENLV(5,1,X,N))-
```

```
      (A(I,5)*TOPV &*ENLV(5,2,X,N))
   70 CONTINUE
      GOTO 1000
C
C    eqns. for the stripping section
C                  M=M+NC
  100 CONTINUE
      DO 110 I=1,4
      DO 110 K=1,NC
      M=K
      DO 110 J=2,4
      FA1(I,K)=A(I,J)*X(M)*X(N2-1+J)+FA1(I,K)
      M=M+NC
  110 CONTINUE
      DO 120 I=1,5
      DO 120 K=LN,LN+NC-1
      M=K+NC
      DO 120 J=2,4
      FB1(I,K)=A(I,J)*X(M)*X(N2+NC-1+J)+FB1(I,K)
      M=M+NC
  120 CONTINUE
      DO 125 I=1,4
      DO 125 J=2,5
      BL(I)=A(I,J)*X(N2-1+J)+BL(I) EL(I)=A(I,J)*X(N2-
      1+J)*ENLV(J,1,X,N)+EL(I) BV(I)=A(I,J)*X(N2+3+J)+BV(I)
      EV(I)=A(I,J)*X(N2+3+J)*ENLV(J,2,X,N)+EV(I)
  125 CONTINUE
      J=1
      DO 130 I=1,4
      DO 130 K=1,NC
      F(J)=FA1(I,K)-FB1(I,K+N1)+(A(I,1)*XTOP(K)*SL1)+
      (A(I,5)*X(N1-NC+K)*(X(N2+4)-X(N2+8)*XBOT1(K,X,N)))-
      (A(I,1)*SV1*X(N1+K))
      J=J+1
  130 CONTINUE
      J=N1+1
      DO 140 I=2,5
      DO 140 K=1,NC
      IF(I.EQ.5) THEN
      F(J)= -(1.0/STH)*(FB1(I,K+N1))-
      (A(I,5)*XBOT1(K,X,N)*X(N1-NC+K)* &X(N2+8)/STH)-
      GOK(I,X,N)*(XBOT1(K,X,N)*X(N1-NC+K)-YSTAR1(K,I,X,N))
     &-(A(I,1)*SV1*X(N1+K)/STH)
      ELSE
      F(J)= -(1.0/STH)*(FB1(I,K+N1))-
      (A(I,5)*XBOT1(K,X,N)*X(N1-NC+K)* &X(N2+8)/STH)-
      GOK(I,X,N)*(X(J+NC)-YSTAR1(K,I,X,N))-(A(I,1)*SV1*
     &X(N1+K)/STH)
      ENDIF
      J=J+1
  140 CONTINUE
      DO 150 I=1,4
```

```
      F(N2+I)=BL(I)-BV(I)+(A(I,1)*(SL1-SV1))
  150 CONTINUE
      DO 160 I=1,4 F(N2+4+I)=EL(I)-
      EV(I)+(A(I,1)*SL1*ENLV(1,1,X,N))-(A(I,1)*SV1
     &*ENLV(1,2,X,N))
  160 CONTINUE
C
 1000 RETURN
      END
***
*   function gok is used to calculate the overall gas phase
*   mass transfer coefficient.
*
***
      FUNCTION GOK(K,X,N)
*
      IMPLICIT REAL *8 (A-H,O-Z)
      COMMON/ENRCHC/ TOPL,TOPV,TEMP(5),FT(5)
      COMMON/ENRCHI/ STRA,STRH,REFR,YBOT(20),DT,IM
      COMMON/STRIP1/ STA,SL1,SV1,IS,STH,XTOP(20)
      COMMON/V4/ MIX,NPT,IEOS,IN,IO,LP,IP,NC,KY,INPT
      DOUBLE PRECISION X(N)
      N2=N-2*4
      IF(IS.EQ.1) THEN
      GOK=0.74*(X(N2+K)/STRA)**(1.175)
      IF(K.EQ.5) GOK=0.74*(TOPL/STRA)**(1.175)
      GOK=GOK*STRA
      ENDIF
      IF(IS.EQ.2) THEN
      GOK=0.5*(X(N2+NC-1+K)/STA)**(1.29)
      GOK=GOK*STA
      ENDIF
      RETURN
      END

***
*  this function ENLV is used to estimate the enthalpy of *
the liquid and vapor at each collocation point.
*
***
      FUNCTION ENLV(K,M,X,N)
*
      IMPLICIT REAL *8 (A-H,O-Z)
      COMMON/V4/ MIX,NPT,IEOS,IN,IO,LP,IP,NC,KY,INPT
      COMMON/VE/ XE(5,20),YE(5,20),ZE(5,20),KE(5,20),
      C(20,20)
      COMMON/VC/ XC(5,20),YC(5,20),ZZ(5,20),KC(5,20),
      D(20,20)
      COMMON/V1/ RHOL(5),RHOV(5),RHOLC(5),RHOVC(5),WTM(5),
     &           T(5),P(5),PP(5),ALFAS(5)
      COMMON/ENRCHC/ TOPL,TOPV,TEMP(5),FT(5)
      COMMON/ENRCHI/ STRA,STRH,REFR,YBOT(20),DT,IM
```

```
      COMMON/ENTH1/ VMENTH,FMENTH
      COMMON/STRIP1/ STA,SL1,SV1,IS,STH,XTOP(20)
      DOUBLE PRECISION X(N)
C      J1=J1+1
      N1=K*NC-NC
      N2=(N-2*4)/2
      N3=K*NC-2*NC
      N4=NC*(K-2)
      N5=NC*(K-1)
C
      DO 10 I=1,NC
      IF(IS.EQ.1) THEN
      IF(K.LE.4) XC(1,I)=X(N1+I)
      IF(K.EQ.5) XC(1,I)=X(2*N1-4+I)
      IF(K.EQ.1) YC(1,I)=YBOT(I)
      IF(K.GT.1) YC(1,I)=X(N2+N3+I)
      ENDIF
      IF(IS.EQ.2) THEN
      IF(K.EQ.1) XC(1,I)=XTOP(I)
      IF(K.GT.1) XC(1,I)=X(N4+I)
      IF(K.LE.4) YC(1,I)=X(N2+N5+I)
      IF(K.EQ.5) YC(1,I)=XBOT1(I,X,N)*X(N2-NC+I)
      ENDIF
   10 CONTINUE
*  Warning ; if collocation points are changed, modify *
algorithm.
      T(1)=TEMP(K)
      IF(FT(K).GT.0.0) T(1)=FT(K)
      IF(K.EQ.1) T(1)=TEMP(K)
      CALL ENTHALPY
      IF(M.EQ.1) ENLV=FMENTH
   20 IF(M.EQ.2) ENLV=VMENTH
C
      RETURN
      END
***
*  function xbot calculates the mole fraction of vapor *
entering the column at the bottom using the bubble point *
temperature method.
***
*
      FUNCTION XBOT(M,X,N)
*
      IMPLICIT REAL *8 (A-H,O-Z)
      COMMON/V4/ MIX,NPT,IEOS,IN,IO,LP,IP,NC,KY,INPT
      COMMON/VE/ XE(5,20),YE(5,20),ZE(5,20),KE(5,20),
      C(20,20)
      COMMON/VC/ XC(5,20),YC(5,20),ZZ(5,20),KC(5,20),
      D(20,20)
      COMMON/V1/ RHOL(5),RHOV(5),RHOLC(5),RHOVC(5),WTM(5),
     &           T(5),P(5),PP(5),ALFAS(5)
      COMMON/STRIP1/ STA,SL1,SV1,IS,STH,XTOP(20)
```

```
      COMMON/ENRCHC/ TOPL,TOPV,TEMP(5),FT(5)
      DOUBLE PRECISION X(N),BOT(20)
*
      N1=(N-2*4)/2
      IF(M.EQ.1) THEN
      DO 10 I=1,NC
      ZE(1,I)=X(N1-NC+I)
   10 CONTINUE
      T(1)=TEMP(5)
      IF(FT(5).GT.0.0) T(1)=FT(5)
      CALL VLE
      CALL OUTPUT
*
      DO 20 J=1,NC DUM=X(2*N1+2*4)+(X(2*N1+4)-
      X(2*N1+2*4))*(XC(1,J)/YC(1,J))
   20 BOT(J)=X(2*N1+4)/(DUM)
      ENDIF
*
      XBOT=BOT(M)
      RETURN
      END

***
*  function xbot1 calculates the mole fraction of vapor *
entering the column at the bottom using constant *
relative volatilities.
***
*
      FUNCTION XBOT1(L,X,N)
*
      IMPLICIT REAL *8 (A-H,O-Z)
      COMMON/V4/ MIX,NPT,IEOS,IN,IO,LP,IP,NC,KY,INPT
      COMMON/STRIP1/ STA,SL1,SV1,IS,STH,XTOP(20)
      DOUBLE PRECISION X(N),ALFA(4)
      DATA ALFA/ 2.8,2.2,1.0,0.95 /
*  NOTE:  modify this subroutine
      N1=(N-2*4)/2
      IF(L.NE.1) GOTO 20
      SUM=0.0
      DO 10 I=1,NC
      SUM=SUM+ALFA(I)*X(N1-NC+I)
   10 CONTINUE
   20 DUM=(X(2*N1+4)-X(2*N1+2*4))*(SUM/ALFA(L))
      XBOT1=X(2*N1+4)/(X(2*N1+2*4)+DUM)
      RETURN
      END
*********
*
*        function ystar calculates the bubble point at each
*        collocation point.
*
*********
```

```
      FUNCTION YSTAR(L,M,X,N)
*
      IMPLICIT REAL *8 (A-H,O-Z)
      COMMON/V4/ MIX,NPT,IEOS,IN,IO,LP,IP,NC,KY,INPT
      COMMON/VE/
      XE(5,20),YE(5,20),ZE(5,20),KE(5,20),C(20,20)
      COMMON/VC/
      XC(5,20),YC(5,20),ZZ(5,20),KC(5,20),D(20,20)
      COMMON/V1/ RHOL(5),RHOV(5),RHOLC(5),RHOVC(5),WTM(5),
     &           T(5),P(5),PP(5),ALFAS(5)
      COMMON/ENRCHC/ TOPL,TOPV,TEMP(5),FT(5)
      COMMON/STRIP1/ STA,SL1,SV1,IS,STH,XTOP(20)
      DOUBLE PRECISION X(N)
C
C
      N1=0
      IF(IS.EQ.1) N1=NC
      N2=(M-2)*NC
C
      IF (L.EQ.1) THEN
      DO 50 I=1,NC
      IF (IS.EQ.1.AND.M.EQ.5) N2=6*NC
      ZE(1,I)=X(N1+N2+I)
   50 CONTINUE
      T(1)=TEMP(M)
      CALL VLE
      FT(M)=T(1)
      CALL OUTPUT
      ENDIF
*   allot the respective equilibrium mole fractions ystar.
      YSTAR=YC(1,L)
*
      RETURN
      END
*
*     this is an alternate method of estimating the
*     equilibrium mole fractions ystar, using
*     constant relative volatilities.
*
      FUNCTION YSTAR1(K,L,X,N)
*
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON/V4/ MIX,NPT,IEOS,IN,IO,LP,IP,NC,KY,INPT
      COMMON/STRIP1/ STA,SL1,SV1,IS,STH,XTOP(20)
      DOUBLE PRECISION ALFA(4),X(N)
*   relative volatilities
      DATA ALFA/ 2.8,2.2,1.0,0.95 /
* if stripping use n1=0 :  enriching n1=4
      N1=0
      IF(IS.EQ.1) N1=NC
      N2=(L-2)*NC
      IF (K.EQ.1) THEN
```

```
      SUM=0.0
      DO 10 I=1,NC
      IF (IS.EQ.1.AND.L.EQ.5) N2=6*NC
      SUM=SUM+ALFA(I)*X(N1+N2+I)
   10 CONTINUE
      ENDIF
      YSTAR1=ALFA(K)*X(N1+N2+K)/SUM
C      WRITE(*,*) YSTAR1
      RETURN
      END
*
**********
*                       SUBPROGRAM IDENTIFICATION
**********
*
*         Subroutine PLANAR computes the matrices without *
symmetry needed to run the ortoghonal collocation *
technique. This code comes from the book by Bruce *
A.  Finlayson.
*
**********
*                       VARIABLES IDENTIFICATION
**********
*
*         A    =  Matrix for first derivatives
*         B    =  Matrix for second derivatives
*         Q    =  Matrix for the Q inverse
*         XC   =  Vector of collocation points
*         W    =  Vector of Weights
*         R,S  =  Temporary arrays
*
**********
*                       SUBROUTINE CALLS
**********
*
*         JACOBI    =  Calculates the collocation points
*
*
**********
*                       TYPE DECLARATIONS AND STORAGE *
ALLOCATION **********
*
      SUBROUTINE PLANAR
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON /COLLO1/
      A(20,20),B(20,20),Q(20,20),XC(20),W(20)
      DIMENSION  R(30,30),S(30)
C
C      WRITE(*,*) 'NO. OF COLLOCATION PTS.'
C      READ(*,*) N
C
C    CHANGE N TO CHANGE NO. OF COLLOCATION POINTS.
```

```
C     DEFAULT VALUE OF N AS IN THE NEXT LINE IS 3
       N=3
       NP=N+2
*
**********
* BLOCK 0000             CALCULATE COLLOCATION POINTS
**********
*
      NCOL = NP-2
      CALL JACOBI(NP,NCOL,0,0,XC)
      IF(NP.GT.20) GO TO 100
      WRITE(6,90) (I, XC(I), I=1,NP)
 90   FORMAT(//,T15,' ** COLLOCATION POINTS **',/,T10,'
POINT',
     1       T20,'ORDINATE',/, (T10,I5,T20,E15.8))
*
*********
* BLOCK 0100             A AND B MATRIXES
*********
*
 100  DO 130 I=1, NP
         R(I,I) = 0.0
         A(I,I) = 0.0
         S(I)   = 1.0
         B(I,I) = 0.0
         DO 110 J=1, NP
            IF(I.EQ.J)  GO TO 110
            R(I,J) = 1.0/(XC(I)-XC(J))
            S(I) = S(I)*R(I,J)
 110        CONTINUE
         DO 120 J=1,NP
            JX = NP-J+1
            IF(JX.LT.J) THEN
               GO TO 130
            ELSEIF(JX.EQ.J) THEN
               A(I,I) = A(I,I) + R(I,J)
            ELSE
               A(I,I) = A(I,I) + R(I,J) + R(I,JX)
            ENDIF
 120        CONTINUE
 130     CONTINUE
      DO 150 I=1, NP
         DO 140 J=1,NP
            IF(I.EQ.J) GO TO 140
            A(I,J) = S(J)*R(I,J)/S(I)
            B(I,J) = 2.0*A(I,J)*(A(I,I)-R(I,J))
            B(I,I) = B(I,I) + R(I,J)*(A(I,I)-R(I,J))
 140        CONTINUE
 150     CONTINUE
*
*********
* BLOCK 0200            Q  MATRIX AND W VECTOR
```

```
*********
*
      DO 300 I=1, NP
         Q(1,I) = S(I)
         K = 1
         W(I) = 0.0
         DO 270 J=1, NP
            IF(J.EQ.I) GO TO 270
            L = K
            K = K + 1
            Q(K,I) = Q(L,I)
 260        IF( L.NE.1) THEN
                M = L-1
                Q(L,I) = Q(M,I) - XC(J)*Q(L,I)
                L = M
                GO TO 260
            ENDIF
            Q(1,I) = -XC(J)*Q(1,I)
 270        CONTINUE
         DO 280 J=1, NP
 280        W(I) =  W(I) + Q(J,I)/FLOAT(J)
 300     CONTINUE
      WRITE(*,*) ((A(I,J),J=1,NP),I=1,NP)
      RETURN
      END
*
*
      SUBROUTINE JACOBI(ND,N,ALFA,BETA,ROOT)
*
**********
*                       PROGRAM DESCRIPTION
**********
*
*         JACOBI is a modification of subroutine A1 in : *
Villadsen, J., M.  L.  Michelsen, "Solution of *
Differential Equation Models by Polynomial *
Approximation", Prentice-Hall, Inc., U.S.A., *
1978.  It is used here to calculate the *
collocation points in each element.  The section *
which calculates the derivatives has being *
eliminated.
*
**********
*                       VARIABLES IDENTIFICATION
**********
*
*         ND         =  Dimension of vector ROOT
*         N          =  The degrre of the Jacobi polynomial
*         ALFA,BETA  =  Exponents in the Weighting function
*                       of Jacobi Polynomial.
*         ROOT       =  Roots of the Jacobi Polynomial.
*         DIF1,DIF2  =  Temporary arrays.
```

```
*
**********
*                      TYPE DECLARATION AND STORAGE *
ALLOCATION
**********
*
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION ROOT(20), DIF1(20), DIF2(20)
*
**********
*   BLOCK 0000         EVALUATION OF COEFFICIENTS
*********
*
      AB = ALFA + BETA
      AD = BETA - ALFA
      AP = BETA * ALFA
      DIF1(1) = (AD/(AB+2)+1)/2
      DIF2(1) = 0.
      IF( N.LT.2) GO TO 100
      DO 10 I=2,N
            ZI = I - 1
            Z  = AB + 2*ZI
            DIF1(I) = (AB*AD/Z/(Z+2)+1)/2
            IF(I.EQ.2) THEN
               DIF2(I)=(AB+AP+ZI)/Z/Z/(Z+1)
            ELSE
               Z = Z*Z
               Y = ZI*(AB+ZI)
               Y = Y*(AP+Y)
               DIF2(I)=Y/Z/(Z-1)
            ENDIF
 10   CONTINUE
*
*********
*    BLOCK 0100        ROOT DETERMIMATION BY NEWTON'S METHOD
*********
*
 100  X = 0.
      DO 190 I=1,N
 105        XD = 0.0
            XN = 1.0
            XD1 = 0.0
            XN1 = 1.0
            DO 130 J=1,N
               XP=(DIF1(J)-X)*XN-DIF2(J)*XD XP1=(DIF1(J)-
               X)*XN1-DIF2(J)*XD1-XN
               XD=XN
               XD1=XN1
               XN=XP
 130           XN1=XP1
           ZC=1.0
           Z=XN/XN1
```

```
          IF(I.NE.1) THEN
              DO 140 J=2,I
 140              ZC=ZC-Z/(X-ROOT(J-1))
          ENDIF
          Z=Z/ZC
          X=X-Z
          IF( DABS(Z).GT.1.D-09) GO TO 105
          ROOT(I) = X
          X = X+0.0001
 190  CONTINUE
*
*********
*   BLOCK 0300        ADD POINTS AT X=0 AND X=1
*********
*
      NT = N+2
      DO 310 I=1,N
         J=N+1-I
 310     ROOT(J+1) = ROOT(J)
         ROOT(1) = 0.0
         ROOT(NT)= 1.0
*
*********
*   BLOCK 0400        CLOSE THE PROGRAM
*********
*
      RETURN
      END
C
C     NC   :  NO OF COMPONENTS IN THE SYSTEM (MAX=20)
C     NPTS :  NO PTS OF DATA (MAX=50)
C     TC,PC,OMG,W  = PURE FLUID  PROPERTIES ( EOS INPUT C
VARIABLES)
C     T,P(PP)      = TEMPERATURE, PRESSURE
C     XE,YE,ZE     = COMPOSITION FOR LIQUID, VAPOR, AND C
FEED
C     LV           = 1 PREDICT LIQUID,     LV =2 PREDICT
C                    VAPOR
C
C     K           = EQUILIBRIUM CONSTANT
C     RHO(L/V)    = DENSITY
C     FUG(L/V)    = FUGACITY
C     PHI(L/V)    = FUGACITY COEFFICIENT
C     CIJ         = 1ST EOS INTERACTION PARAMETER
C     DIJ         = 2ND EOS INTERACTION PARAMETER
C
*
      SUBROUTINE INPUT
*
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON/CVLE/ X(20),XMAX(20),XMIN(20),DELTC(20),
      DELMN(20),NV,MAXIT,NPTS
```

```
      COMMON/V0/ TC(20),PC(20),OMG(20),TB(20),WT(20),
      ZRA(20),A1(20),AL(20),B1(20),BL(20)
      COMMON/V1/ RHOL(5),RHOV(5),RHOLC(5),RHOVC(5),WTM(5),
     &           T(5),P(5),PP(5),ALFAS(5)
      COMMON/VE/ XE(5,20),YE(5,20),ZE(5,20),KE(5,20),
      C(20,20)
      COMMON/VC/ XC(5,20),YC(5,20),ZZ(5,20),KC(5,20),
      D(20,20)
      COMMON/VF/ PHL(5,20),PHV(5,20),FUGL(5,20),FUGV(5,20),
      KO(5,20)
      COMMON/V2/ LAMB,PHI,OMGM,PCM
      COMMON/V3/ OMGB,GC,OMGM2,OMGM3
      COMMON/V4/ MIX,NPT,IEOS,IN,IO,LP,IP,NC,KY,INPT
      COMMON/V5/ AN(20,5),TITLE(15)
      COMMON/V6/ A,AAL,B,BBL,U,UU,W,WW,ZC,R,TOL,LV,
      LL,MODE,KM,IERR,IPR OP
      COMMON/VP/ PVAP(20),VPB1(20),VPB2(20),VPB3(20),
      VPB4(20)
      COMMON/LD/ CVOL(20),HW(20),RHOPL(20)
      COMMON/DIAM/ FLV,DREF,PF,ND,ALPH,BETA,DELP,COLD,WL
      COMMON/TRAP/ ID(20),NC1
      COMMON/VDIF/ VC(20)
      COMMON/ENTH/ HA(20),HB(20),HC(20),HD(20),HE(20),
      HF(20), DELH(20)
      COMMON/HETPC/ IPP,HP,SLP,HETPA
      COMMON/ENRCHI/ STRA,STRH,REFR,YBOT(20),DT,IM
      COMMON/STRIP1/ STA,SL1,SV1,IS,STH,XTOP(20)
      DOUBLE PRECISION KO,KC,KE,DUMMY(35)
C*****
C       INSERT INPUT PORTION
      MODE=1
*
*      Introduction and choice of method
*
      WRITE(*,*) '***************************************'
      WRITE(*,*) 'WELCOME TO THE PACKED COLUMN SIMULATOR'
      WRITE(*,*) '***************************************'
      WRITE(*,*)
      WRITE(*,*) 'PLEASE SPECIFY THE CALCULATION DESIRED'
      WRITE(*,*) '1=DISTILLATION USING COLLOCATION'
      WRITE(*,*) '2=DIAMETER AND HETP CALCULATION'
      READ(*,*) IM
*
*   Input for the enriching section of the distillation
*    unit
*
      IEOS=2
      IPROP=3


      WRITE(*,*) ' ENTER NUMBER OF COMPONENTS IN THE
      SYSTEM(MAX=20) ' READ(*,*) NC
```

```
      NC1=NC
C
      NPTS=1
      NPT=NPTS
      INPT=2
C
      WRITE(*,*) ' ENTER INPUT UNITS '
      WRITE(*,*) ' 1= T(K), P(BAR), DEN(G/CC) '
      WRITE(*,*) ' 2= T(F), P(PSIA), DEN(GM/CC) '
      READ(*,*) IUNIT
C
      DO 10 J=1,NC
      WRITE(*,*) J,' COMPONENT ID '
   10 READ(*,*) ID(J)
      ID(NC+1)=61
C

      DO 20 K=1,61
      READ(10,1000) (DUMMY(J),J=1,30)
      DO 15 L=1,NC+1
      IF(K.EQ.ID(L)) THEN
      TC(L)=DUMMY(3)
      PC(L)=DUMMY(4)
      OMG(L)=DUMMY(5)
      TB(L)=DUMMY(6)
      WT(L)=DUMMY(7)
      ZRA(L)=DUMMY(8)
      VPB1(L)=DUMMY(9)
      VPB2(L)=DUMMY(10)
      VPB3(L)=DUMMY(11)
      VPB4(L)=DUMMY(12)
      HW(L)=DUMMY(13)
      CVOL(L)=DUMMY(14)
      VC(L)=DUMMY(17)
      HA(L)=DUMMY(18)
      HB(L)=DUMMY(19)
      HC(L)=DUMMY(20)
      HD(L)=DUMMY(21)
      HE(L)=DUMMY(22)
      HF(L)=DUMMY(23)
      DELH(L)=DUMMY(24)
C***    ADD ADDITIONAL DATA HERE      ****
      ENDIF
   15 CONTINUE
   20 CONTINUE
*
      NCM=NC-1
      IF(NC.EQ.1) NCM=1
      DO 25 K=1,NCM
      JJ=K+1
      DO 25 J=JJ,NC
      C(K,J)=0.0
```

```
      D(K,J)=0.0
   25 CONTINUE
      NV=NC*(NC-1)
      IF(NC.EQ.1) NV=1


*
*   goto 50 for dia,HETP input
*
      IF(IM.EQ.2) GOTO 50
      WRITE(*,*) ' ENTER SECTION TO BE SOLVED '
      WRITE(*,*) ' 1 = ENRICHING  :  2 = STRIPPING '
      READ(*,*) IS
*  input for enriching section
      IF(IS.EQ.1) THEN
      WRITE(*,*) 'ENTER THE ENRICHING SECTION AREA AND
      HEIGHT (ft/ft2)' READ(*,*) STRA,STRH
      WRITE(*,*) 'ENTER THE DISTILLATE RATE lbmole/hr'
      READ(*,*) DT
      WRITE(*,*) 'ENTER THE REFLUX RATIO '
      READ(*,*) REFR
      DO 30 K=1,NC
      WRITE(*,*) 'ENTER VAPOR COMPOSITION AT THE FEED
      POINT'
      WRITE(*,*) 'FOR COMPONENT ',K
      READ(*,*) YBOT(K)
   30 CONTINUE
      ENDIF
      WRITE(*,*) 'ENTER THE PRESSURE IN THE COLUMN'
      PP(1)=1.03
*  input for stripping section
      IF(IS.EQ.2) THEN
      WRITE(*,*) 'PLEASE ENTER THE AREA AND HEIGHT '
      WRITE(*,*) ' OF THE STRIPPING SECTION  '
      READ(*,*) STA,STH
      WRITE(*,*) ' PLEASE ENTER LIQUID RATE AT THE FEED
      POINT'
      READ(*,*) SL1
      WRITE(*,*) ' PLEASE ENTER VAPOR RATE AT THE FEED
      POINT'
      READ(*,*) SV1
      DO 40 K=1,NC
      WRITE(*,*) 'ENTER LIQUID COMPOSITION AT THE FEED
      POINT'
      WRITE(*,*) 'FOR COMPONENT ',K
   40 READ(*,*) XTOP(K)
      ENDIF
      GOTO 2100

*
*   Input for VLE , diameter and HETP of the packed column.
*
```

```
   50 WRITE(*,*) 'ENTER EOS TO BE USED'
      WRITE(*,*) '1=VP,2=SRK,3=PR '
      READ(*,*) IEOS
      WRITE(*,*) ' ENTER TYPE OF VLE CALCULATION '
      WRITE(*,*) ' 1=FLASH CALCULATIONS '
      WRITE(*,*) ' 2=BUBBLE POINT PRESSURE '
      WRITE(*,*) ' 3=BUBBLE POINT TEMPERATURE '
      WRITE(*,*) ' 4=DEW POINT PRESSURE '
      WRITE(*,*) ' 5=DEW POINT TEMPERATURE '
      READ(*,*) IPROP

      DO 400 I=1,NPT
      WRITE(*,*) ' ENTER T,P & Z s '
      READ (*,*) T(I),PP(I),(ZE(I,J),J=1,NC)
C
      SUM=0.0
      DO 70 J=1,NC
        SUM=SUM+ZE(I,J)
   70 CONTINUE
C
      DO 100 J=1,NC
      ZE(I,J)=ZE(I,J)/SUM
      IF(IUNIT.EQ.1) GOTO 100
      TB(J)=(TB(J)+459.67)/1.8
      TC(J)=(TC(J)+459.67)/1.8
      PC(J)=PC(J)/14.5038
  100 CONTINUE
C
      NCM=NC-1
      IF(NC.EQ.1) NCM=1
      DO 150 K=1,NCM
      JJ=K+1
      DO 150 J=JJ,NC
      C(K,J)=0.0
      D(K,J)=0.0
  150 CONTINUE
      NV=NC*(NC-1)
      IF(NC.EQ.1) NV=1
C
  170 CONTINUE
      IF(IUNIT.EQ.1) GOTO 171
      T(I)=(T(I)+459.67)/1.8
      PP(I)=PP(I)/14.5038
  171 P(I)=PP(I)
  300 CONTINUE
  400 CONTINUE
C
 1000
     FORMAT(/1X,2A4,1X,3F8.4/1X,5F8.4,1X/1X,5F8.4,1X/1X,5F1
     0.5, &1X/1X,5F10.5,1X/1X,5F4.2,1X/)
C*****
C THIS IS THE END OF THE INPUT SECTION FOR THE VLE CALC.
```

```
C*****
      PAUSE
C --- DIAMETER CALC. INPUT---
      WRITE(*,*) 'PLEASE ENTER PACKING ID NO.'
      READ(*,*) IPP
      WRITE(*,*) 'PLEASE ENTER L/V AT THIS SECTION OF THE
      COLUMN' READ(*,*) FLV
      WRITE(*,*) 'PLEASE ENTER REFLUX (D) IBMOL/HR'
      READ (*,*) DREF
      WRITE(*,*) 'WOULD YOU LIKE TO CARRY OUT PRESSURE
      BASED (1)' WRITE(*,*) ' OR %FLOOD BASED (2)
      CALCULATIONS'
      READ(*,*) ND
      DO 500 K=1,30
      READ(12,2000) (DUMMY(J),J=1,10)
      IF(K.EQ.IPP) THEN
      PF=DUMMY(3)
      ALPH=DUMMY(4)
      BETA=DUMMY(5)
      ENDIF
  500 CONTINUE
      IF(ND.EQ.1) THEN
      WRITE(*,*) 'PLEASE SPECIFY THE PRESSURE DROP'
      READ(*,*) DELP
      ENDIF
C***
C HETP CALCULATION INPUT
C***
      WRITE(*,*) 'PLEASE ENTER THE SLOPE OF THE EQUILIBRIUM
      CURVE' READ(*,*) SLP
      WRITE(*,*) 'PLEASE ENTER THE HEIGHT OF THE PACKING'
      READ(*,*) HP
C
C-----END OF INPUT-----------
C
 2000 FORMAT(/1X,2A4,1X,3F8.4,1X/1X,5F8.4,1X/)
      PAUSE
 2100 RETURN
      END ***
      SUBROUTINE VLE
***
      IMPLICIT REAL*8 (A-H,O-Z)
C-----
      COMMON/CVLE/ X(20),XMAX(20),XMIN(20),DELTC(20),
      DELMN(20),NV,MAXIT,NPTS
      COMMON/V0/ TC(20),PC(20),OMG(20),TB(20),WT(20),
      ZRA(20),A1(20),AL(20),B1(20),BL(20)
      COMMON/V1/ RHOL(5),RHOV(5),RHOLC(5),RHOVC(5),WTM(5),
     &           T(5),P(5),PP(5),ALFAS(5)
      COMMON/VE/ XE(5,20),YE(5,20),ZE(5,20),KE(5,20),
      C(20,20)
      COMMON/VC/ XC(5,20),YC(5,20),ZZ(5,20),KC(5,20),
```

```
      D(20,20)
      COMMON/VF/ PHL(5,20),PHV(5,20),FUGL(5,20),FUGV(5,20),
      KO(5,20)
      COMMON/V2/ LAMB,PHI,OMGM,PCM
      COMMON/V3/ OMGB,GC,OMGM2,OMGM3
      COMMON/V4/ MIX,NPT,IEOS,IN,IO,LP,IP,NC,KY,INPT
      COMMON/V5/ AN(20,5),TITLE(15)
      COMMON/V6/ A,AAL,B,BBL,U,UU,W,WW,ZC,R,TOL,LV,LL,
      MODE,KM,IERR,IPR OP
      COMMON/ENRCHI/ STRA,STRH,REFR,YBOT(20),DT,IM
      DOUBLE PRECISION KO,KC,KE
C
      LL=LL+1
      K =0
      NCM=NC-1
      IF(NC.EQ.1) NCM=1
      DO 1 I=1,NCM
      JJ=I+1
      DO 1 J=JJ,NC
      K=K+1
      IF(LL.EQ.1) THEN
      X(K)=C(I,J)
      X(K+NV/2)=D(I,J)
      ELSE
      C(I,J)=X(K)
      D(I,J)=X(K+NV/2)
      ENDIF
    1 CONTINUE
C
      DO 600 I=1,NPT
      KM=0
      KY=0
   10 CONTINUE
      KM=KM+1
      IF(IEOS.EQ.1) GOTO 64
      IF(KM.EQ.1) CALL INITIAL(I)
C
      LV=1
      DO 61 J=1,NC
   61 ZZ(I,J)=XC(I,J)
      CALL MIXING(I)
      CALL EOS
                              RHOLC(I)=P(I)*WTM(I)/(ZCT(I))
      CALL FUGACITY(I)
C
      LV=2
      DO 62 J=1,NC
   62 ZZ(I,J)=YC(I,J)
      CALL MIXING(I)
      CALL EOS
                              RHOVC(I)=P(I)*WTM(I)/(ZCT(I))
      CALL FUGACITY(I)
```

```
   64 IF(IEOS.EQ.1) CALL VAPPR(I)
      GOTO (71,72,72,73,73), IPROP
   71 CALL FLASH(I)
      CALL UPDATE(I)
      IERRM=IERR
      GOTO 80
   72 CALL BUBBL(I)
      IERRM=IERR
      GOTO 80
C *******     INSERT DEW PT.  HERE *****
   73 CALL DEW(I)
      IERRM=IERR
      GOTO 80
   80 IF(KM.GT.100) WRITE(6,*) I,KM,'NO VLE CONVERGENCE'
      IF(IERRM.EQ.1) GOTO 10
      IF(IM.EQ.2) CALL HANKTHM(I)
  600 CONTINUE
      RETURN
      END
***
      SUBROUTINE UPDATE(I)
***
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON/V1/ RHOL(5),RHOV(5),RHOLC(5),RHOVC(5),WTM(5),
     &           T(5),P(5),PP(5),ALFAS(5)
      COMMON/VE/ XE(5,20),YE(5,20),ZE(5,20),KE(5,20),
      C(20,20)
      COMMON/VC/ XC(5,20),YC(5,20),ZZ(5,20),KC(5,20),
      D(20,20)
      COMMON/VF/ PHL(5,20),PHV(5,20),FUGL(5,20),FUGV(5,20),
      KO(5,20)
      COMMON/V4/ MIX,NPT,IEOS,IN,IO,LP,IP,NC,KY,INPT
      COMMON/V6/ A,AAL,B,BBL,U,UU,W,WW,ZC,R,TOL,LV,
      LL,MODE,KM,IERR,IPR OP
      COMMON/VP/ PVAP(20),VPB1(20),VPB2(20),VPB3(20),
      VPB4(20)
      DOUBLE PRECISION KO,KC,KE
C
      IERR=0
  10  TOL=0.0001
      DO 140 J=1,NC
         KO(I,J)=KC(I,J)
         IF(IEOS.EQ.1) THEN
         KC(I,J)=PVAP(J)/P(I)
         GOTO 20
         ENDIF
         KC(I,J)=PHL(I,J)/PHV(I,J)
  20     ERR=( KC(I,J)/KO(I,J) - 1.0)
         IF(DABS(ERR).GT.TOL) IERR=1
 140  CONTINUE
      RETURN
      END
```

```
***
      SUBROUTINE INITIAL(I)
***
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON/V0/ TC(20),PC(20),OMG(20),TB(20),WT(20),
      ZRA(20),A1(20),AL(20),B1(20),BL(20)
      COMMON/V1/ RHOL(5),RHOV(5),RHOLC(5),RHOVC(5),WTM(5),
     &           T(5),P(5),PP(5),ALFAS(5)
      COMMON/VE/ XE(5,20),YE(5,20),ZE(5,20),KE(5,20),
      C(20,20)
      COMMON/VC/ XC(5,20),YC(5,20),ZZ(5,20),KC(5,20),
      D(20,20)
      COMMON/VF/ PHL(5,20),PHV(5,20),FUGL(5,20),FUGV(5,20),
      KO(5,20)
      COMMON/V2/ LAMB,PHI,OMGM,PCM
      COMMON/V3/ OMGB,GC,OMGM2,OMGM3
      COMMON/V4/ MIX,NPT,IEOS,IN,IO,LP,IP,NC,KY,INPT
      COMMON/V5/ AN(20,5),TITLE(15)
      COMMON/V6/ A,AAL,B,BBL,U,UU,W,WW,ZC,R,TOL,LV,
      LL,MODE,KM,IERR,IPR OP
      DOUBLE PRECISION KO,KC,KE
C
C INITIAL GUESS FOR K VALUE FOR INITIAL FLASH CALCULATION
C
      GOTO (102,101,101,101,101),IPROP
  101 CONTINUE
      ALFA=0.5
         SUMX=0.0
         SUMY=0.0
      DO 10 J=1,NC
         WRITE(*,*) 'T,P',T(1),P(1),PC(J),TC(J)
         P(I)=PP(I)
         PR=P(I)/PC(J)
         TR=T(I)/TC(J)
         WRITE(*,*) TR,PR
         IF(INPT.EQ.1) GOTO 5
         KC(I,J)=DLOG(1./PR) + 5.373*(1.+OMG(J))*(1.-1./TR)
         KC(I,J)=DEXP(KC(I,J))
         YC(I,J)=KC(I,J)*ZE(I,J)/(ALFA+(1.-ALFA)*KC(I,J))
         XC(I,J)=ZE(I,J)/(ALFA+(1.-ALFA)*KC(I,J))
         GOTO 6
   5     KC(I,J)=YE(I,J)/XE(I,J)
         YC(I,J)=YE(I,J)
         XC(I,J)=XE(I,J)
   6     SUMX=SUMX+XC(I,J)
         SUMY=SUMY+YC(I,J)
  10  CONTINUE
      DO 20 J=1,NC
         XC(I,J)=XC(I,J)/SUMX
         YC(I,J)=YC(I,J)/SUMY
  20  CONTINUE
      RETURN
```

```
  102 CONTINUE
         P(I)=PP(I)
      DO 200 J=1,NC
         PR=P(I)/PC(J)
         TR=T(I)/TC(J)
         XC(I,J)=XE(I,J)
         YC(I,J)=YE(I,J)
         KC(I,J)=YC(I,J)/XC(I,J)
  200 CONTINUE
      RETURN
      END
***
      SUBROUTINE FLASH(I) ***
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON/V0/
      TC(20),PC(20),OMG(20),TB(20),WT(20),ZRA(20),
     &           A1(20),AL(20),B1(20),BL(20)
      COMMON/V1/ RHOL(5),RHOV(5),RHOLC(5),RHOVC(5),WTM(5),
     &           T(5),P(5),PP(5),ALFAS(5)
      COMMON/VE/ XE(5,20),YE(5,20),ZE(5,20),KE(5,20),
      C(20,20)
      COMMON/VC/ XC(5,20),YC(5,20),ZZ(5,20),KC(5,20),
      D(20,20)
      COMMON/VF/ PHL(5,20),PHV(5,20),FUGL(5,20),FUGV(5,20),
      KO(5,20)
      COMMON/V2/ LAMB,PHI,OMGM,PCM
      COMMON/V3/ OMGB,GC,OMGM2,OMGM3
      COMMON/V4/ MIX,NPT,IEOS,IN,IO,LP,IP,NC,KY,INPT
      COMMON/V5/ AN(20,5),TITLE(15)
      COMMON/V6/ A,AAL,B,BBL,U,UU,W,WW,ZC,R,TOL,LV
      ,LL,MODE,KM,IERR,IPR OP
      COMMON/VP/ PVAP(20),VPB1(20),VPB2(20),VPB3(20),
      VPB4(20)
      DOUBLE PRECISION KO,KC,KE
      LIMIT=20
      TOL=0.00001
C
C BUBLE AND DEW POINT CHECK
C
      SUMB=0.0
      SUMD=0.0
      DO 40 J=1,NC
        IF(IEOS.EQ.1) KC(I,J)=PVAP(J)/P(I)
         BUB=ZE(I,J)*KC(I,J)
         DEW=ZE(I,J)/KC(I,J)
         SUMD=SUMD+DEW
         SUMB=SUMB+BUB
 40   CONTINUE
C
C
      IF(SUMB.LT.1.0) GOTO 100
      IF(SUMD.LT.1.0) GOTO 200
```

```
C
C FLASH CALCUALATIONS
C
      ALFA=0.5
      KK  =0.0
  60  CONTINUE
      SUMFF=0.0
      SUMDF=0.0
      DO 80 J=1,NC
         DD=ALFA+(1.-ALFA)*KC(I,J)
         FF=ZE(I,J)*(1.-KC(I,J))/DD
         DF=( ZE(I,J)*(1.-KC(I,J))**2 )/DD/DD
         SUMFF=SUMFF+FF
         SUMDF=SUMDF-DF
  80  CONTINUE
C
      IF(DABS(SUMFF).LT.TOL) GOTO 300
      ALFAO=ALFA
      ALFA=ALFA-SUMFF/SUMDF
      IF(ALFA.LT.0.0) ALFA=ALFAO/2.
      IF(ALFA.GT.1.0) ALFA=(1.+ALFAO)/2.
      KK=KK+1
      IF(KK.LE.20) GOTO 60
      IF(KK.GT.20.AND.KM.EQ.60) WRITE(6,*) I,'NO
      CONVERGENCE IN FLASH' GO TO 300
C
 100  ALFA=1.0
      IF(KM.EQ.100) WRITE(6,*) I,KM,'SUBCOOLED LIQUID'
      GOTO 300
C
 200  ALFA=0.0
      IF(KM.EQ.100) WRITE(6,*) I,KM,'SUPERHEAT VAPOR'
 300  SUMX=0.0
      SUMY=0.0
      ALFAS(I)=ALFA
      DO 400 J=1,NC
         YC(I,J)=KC(I,J)*ZE(I,J)/(ALFA+(1.-ALFA)*KC(I,J))
         XC(I,J)=ZE(I,J)/(ALFA+(1.-ALFA)*KC(I,J))
         SUMX=SUMX+XC(I,J)
         SUMY=SUMY+YC(I,J)
  400 CONTINUE
      DO 500 J=1,NC
         XC(I,J)=XC(I,J)/SUMX
         YC(I,J)=YC(I,J)/SUMY
  500 CONTINUE
      RETURN
      END
C
***
      SUBROUTINE BUBBL(I) ***
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON/V0/ TC(20),PC(20),OMG(20),TB(20),WT(20),
```

```
      ZRA(20),A1(20),AL(20),B1(20),BL(20)
      COMMON/V1/ RHOL(5),RHOV(5),RHOLC(5),RHOVC(5),WTM(5),
     &           T(5),P(5),PP(5),ALFAS(5)
      COMMON/VE/ XE(5,20),YE(5,20),ZE(5,20),KE(5,20),
      C(20,20)
      COMMON/VC/ XC(5,20),YC(5,20),ZZ(5,20),KC(5,20),
      D(20,20)
      COMMON/VF/ PHL(5,20),PHV(5,20),FUGL(5,20),FUGV(5,20),
      KO(5,20)
      COMMON/V2/ LAMB,PHI,OMGM,PCM
      COMMON/V3/ OMGB,GC,OMGM2,OMGM3
      COMMON/V4/ MIX,NPT,IEOS,IN,IO,LP,IP,NC,KY,INPT
      COMMON/V5/ AN(20,5),TITLE(15)
      COMMON/V6/ A,AAL,B,BBL,U,UU,W,WW,ZC,R,TOL,LV,
      LL,MODE,KM,IERR,IPR OP
      COMMON/VP/ PVAP(20),VPB1(20),VPB2(20),VPB3(20),
      VPB4(20)
      DOUBLE PRECISION KO,KC,KE,TYE(10,20)
      TOL=0.0001

      TOL1=0.1
      ALFAS(I)=1.0

      IERR=0
      SUM=0.0
      DO 10 IL=1,NC
      TYE(1,IL)=YC(1,IL)
      IF(IEOS.EQ.1) THEN
      KC(1,IL)=PVAP(IL)/P(1)
      GOTO 5
      ENDIF
      KC(1,IL)=PHL(1,IL)/PHV(1,IL)
    5 YC(1,IL)=ZE(1,IL)*KC(1,IL)
      XC(1,IL)=ZE(1,IL)
   10 CONTINUE
      DO 20 J=1,NC
      SUM=SUM+YC(1,J)
   20 CONTINUE
      WRITE(*,*)SUM
      YM=1.0-SUM
      IF(DABS(YM).GT.TOL) GOTO 22
      GOTO 30
   22 CONTINUE
      IF(IPROP.EQ.2) THEN
      CALL PRESSURE(YM)
      IERR=1
      GOTO 40
      ENDIF
      IF(IPROP.EQ.3) THEN
      WRITE(*,*) 'T(1)=',T(1)
      CALL TEMP(YM)
      WRITE(*,*) 'YM=',YM
```

```
      IERR=1
      GOTO 40
      ENDIF
   30 CONTINUE
      DO 35 K=1,NC
      IF(DABS(YC(1,K)-TYE(1,K)).GT.TOL1) WRITE(*,*)
      YC(1,K),TYE(1,K)
   35 CONTINUE
   40 CONTINUE
      RETURN
      END ***
      SUBROUTINE MIXING(I) ***
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON/V0/
      TC(20),PC(20),OMG(20),TB(20),WT(20),ZRA(20),
     &           A1(20),AL(20),B1(20),BL(20)
      COMMON/V1/ RHOL(5),RHOV(5),RHOLC(5),RHOVC(5),WTM(5),
     &           T(5),P(5),PP(5),ALFAS(5)
      COMMON/VE/ XE(5,20),YE(5,20),ZE(5,20),KE(5,20),
      C(20,20)
      COMMON/VC/ XC(5,20),YC(5,20),ZZ(5,20),KC(5,20),
      D(20,20)
      COMMON/VF/ PHL(5,20),PHV(5,20),FUGL(5,20),FUGV(5,20),
      KO(5,20)
      COMMON/V2/ LAMB,PHI,OMGM,PCM
      COMMON/V3/ OMGB,GC,OMGM2,OMGM3
      COMMON/V4/ MIX,NPT,IEOS,IN,IO,LP,IP,NC,KY,INPT
      COMMON/V5/ AN(20,5),TITLE(15)
      COMMON/V6/ A,AAL,B,BBL,U,UU,W,WW,ZC,R,TOL,LV,
      LL,MODE,KM,IERR,IPR OP
      DOUBLE PRECISION KO,KC,KE
C-----
      R=83.14
      TOL=0.00001
      B=0.
      OMGM=0.
      SWTM=0.
C
      DO 20 J=1,NC
      TR=T(I)/TC(J)
      TR2=TR*TR
      PR=P(I)/PC(J)
      OMGM=OMG(J)
      OMGM2=OMGM*OMGM
      OMGM3=OMGM2*OMGM
C
C-----EOS A AND B DEFINITIONS
C
      IF (IEOS.EQ.1) THEN
C************* INSERT VAPOR PRESSURE CALC.****************
      ELSE IF(IEOS.EQ.2) THEN
        FA=0.48+1.574*OMGM+0.176*OMGM2
```

```
          OMGB=0.08664
          OMGA=0.42747
        ELSE IF(IEOS.EQ.3)THEN
          FA=(0.37646+1.54226*OMGM-0.26992*OMGM**2)
          OMGA=0.457235
          OMGB=0.077796
        END IF
C
C-----RK MIXING RULES
C
        ALPH=(1+FA*(1-TR**0.5))**2
        A1(J)=OMGA*PR*ALPH/TR2
                                AL(J)=OMGA*ALPHR*TC(J)*TC(J)/PC(J)
        B1(J)=OMGB*PR/TR
                                               BL(J)=OMGBTC(J)/PC(J)
   20 CONTINUE
        SUMA=0.0
        SUMB=0.0
        SUMAL=0.0
        SUMBL=0.0
        SUMO=0.0
        SUMW=0.0
        DO 22 J=1,NC
        DO 21 K=1,NC
        C(K,K)=0.0
        D(K,K)=0.0
        C(K,J)=C(J,K)
        D(K,J)=D(J,K)
        AA=(1.-C(K,J))*(A1(K)*A1(J))**0.5
        BB=(1.+D(K,J))*(B1(K)+B1(J))*0.5 AAL=(1.-
        C(K,J))*(AL(K)*AL(J))**0.5
        BBL=(1.+D(K,J))*(BL(K)+BL(J))*0.5
        SUMA=SUMA+ZZ(I,K)*ZZ(I,J)*AA
        SUMB=SUMB+ZZ(I,K)*ZZ(I,J)*BB
        SUMAL=SUMAL+ZZ(I,K)*ZZ(I,J)*AAL
  21    SUMBL=SUMBL+ZZ(I,K)*ZZ(I,J)*BBL
        SUMW=SUMW+WT(J)*ZZ(I,J)
  22    SUMO=SUMO+OMG(J)*ZZ(I,J)
C-----
        A=SUMA
        B=SUMB
        AAL=SUMAL
        BBL=SUMBL
        OMGM=SUMO
        WTM(I)=SUMW
C
C-----EOS SELECTION SETUP, DEFINITIONS OF U AND W
C
   25 IF (IEOS.EQ.1) THEN
        U=1
        W=0
        ELSE IF(IEOS.EQ.2) THEN
```

```
      U=1
      W=0
      ELSE IF(IEOS.EQ.3)THEN
      U=2
      W=-1
      END IF
      RETURN
      END ***
      SUBROUTINE EOS ***
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON/V1/ RHOL(5),RHOV(5),RHOLC(5),RHOVC(5),WTM(5),
     &           T(5),P(5),PP(5),ALFAS(5)
      COMMON/V6/ A,AAL,B,BBL,U,UU,W,WW,ZC,R,TOL,LV,
      LL,MODE,KM,IERR,IPR OP
      REAL LAMB
      KK=0
      D=U*B-B-1
      E=W*B**2-U*B**2-U*B+A
      F=W*B**3+W*B**2+B*A
      LAMB=4*D**2-12*E
      IF(LAMB.LE.0.) THEN
        IF(LV.EQ.1)ZI=0.1
        IF(LV.EQ.2)ZI=1.0
      ELSE
        Z1=(-2*D-LAMB**0.5)/6
        Z2=(-2*D+LAMB**0.5)/6
        FZ1=Z1**3+D*Z1**2+E*Z1-F
        FZ2=Z2**3+D*Z2**2+E*Z2-F
             IF(LV.EQ.1.AND.FZ1.GT.0.0) ZI=(Z1+B)/2.
             IF(LV.EQ.1.AND.FZ1.LT.0.0) ZI=(Z2+1.)/2.
             IF(LV.EQ.2.AND.FZ2.LT.0.0) ZI=(Z2+1.)/2.
             IF(LV.EQ.2.AND.FZ2.GT.0.0) ZI=(Z1+B)/2.
      END IF
   99 ZC=ZI
  100 CONTINUE
      FZC=ZC**3+D*ZC**2+E*ZC-F
      DFC=3*ZC**2+2*D*ZC+E
      ZCN=ZC-FZC/DFC
C
      IF(ZC.LE.B) ZC=1.01*B
C
      ZTEST=(ZCN-ZC)
      TEST=DABS(ZTEST)
      KK=KK+1
      IF(TEST.GT.TOL.AND.KK.LT.50) THEN
      ZC=ZCN
      GO TO 100
      ELSE
      IF(KK.EQ.50) WRITE(6,*) 'NO CUBIC CONVERAGENCE IN 50
      ITERATIONS' END IF
      RETURN
      END ***
```

```
      SUBROUTINE OUTPUT ***
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON/V0/
      TC(20),PC(20),OMG(20),TB(20),WT(20),ZRA(20),
     &           A1(20),AL(20),B1(20),BL(20)
      COMMON/V1/ RHOL(5),RHOV(5),RHOLC(5),RHOVC(5),WTM(5),
     &           T(5),P(5),PP(5),ALFAS(5)
      COMMON/VE/ XE(5,20),YE(5,20),ZE(5,20),KE(5,20),
      C(20,20)
      COMMON/VC/ XC(5,20),YC(5,20),ZZ(5,20),KC(5,20),
      D(20,20)
      COMMON/V2/ LAMB,PHI,OMGM,PCM
      COMMON/V3/ OMGB,GC,OMGM2,OMGM3
      COMMON/V4/ MIX,NPT,IEOS,IN,IO,LP,IP,NC,KY,INPT
      COMMON/V5/ AN(20,5),TITLE(15)
      COMMON/V6/ A,AAL,B,BBL,U,UU,W,WW,ZC,R,TOL,LV,
      LL,MODE,KM,IERR,IPR OP
      DOUBLE PRECISION KO,KC,KE
C
      IF(IEOS.EQ.1) WRITE(LP,1251)
      IF(IEOS.EQ.2) WRITE(LP,1252)
      IF(IEOS.EQ.3) WRITE(LP,1253)
      WRITE(LP,1000) (TITLE(I),I=1,15)
      WRITE(LP,1350)
      WRITE(LP,2000)
      WRITE(LP,1350)
      DO 600 I=1,NPT
      DO 600 J=1,NC
      IF(J.EQ.1) WRITE(LP,2100)
      I,J,T(I),P(I),ZE(I,J),XC(I,J),YC(I,J),
     &KC(I,J),RHOLC(I),RHOVC(I),ALFAS(I)
  600 IF(J.NE.1) WRITE(LP,2200)
      J,ZE(I,J),XC(I,J),YC(I,J),KC(I,J)
      WRITE(LP,1350)
C
 900  WRITE(LP,1500)
C
C
 1000 FORMAT(1H,15A4)
 1251 FORMAT(1H,'VAPOR-PRESSURE EOS PREDICTIONS        ')
 1252 FORMAT(1H,'SOAVE-RK EQUATION OF STATE PREDICTIONS')
 1253 FORMAT(1H,'PENG-ROBINSON EQUATION OF STATE
 PREDICTIONS')
 1350 FORMAT(1H,'----------------------------------------
     ------------&----------------------')
 1500 FORMAT(1H, ' ')
 2000 FORMAT(' I COMP. T(K)   P(BAR)   Z(I)   X(I)   Y(I)
     K(I)   DL(G &/CC) DV(G/CC)  L/N')
 2100 FORMAT(2I3,2X,F6.1,F7.2,7F8.4)
 2200 FORMAT(3X,I3,15X,7F8.4)
C******
      RETURN
```

```
      END ***
      SUBROUTINE FUGACITY(I) ***
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON/V0/ TC(20),PC(20),OMG(20),TB(20),WT(20),
      ZRA(20),A1(20),AL(20),B1(20),BL(20)
      COMMON/V1/ RHOL(5),RHOV(5),RHOLC(5),RHOVC(5),WTM(5),
     &           T(5),P(5),PP(5),ALFAS(5)
      COMMON/VE/ XE(5,20),YE(5,20),ZE(5,20),KE(5,20),
      C(20,20)
      COMMON/VC/ XC(5,20),YC(5,20),ZZ(5,20),KC(5,20),
      D(20,20)
      COMMON/VF/ PHL(5,20),PHV(5,20),FUGL(5,20),FUGV(5,20),
      KO(5,20)
      COMMON/V2/ LAMB,PHI,OMGM,PCM
      COMMON/V3/ OMGB,GC,OMGM2,OMGM3
      COMMON/V4/ MIX,NPT,IEOS,IN,IO,LP,IP,NC,KY,INPT
      COMMON/V5/ AN(20,5),TITLE(15)
      COMMON/V6/ A,AAL,B,BBL,U,UU,W,WW,ZC,R,TOL,LV,
      LL,MODE,KM,IERR,IPR OP
      DOUBLE PRECISION KO,KC,KE
C-----
      DO 100 J=1,NC
CT4
      SUMA=0.0
      DO 10 K=1,NC
      SUMA=SUMA+ZZ(I,K)*(1.-C(J,K))*AL(K)**.5
   10 CONTINUE
      T4= (2*SUMA*DSQRT(AL(J))/AAL) - (BL(J)/BBL)
CT3
      BX=U*U-4.0*W
      BX=BX**0.5
      BB=(2.*ZC+B*(U+BX))/(2.*ZC+B*(U-BX))
      IF(BB.LE.0.0) BB=1.D-20
      CC=DLOG(BB)
      T3=CC*A/(B*BX)
CT2
      DD=ZC-B
      IF(DD.LE.0.0) DD=1.D-20
      T2=DLOG(DD)
CT1
      T1=BL(J)*(ZC-1.0)/BBL
CSUM
      FUG=T1-T2-T3*T4
      IF(FUG.GT.174.) FUG=170.
      IF(FUG.LT.-174.) FUG=-170.
      FUG=DEXP(FUG)
      IF(LV.EQ.1) PHL(I,J)=FUG
      IF(LV.EQ.1) FUGL(I,J)=FUG*P(I)*XC(I,J)
      IF(LV.EQ.2) PHV(I,J)=FUG
      IF(LV.EQ.2) FUGV(I,J)=FUG*P(I)*YC(I,J)
  100 CONTINUE
      RETURN
```

```
      END ***
      SUBROUTINE TEMP(XM) ***
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON/V1/ RHOL(5),RHOV(5),RHOLC(5),RHOVC(5),WTM(5),
     &           T(5),P(5),PP(5),ALFAS(5)
      COMMON/V6/ A,AAL,B,BBL,U,UU,W,WW,ZC,R,TOL,LV,
      LL,MODE,KM,IERR,IPR OP
      WRITE(*,*) 'IN SUB T(1)=',T(1)
      TM=T(1)
      WRITE(*,*) 'TM=',TM,KM
      IF(KM.EQ.1) THEN
      TM1=1.05*TM
      WRITE(*,*) 'KM=1, TM1=',TM1
      GOTO 30
      ENDIF
   10 CONTINUE
      TM1=TM-(((TM-TM0)*XM)/(XM-XM0))
      DTM=TM1-TM
      IF(DABS(TM1-TM).LT.10) GOTO 30
      IF(DTM.GT.0) TM1=TM+10
      IF(DTM.LT.0) TM1=TM-10
   30 CONTINUE
      TM0=TM
      XM0=XM
      WRITE(*,*) 'TM1=',TM1
      T(1)=TM1
      RETURN
      END
*** SUBROUTINE PRESSURE(ZM) ***
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON/V1/ RHOL(5),RHOV(5),RHOLC(5),RHOVC(5),WTM(5),
     &           T(5),P(5),PP(5),ALFAS(5)
      COMMON/V6/ A,AAL,B,BBL,U,UU,W,WW,ZC,R,TOL,LV,
      LL,MODE,KM,IERR,IPR OP
      DOUBLE PRECISION PM,PM1,PM0,ZM,ZM0
      WRITE(*,*) 'IN SUB P(1)=',P(1)
      PM=P(1)
      WRITE(*,*) 'PM=',PM
      IF(KM.EQ.1) THEN
      PM1=1.05*PM
      WRITE(*,*) 'KM=1,PM1=',PM1
      GOTO 30
      ENDIF
   10 CONTINUE
      PM1=DEXP(DLOG(PM)-(((DLOG(PM)-DLOG(PM0))*ZM)/(ZM-
      ZM0)))
      DPM=DLOG(PM1)-DLOG(PM)
      IF(DABS(DPM).LT.1.5) GOTO 30
      IF(DPM.GT.0.) PM1=DEXP(DLOG(PM)+1.5)
      IF(DPM.LT.0.) PM1=DEXP(DLOG(PM)-1.5)
   30 CONTINUE
      PM0=PM
```

```
      ZM0=ZM
      P(1)=DEXP(DLOG(PM1))
      RETURN
      END ***
      SUBROUTINE DEW(I) ***
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON/V0/
      TC(20),PC(20),OMG(20),TB(20),WT(20),ZRA(20),
     &           A1(20),AL(20),B1(20),BL(20)
      COMMON/V1/ RHOL(5),RHOV(5),RHOLC(5),RHOVC(5),WTM(5),
     &           T(5),P(5),PP(5),ALFAS(5)
      COMMON/VE/ XE(5,20),YE(5,20),ZE(5,20),KE(5,20),
      C(20,20)
      COMMON/VC/ XC(5,20),YC(5,20),ZZ(5,20),KC(5,20),
      D(20,20)
      COMMON/VF/ PHL(5,20),PHV(5,20),FUGL(5,20),FUGV(5,20),
      KO(5,20)
      COMMON/V2/ LAMB,PHI,OMGM,PCM
      COMMON/V3/ OMGB,GC,OMGM2,OMGM3
      COMMON/V4/ MIX,NPT,IEOS,IN,IO,LP,IP,NC,KY,INPT
      COMMON/V5/ AN(20,5),TITLE(15)
      COMMON/V6/ A,AAL,B,BBL,U,UU,W,WW,ZC,R,TOL,LV,
      LL,MODE,KM,IERR,IPR OP
      COMMON/VP/ PVAP(20),VPB1(20),VPB2(20),VPB3(20),
      VPB4(20)
      DOUBLE PRECISION KO,KC,KE,TXE(10,20)
      TOL=0.0001

      TOL1=0.1
      ALFAS(I)=0.0

      IERR=0
      SUM=0.0
      DO 10 IL=1,NC
      TXE(1,IL)=XC(1,IL)
      IF(IEOS.EQ.1) THEN
      WRITE(*,*) PVAP(IL),P(I)
      KC(1,IL)=PVAP(IL)/P(I)
      WRITE(*,*) KC(1,IL)
      GOTO 5
      ENDIF
      KC(1,IL)=PHL(1,IL)/PHV(1,IL)
    5 XC(1,IL)=ZE(1,IL)/KC(1,IL)
      YC(1,IL)=ZE(1,IL)
   10 CONTINUE
      DO 20 J=1,NC
      SUM=SUM+XC(1,J)
   20 CONTINUE
      WRITE(*,*) SUM
      YM=SUM-1.0
      IF(DABS(YM).GT.TOL) GOTO 22
      GOTO 30
```

```
   22 CONTINUE
      IF(IPROP.EQ.4) THEN
      CALL PRESSURE(YM)
      IERR=1
      GOTO 40
      ENDIF
      IF(IPROP.EQ.5) THEN
      WRITE(*,*) 'T(1)=',T(1)
      CALL TEMP(YM)
      WRITE(*,*) 'YM=',YM
      IERR=1
      GOTO 40
      ENDIF
   30 CONTINUE
      DO 35 K=1,NC
      IF(DABS(XC(1,K)-TXE(1,K)).GT.TOL1)
      WRITE(*,*) XC(1,K),TXE(1,K)
   35 CONTINUE
   40 CONTINUE
      RETURN
      END
***
      SUBROUTINE VAPPR(I) ***
C        CONTAINS WAGNER EQUATION FOR VAPOR PRESSURES ***
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON/V1/ RHOL(5),RHOV(5),RHOLC(5),RHOVC(5),WTM(5),
     &           T(5),P(5),PP(5),ALFAS(5)
      COMMON/V0/ TC(20),PC(20),OMG(20),TB(20),WT(20),
      ZRA(20),A1(20),AL(20),B1(20),BL(20)
      COMMON/VP/ PVAP(20),VPB1(20),VPB2(20),VPB3(20),
      VPB4(20)
      COMMON/V4/ MIX,NPT,IEOS,IN,IO,LP,IP,NC,KY,INPT
      DOUBLE PRECISION Q,VPB
      DO 10 IJ=1,NC
      WRITE(*,*) '*',VPB1(IJ),VPB2(IJ),VPB3(IJ),VPB4(IJ)
      Q=1.0-(T(I)/TC(IJ))
      VPB=VPB1(IJ)*Q+VPB2(IJ)*Q**(3/2)+VPB3(IJ)*Q**3+VPB4(I
      J)*Q**6
      PVAP(IJ)=DEXP(DLOG(100*PC(IJ))+VPB*(TC(IJ)/T(I)))
      PVAP(IJ)=0.01*PVAP(IJ)
      WRITE(*,*) PVAP(IJ)
   10 CONTINUE
      RETURN
      END
***
      SUBROUTINE HANKTHM(I)
C***************************************************
C              HANKINSON THOMSON METHOD
C                   FOR MIXTURES
C        CVOL :CHARACTERISTIC VOLUME (LTR/MOLE)
C        HW: H-T ACENTRIC FACTOR
C***************************************************
```

```
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON/VC/ XC(5,20),YC(5,20),ZZ(5,20),KC(5,20),
      D(20,20)
      COMMON/LD/ CVOL(20),HW(20),RHOPL(20)
      COMMON/V1/ RHOL(5),RHOV(5),RHOLC(5),RHOVC(5),WTM(5),
     &           T(5),P(5),PP(5),ALFAS(5)
      COMMON/V0/ TC(20),PC(20),OMG(20),TB(20),WT(20),
      ZRA(20),A1(20),AL(20),B1(20),BL(20)
      COMMON/V4/ MIX,NPT,IEOS,IN,IO,LP,IP,NC,KY,INPT
      DOUBLE PRECISION C(10)
      C(1)=-1.52816
      C(2)=1.43907
      C(3)=-0.81446
      C(4)=0.190454
      C(5)=-0.296123
      C(6)=0.386914
      C(7)=-0.0427258
      C(8)=-0.0480645
      XV=0.0
      XV23=0.0
      XV13=0.0
      WSRK=0.0
      WM=0.0
C
      DO 10 II=1,NC
      XV=XC(1,II)*CVOL(II)+XV
      XV23=XC(1,II)*CVOL(II)**(2.0/3.0)+XV23
      XV13=XC(1,II)*CVOL(II)**(1.0/3.0)+XV13
      WSRK=XC(1,II)*HW(II)+WSRK
      WM=XC(1,II)*WT(II)+WM
   10 CONTINUE
      VM0=0.25*(XV+(3*XV23*XV13))
      DO 20 L=1,NC
      DO 20 K=1,NC
      VTXX=XC(1,L)*XC(1,K)*(CVOL(L)*TC(L)*CVOL(K)*TC(K))
      **(1.0 /2.0)+VTXX 20 CONTINUE
      TCM=VTXX/VM0
      TR=T(I)/TCM
      TQ=1.0-TR
      TS=TQ**(1.0D0/3.0D0)
      VR0=1+TS*(C(1)+C(2)*TS)+TQ*C(3)+C(4)*TS**(4.0D0)
      VRD=(C(5)+C(6)*TR+C(7)*TR*TR+C(8)*TR*TR*TR)/(TR-
      1.00001) VS=(VM0*VR0*(1-WSRK*VRD))
      DM=1.0D0/VS
      RHOLC(1)=DM*WM/1000.0
      WRITE(*,*) 'LIQUID MIXTURE DENSITY (GM/CC)',RHOLC(1)
C
C ***************************************************** C
** HANKINSON AND THOMSON **
C                         FOR PURE LIQUIDS
C ******************************************************
      DO 50 IK=1,NC
```

```
      TR=T(I)/TC(IK)
      TQ=1.0-TR
      TS=TQ**(1.0D0/3.0D0)
      VR0=1+TS*(C(1)+C(2)*TS)+TQ*C(3)+C(4)*TS**(4.0D0)
      VRD=(C(5)+C(6)*TR+C(7)*TR*TR+C(8)*TR*TR*TR)/(TR-
      1.00001) VS=(CVOL(IK)*VR0*(1-HW(IK)*VRD))
      DM=1.0D0/VS
      RHOPL(IK)=DM*WT(IK)/1000.0
      WRITE(*,*) 'PURE LIQUID DENSITY',RHOPL(IK)
   50 CONTINUE
C
      RETURN
      END
***
      SUBROUTINE DIA ***
C     THIS SUBROUTINE WILL BE USED TO ESTIMATE THE COLUMN
C     DIAMETER USING EITHER THE SPECIFIED PRESSURE DROP
C     OR THE % FLOODING. FL IS LIQUID FLOWRATE C
(lbMOLES/SEC)
C     FV IS VAPOR FLOWRATE (lbMOLES/SEC),FL/FV IS THE C
INTERNAL
C     REFLUX RATIO TO BE SPECIFIED BY THE USER.
C     ND=1 PRESSURE DROP SPECIFIED
C     ND=2 % FLOODING SPECIFIED
C     PSI=RHOLC(1)/RHOW
C
C
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON/VC/ XC(5,20),YC(5,20),ZZ(5,20),KC(5,20),
      D(20,20)
      COMMON/LD/ CVOL(20),HW(20),RHOPL(20)
      COMMON/V1/ RHOL(5),RHOV(5),RHOLC(5),RHOVC(5),WTM(5),
     &           T(5),P(5),PP(5),ALFAS(5)
      COMMON/V0/ TC(20),PC(20),OMG(20),TB(20),WT(20),
      ZRA(20),A1(20),AL(20),B1(20),BL(20)
      COMMON/V4/ MIX,NPT,IEOS,IN,IO,LP,IP,NC,KY,INPT
      COMMON/DIAM/ FLV,DREF,PF,ND,ALPH,BETA,DELP,COLD,WL
      COMMON/SRF1/ WML
      COMMON/DIF/ VISCL,VISCV,RHOW,VISCW
      WRITE(*,*) 'PF,ALPH,BETA',PF,ALPH,BETA,FLV,DREF,DELP
C  CONVERT DENSITIES TO lbs/cft
      RHOVC(1)=RHOVC(1)*1000/16.0185
      RHOLC(1)=RHOLC(1)*1000/16.0185
C
      PI=3.1415926
      WML=0.0
      WMV=0.0
      DO 10 K=1,NC
      WML=XC(1,K)*WT(K)+WML
      WMV=YC(1,K)*WT(K)+WMV
   10 CONTINUE
C
```

```
      CALL PROP
C
      GLD=(FLV*WML/WMV)
      IF(ND.EQ.2) GOTO 40
C   PRESSURE DROP BASED CALCULATIONS BEGIN HERE
      GDI=1.0
   20 EP=10**(BETA*GLD*GDI)
      GDA=((DELP*RHOVC(1))/(ALPH*EP))**(1.0/2.0)
      IF(ABS(GDA-GDI).LE.1.0E-02) GOTO 30
      GDI=GDA
      GOTO 20
   30 CONTINUE
      GOTO 100
C   % FLOODING BASED CALCULATIONS BEGIN HERE
   40 CONTINUE
      VISCV=VISCV/2.4189
      PSI=RHOLC(1)/RHOW
      FLV=GLD*(RHOVC(1)/RHOLC(1))**(1.0/2.0) RS=-1.6678-
      (1.085*DLOG10(FLV))-(0.29655*(DLOG10(FLV))**2.0)
      GDFL=(10**RS)*RHOVC(1)*RHOLC(1)*32.2
      GDFL=GDFL/(PF*PSI*VISCV**0.2)
      GDFL=GDFL**(1.0/2.0)
      GDA=0.5*GDFL
  100 CONTINUE
C THIS SECTION CALCULATES THE DIAMETER
C
C   CONVERT REFLUX D INTO lbmoles/sec
      DREF=DREF/3600
      FL=FLV*DREF/(1-FLV)
      FV=FL+DREF
      AREA=(FV*WMV)/GDA
      WL=FL*WML/AREA
      COLD=((4*AREA)/PI)**(1.0/2.0)
      WRITE(*,*) 'COLUMN DIA. (ft) IS =',COLD
      WRITE(*,*) 'MASS FLUX OF LIQUID (lbmol/ft.s)= ',WL
      RETURN
      END
***
      SUBROUTINE PROP ***
      IMPLICIT REAL *8 (A-H,O-Z)
      COMMON/V1/ RHOL(5),RHOV(5),RHOLC(5),RHOVC(5),WTM(5),
     &           T(5),P(5),PP(5),ALFAS(5)
      COMMON/SRF/ SRFTL,SRFTW
      COMMON/PARAMP/ FR,PSI,PHI,CFL
      COMMON/PTEH/ X(20),TIN,PIN,ETAX,DX
      COMMON/VC/ XC(5,20),YC(5,20),ZZ(5,20),KC(5,20),
      D(20,20)
      COMMON/V0/ TC(20),PC(20),OMG(20),TB(20),WT(20),
      ZRA(20),A1(20),AL(20),B1(20),BL(20)
      COMMON/TRAP/ ID(20),NC1
      COMMON/DIF/ VISCL,VISCV,RHOW,VISCW
      COMMON/DIFLV/ DIFL,DIFV
```

```
      TIN=1.8*T(1)-460
      PIN=PP(1)*14.7
      DO 5 I=1,20
   5  X(I)=YC(1,I)
      CALL VISELY
      VISCV=ETAX
      DO 7 J=1,20
    7 X(J)=XC(1,J)
      WRITE(*,*) 'ENTER PRESSURE /TEMPERATURE STEP'
      READ(*,*) PSTEP,TSTEP
      PIN=PIN+PSTEP
      TIN=TIN+TSTEP
      CALL VISELY
      VISCL=ETAX
      WRITE(*,*) 'VISCOSITY L/V',VISCL,VISCV

C ** DENSITY & VISCOSITY OF WATER
      PIN=PIN-PSTEP
      TIN=TIN-TSTEP
      PC(1)=PC(NC1+1)
      TC(1)=TC(NC1+1)
      OMG(1)=OMG(NC1+1)
      WT(1)=WT(NC1+1)
      TB(1)=TB(NC1+1)
      ZRA(1)=ZRA(NC1+1)
      NC1=1
      X(1)=1.0
      CALL VISELY
      WRITE(*,*) 'FOR WATER DEN/VIS',DX,ETAX
      RHOW=4.61
      VISCW=ETAX
C **
      CALL SRFTN
      WRITE(*,*) 'SURFACE TN.',SRFTL,SRFTW
      CALL DIFF
      WRITE(*,*) 'DIFFUSIVITY L/V',DIFL,DIFV
      DIFL=DIFL*3600/(10000*0.092903)
      DIFV=DIFV*3600/(10000*0.092903)
C       GOTO 50
      RHOLC(1)=RHOLC(1)*1000.0/16.0185
      RETURN
      END

***
      SUBROUTINE HETP ***
C  THIS SUBROUTINE WILL ESTIMATE THE HETP IN ANY GIVEN C
SECTION OF THE PACKED BED.
C  SPECIFY:
C  SLP=SLOPE OF EQUIL. CURVE,
C  HP= HEIGHT OF EACH PACKED SECTION
C  SC=SCHMIDT NO.        PSI,PHI,CFL=CORRELATED
C  VISC=VISCOSITY
```

```
C  DIF=DIFFUSIVITY        IP=PACKING ID NO.
C  COLD=COLUMN DIA.
C  SRFT=SURFACE TENSION. (L-LIQ./W-WATER)
C
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON/DIAM/ FLV,DREF,PF,ND,ALPH,BETA,DELP,COLD,WL
      COMMON/HETPC/ IPP,HP,SLP,HETPA
      COMMON/V1/ RHOL(5),RHOV(5),RHOLC(5),RHOVC(5),WTM(5),
     &           T(5),P(5),PP(5),ALFAS(5)
      COMMON/SRF/ SRFTL,SRFTW
      COMMON/PARAMP/ FR,PSI,PHI,CFL
      COMMON/PTEH/ X(20),TIN,PIN,ETAX,DX
      COMMON/VC/ XC(5,20),YC(5,20),ZZ(5,20),KC(5,20),
      D(20,20)
      COMMON/V0/ TC(20),PC(20),OMG(20),TB(20),WT(20),
      ZRA(20),A1(20),AL(20),B1(20),BL(20)
      COMMON/TRAP/ ID(20),NC1
      COMMON/DIF/ VISCL,VISCV,RHOW,VISCW
      COMMON/DIFLV/ DIFL,DIFV

      IF(IPP.LE.20) THEN
      HB1=1.24
      HB2=0.6
      ELSE
      HB1=1.11
      HB2=0.5
      ENDIF
C***
C    CALL PARAM TO CALCULATE PSI,PHI,CFL
      FR= 0.50
      CALL PARAM
C      WRITE(*,*) PSI,PHI,CFL
      WL=WL/3600
C
      WRITE(*,*) 'DEN: L/V ',RHOLC(1),RHOVC(1)
      SCV=VISCV/(RHOVC(1)*DIFV)
      SCL=VISCL/(RHOLC(1)*DIFL)
      IF(COLD.LE.2.0) GOTO 10
      COLD=2.0
C      WRITE(*,*) 'HETP',SCV,SCL,COLD
   10 UP=PHI*(COLD**HB1)*((HP/10)**(1.0/3.0))*(SCV**(1.0/2.
      0))
      DOW=3600*WL*((VISCL/VISCW)**0.16)*((RHOLC(1)/RHOW)**(
      -1.25)) DOW=(DOW*(SRFTL/SRFTW)**(-0.8))**HB2
      HG=UP/DOW
      HL=PSI*CFL*((HP/10)**0.15)*(SCL**0.5)
      THETA=SLP/FLV
      HOG=HG+(THETA*HL)
      WRITE(*,*) 'HG,HL,HOG,THETA',HG,HL,HOG,THETA
      HETPA=(HOG*DLOG(THETA))/(THETA-1)
      WRITE(*,*) 'HETP IS =',HETPA
   50 RETURN
```

```
      END
***
      SUBROUTINE SRFTN ***
C     THIS SUBROUTINE CALCULATES THE SURFACE TENSION
C     OF THE LIQUID MIXTURE. PURE LIQUID SURFACE TENSION
C     IS CALCULATED USING THE CORRELATION OF BROCK ANDBIRD.
C
C

      IMPLICIT REAL*8(A-H,O-Z)
      COMMON/VC/ XC(5,20),YC(5,20),ZZ(5,20),KC(5,20),
      D(20,20)
      COMMON/V1/ RHOL(5),RHOV(5),RHOLC(5),RHOVC(5),WTM(5),
     &           T(5),P(5),PP(5),ALFAS(5)
      COMMON/V0/ TC(20),PC(20),OMG(20),TB(20),WT(20),
      ZRA(20),A1(20),AL(20),B1(20),BL(20)
      COMMON/V4/ MIX,NPT,IEOS,IN,IO,LP,IP,NC,KY,INPT
      COMMON/SRF/ SRFTL,SRFTW
      COMMON/LD/ CVOL(20),HW(20),RHOPL(20)
      COMMON/SRF1/ WML
      DOUBLE PRECISION SRFT(20),TBR(20),TR(20)

      SRFTL=0.0
      RHOLC(1)=RHOLC(1)*16.0185/1000.
C   CALCULATES PURE LIQUID SURFACE TENSION
      DO 10 I=1,NC
      TBR(I)=TB(I)/TC(I)
      TR(I)=T(1)/TC(I)
      Q1=TBR(I)*DLOG(PC(I)/1.01325)/(1-TBR(I))
      Q=(0.1196*(1+Q1))-0.279
      SRFT(I)=PC(I)**(2.0/3.0)*TC(I)**(1.0/3.0)*Q*(1-
      TR(I))**(11./9.)
C      WRITE(*,*) 'SURFACE TN.',I,'=',SRFT(I)
   10 CONTINUE
C   CALCULATES LIQUID MIXTURE SURFACE TENSION
C    EQN. 12-5.3  REID ET. AL.
      DO 20 J=1,NC
      SRFTL=SRFTL+(XC(1,J)*WT(J)*(SRFT(J)**(1.0/4.0))/RHOPL
      (J))
C      WRITE(*,*) 'SRFTL',SRFTL,RHOPL(J)
   20 CONTINUE
C      WRITE(*,*) 'RHO',RHOLC(1),WML
      SRFTL=(RHOLC(1)*SRFTL/WML)**(4.0)
C   CALCULATES SURFACE TENSION OF WATER
      TW=T(1)-273
      SRFTW=75.83-0.1477*TW
C
      RETURN
      END
***
      SUBROUTINE DIFF ***
C THIS SUBROUTINE WILL BE USED TO ESTIMATE THE DIFFUSION
```

```
C COEFFICIENTS OF GAS AND LIQUID MIXTURES.
C FOR LIQUID MIXTURES THE MODIFIED WILKE-CHANG EQUATION
C IS USED HERE.
C FOR VAPOR MIXTURES THE WILKE-LEE EQUATION IS USED FOR C
BINARIES
C AND SIMPLIFIED MAXWELL FOR MIXING THE BINARY COMBINATIONS
C   IDIL=DILUTE COMPONENT NUMBER.
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON/VC/ XC(5,20),YC(5,20),ZZ(5,20),KC(5,20),
      D(20,20)
      COMMON/V1/ RHOL(5),RHOV(5),RHOLC(5),RHOVC(5),WTM(5),
     &           T(5),P(5),PP(5),ALFAS(5)
      COMMON/V0/ TC(20),PC(20),OMG(20),TB(20),WT(20),
      ZRA(20),A1(20),AL(20),B1(20),BL(20)
      COMMON/V4/ MIX,NPT,IEOS,IN,IO,LP,IP,NC,KY,INPT
      COMMON/DIFLV/ DIFL,DIFV
      COMMON/LD/ CVOL(20),HW(20),RHOPL(20)
      COMMON/DIF/ VISCL,VISCV,RHOW,VISCW
      COMMON/VDIF/ VC(20)
      DOUBLE PRECISION DIF(20,20),SIG(20),EPHK(20)
C  VISCOSITY OF LIQ. MIXTURE REQUIRED. (VISCL)
C  CONSTANTS FOR RHOD
      C1=1.06036
      C2=0.15610
      C3=0.19300
      C4=0.47635
      C5=1.03587
      C6=1.52996
      C7=1.76474
      C8=3.89411

C
      WRITE(*,*) 'ENTER DILUTE COMPONENT NO.'
      READ(*,*) IDIL
C  CALCULATES LIQUID MIXTURE DIFFUSIVITY
C  DIFL=DIFFUSIVITY OF DILUTE COMP. W.R.T. THE MIXTURE
      PHIM=0.0
      PHIJ=1.0
      VISCL=VISCL/2.4189
      VA=0.285*VC(IDIL)**(1.048)
      DO 10 J=1,NC
      IF(J.NE.IDIL) THEN
      PHIM=PHIM+(XC(1,J)*PHIJ*WT(J))
      ENDIF
   10 CONTINUE
      DIFL=7.4E-08*PHIM**(1./2.)*T(1)/(VISCL*VA**(0.6))
C
C  CALCULATES THE DIFFUSION COEFFICIENT OF THE GAS MIXTURE
C  DIFV=DIFFUSIVITY OF DILUTE COMP. W.R.T. THE MIXTURE
      DO 20 K=1,NC
      SIG(K)=1.18*(WT(K)/RHOPL(K))**(1./3.)
      EPHK(K)=1.15*TB(K)
```

```
   20 CONTINUE
C  CALCULATES DIFFUSIVITY OF EACH BINARY IN THE MIXTURE
      DO 50 I=1,NC
      IF(I.NE.IDIL) THEN
      SIG2=(SIG(IDIL)+SIG(I))/2.
      SIG2=SIG2**(2.0)
      WTAB=2*WT(IDIL)*WT(I)/(WT(IDIL)+WT(I))
      WTAB=WTAB**(1./2.)
      TSTAR=T(1)*(EPHK(IDIL)*EPHK(I))**(-1./2.)
      RHOD=(C1/(TSTAR**C2))+(C3/EXP(C4*TSTAR))
      RHOD=RHOD+(C5/EXP(C6*TSTAR))+(C7/EXP(C8*TSTAR))
      DIF(IDIL,I)=(3.03-(0.98/WTAB))*(1.E-03)*T(1)**(3./2.)
      DIF(IDIL,I)=DIF(IDIL,I)/(PP(1)*WTAB*SIG2*RHOD)
      ENDIF
   50 CONTINUE
C  CALCULATES DIFFUSIVITY OF THE MIXTURE
      DIFV=0.0
      DO 70 K=1,NC
      IF(K.NE.IDIL) THEN
      DIFV=YC(1,K)/DIF(IDIL,K)+DIFV
      ENDIF
   70 CONTINUE
      DIFV=DIFV**(-1.0)
C
      VISCL=VISCL*2.4189
C
      RETURN
      END
***
      SUBROUTINE PARAM ***
      IMPLICIT REAL *8 (A-H,O-Z)
      COMMON/PARDT/ PSIP(30,14),PHIP(30,7)
      COMMON/DIAM/ FLV,DREF,PF,ND,ALPH,BETA,DELP,COLD,WL
      COMMON/PARAMP/ FR,PSI,PHI,CFL
      COMMON/HETPC/ IPP,HP,SLP,HETPA
C
C     change wl to lb/h.ft2
      WL=WL*3600
C      WRITE(*,*) 'WL IN PARAM=',WL,IPP
C   CALCULATE CFL
C
      IF(FR.LE.0.483) THEN
      CFL=1.0
      ELSE
      FR1=FR*FR
      FR2=FR1*FR
      FR3=FR1*FR1
      FR4=FR3*FR CFL=89.6158*FR4-265.839*FR3+311.777*FR2-
      183.759*FR1+54.4098*FR-5.43745
      ENDIF
C
C   CALCULATE PHI
```

```
C
      PF=FR*100
      PF2=PF*PF
      PF3=PF2*PF
      PF4=PF2*PF2
      PF5=PF3*PF2
      PF6=PF3*PF3
      PHI=PHIP(IPP,7)*PF6+PHIP(IPP,6)*PF5+PHIP(IPP,5)*PF4+
     &PHIP(IPP,4)*PF3+PHIP(IPP,3)*PF2+PHIP(IPP,2)*PF
     &+PHIP(IPP,1)
C
C   CALCULATE PSI
C
      WL2=WL*WL
      WL3=WL2*WL
      WL4=WL2*WL2
      WL5=WL3*WL2
      WL6=WL3*WL3
      WL7=WL4*WL3
      WL8=WL4*WL4
     IF(IPP.EQ.6.OR.IPP.EQ.12.OR.IPP.EQ.19.OR.IPP.EQ.23.OR.
     IPP.EQ.24)
     THEN IF(WL.LT.10000) THEN
     PSI=PSIP(IPP,14)*WL8+PSIP(IPP,13)*WL7+PSIP(IPP,12)*WL6
     + PSIP(IPP,11)*WL5+PSIP(IPP,10)*WL4+PSIP(IPP,9)*WL3+
     &PSIP(IPP,8)*WL2+PSIP(IPP,7)*WL+PSIP(IPP,6)
        ELSE
      PSI=PSIP(IPP,5)*WL4+PSIP(IPP,4)*WL3+PSIP(IPP,3)*WL2+
     &PSIP(IPP,2)*WL+PSIP(IPP,1)
        ENDIF
      ENDIF
      PSI=PSIP(IPP,5)*WL4+PSIP(IPP,4)*WL3+PSIP(IPP,3)*WL2+
     &PSIP(IPP,2)*WL+PSIP(IPP,1)
      RETURN
      END
C
C  BLOCK DATA CONTAINS THE COEFFICIENTS OF THE CURVE FIT
C  POLYNOMIALS OF PSI AND PHI
      BLOCK DATA COEFF
      IMPLICIT REAL *8 (A-H,O-Z)
      COMMON/PARDT/ PSIP(30,14),PHIP(30,7)
C
C  METAL RASCHIG RINGS (1/2")
      DATA ((PHIP(J,I),I=1,7),J=2,2)/ -0.146756,2.30633,
     &0.0003305,-0.00112902,1.81652E-05,-9.24823E-08,0.0 /
      DATA ((PSIP(J,I),I=1,14),J=2,2)/ 0.0283273,7.62969E-
     &06,-5.19889E-11,0,0,0,0,0,0,0,0,0,0,0 /
C  METAL RASCHIG RINGS (1.0")
      DATA ((PHIP(J,I),I=1,7),J=5,5)/ -128.643,24.0028, &-
     1.30624,0.0375517,-0.000590067,4.75358E-06, &-
     1.53537E-08 /
      DATA ((PSIP(J,I),I=1,14),J=5,5)/ 0.0376428,3.92178E-
```

```
     &06,-1.70581E-11,0,0,0,0,0,0,0,0,0,0,0 /
C    METAL RASCHIG RINGS (1.5")
        DATA ((PHIP(J,I),I=1,7),J=6,6)/ -118.896,24.7848, &-
     1.31253,0.037506,-0.000596407,4.94541E-06, &-1.66265E-
     08 /
        DATA ((PSIP(J,I),I=1,14),J=6,6)/ 0.0402624,7.78777E-
     &06,-6.85464E-11,0,0,0.0294605,2.15505E-05, &-
     4.33955E-09,5.57882E-13,-3.19568E-17,7.93984E-22, &-
     6.91972E-27,0,0 /
C    METAL RASCHIG RINGS (2.0")
        DATA ((PHIP(J,I),I=1,7),J=7,7)/ 5.39026,9.80438, &-
     0.44123,0.0120643,-0.0002013,1.8294E-06,-6.81115E-&09
     /
        DATA ((PSIP(J,I),I=1,14),J=7,7)/ 0.0476377,7.7637E-
     &06, -2.14559E-10,2.93823E-15,-1.38778E-20,0,0,
     &0,0,0,0,0,0,0 /
C    CERAMIC RASCHIG RINGS (1/2")
        DATA ((PHIP(J,I),I=1,7),J=8,8)/ 35.3721,4.54818, &-
     0.0414699,0,0,0,0 /
        DATA ((PSIP(J,I),I=1,14),J=8,8)/ 0.0305465,8.81516E-
     &06,-6.63468E-11,0,0,0,0,0,0,0,0,0,0,0 /
C    CERAMIC RASCHIG RINGS (1.0")
        DATA ((PHIP(J,I),I=1,7),J=11,11)/ 24.9985,4.05415,-
     &0.0639863,0.000245561,0,0,0 /
        DATA ((PSIP(J,I),I=1,14),J=11,11)/ 0.0413491,
     &4.63675E-06,-2.08984E-11,0,0,0,0,0,0,0,0,0,0,0 /
C    CERAMIC RASCHIG RINGS (1.5")
        DATA ((PHIP(J,I),I=1,7),J=12,12)/ 79.2604,1.58311,
     &0.0920425,-0.00414943,5.65861E-05,-2.58071E-07,0 /
        DATA ((PSIP(J,I),I=1,14),J=12,12)/ 0.0427624,
     &7.78777E-06,-6.85464E-11,0,0,0.0319605,2.15505E-05,
     &-4.33955E-09,5.57882E-13,  -3.19568E-17,7.93984E-
     &22,-6.91972E-27,0,0 /
C    CERAMIC RASCHIG RINGS (2.0")
        DATA ((PHIP(J,I),I=1,7),J=13,13)/ 96.3183,3.78795,
     &0.0214791,-0.00312511,5.01634E-05,-2.46299E-07,0 /
        DATA ((PSIP(J,I),I=1,14),J=13,13)/ 0.0476377,7.7637E-
     &06,-2.14559E-10,2.93823E-15,-1.38778E-20,0,0,
     &0,0,0,0,0,0,0 /
C    METAL PALL RINGS (1.0")
        DATA ((PHIP(J,I),I=1,7),J=18,18)/ -8.01892,5.3931, &-
     0.132003,0.0013934,-5.92692E-06,0,0 /
        DATA ((PSIP(J,I),I=1,14),J=18,18)/ 0.0376428,
     &3.92178E-06,-1.70581E-11,0,0,0,0,0,0,0,0,0,0,0 /
C    METAL PALL RINGS (1.5")
        DATA ((PHIP(J,I),I=1,7),J=19,19)/ -19.8155,9.37264,-
     &0.269776,0.00336971,-1.53114E-05,0,0 /
        DATA ((PSIP(J,I),I=1,14),J=19,19)/ 0.0402624,
     &7.78777E-06, -6.85464E-11,0,0,0.0294605,2.15505E-05,
     &-4.33955E-09,5.57882E-13, -3.19568E-17,7.93984E-22,
     &-6.91972E-27,0,0 /
C    METAL PALL RINGS (2.0")
```

```
      DATA ((PHIP(J,I),I=1,7),J=20,20)/ 35.1649,7.57881, &-
     0.205768, 0.00248036,-1.10948E-05,0,0 /
      DATA ((PSIP(J,I),I=1,14),J=20,20)/ 0.0526122,
     &9.56898E-06,-2.80953E-10,4.2644E-16,9.4619E-20,0,0,
     &0,0,0,0,0,0,0 /
C  CERAMIC BERL SADDLES (1/2")
      DATA ((PHIP(J,I),I=1,7),J=21,21)/ -5.63755,2.10876,
     &-0.0258933,0.000102648,0,0,0 /
      DATA ((PSIP(J,I),I=1,14),J=21,21)/ 0.0363109,
     &7.33042E-06,-3.05995E-10,7.25167E-15,-6.30934E-20,
     &0,0,0,0,0,0,0,0,0 /
C  CERAMIC BERL SADDLES (1.0")
      DATA ((PHIP(J,I),I=1,7),J=23,23)/ -86.2547,15.7506,
     &-0.823457, 0.0236177,-0.000377455,3.12925E-06, &-
     1.04461E-08 /
      DATA ((PSIP(J,I),I=1,14),J=23,23)/ 0.0243579,
     &7.36778E-06,-1.55326E-10,1.32792E-15,0,0.0154622,
     &2.39809E-05,-8.17561E-09,1.99439E-12,-2.8394E-16,
     &2.28572E-20,-9.89035E-25,2.09136E-29,-1.65971E-34 /
C  CERAMIC BERL SADDLES (1.5")
      DATA ((PHIP(J,I),I=1,7),J=24,24)/ -107.898,21.6082,
     &-1.17211, 0.0337958,-0.000535269,4.38511E-06, &-
     1.45052E-08 /
      DATA ((PSIP(J,I),I=1,14),J=24,24)/ 0.0311806,
     &4.47714E-06,-4.26056E-11,0,0,0.0220235,1.53728E-05,
     &-2.79398E-09,3.00366E-13, -1.56582E-17,3.72373E-22,
     &-3.18106E-27,0,0 /
C
C
      END
***
      SUBROUTINE ENTHALPY ***
C
C     THIS SUBROUTINE IS USED TO CALCULATE THE ENTHALPY OF
C     IDEAL GAS AND LIQUID USING THE PROCEDURE OUTLINED
C     IN API-DATABOOK 7A1.1
C     BASE OF ENTHALPY = 0.0 AT T = -200F
C
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON/ENTH/ HA(20),HB(20),HC(20),HD(20),HE(20),
      HF(20),DELH(20)
      COMMON/V1/ RHOL(5),RHOV(5),RHOLC(5),RHOVC(5),WTM(5),
     &          T(5),P(5),PP(5),ALFAS(5)
      COMMON/V0/ TC(20),PC(20),OMG(20),TB(20),WT(20),
      ZRA(20),A1(20),AL(20),B1(20),BL(20)
      COMMON/VC/ XC(5,20),YC(5,20),ZZ(5,20),KC(5,20),
      D(20,20)
      COMMON/ENTH1/ VMENTH,FMENTH
      COMMON/V4/ MIX,NPT,IEOS,IN,IO,LP,IP,NC,KY,INPT
      DOUBLE PRECISION  VENTH(20),FENTH(20),DLBTU(20)
C
C     VAPOR ENTHALPY
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```
C     R=1.8*K
      T1=T(1)*1.8
      DO 10 I=1,NC VENTH(I)=HA(I)+T1*(HB(I)+T1*(HC(I)*1.0E-
      4+T1*(HD(I)*1.0E-7+T1* &(HE(I)*1.0E-
      11+T1*(HF(I)*1.0E-15)))))
      VENTH(I)=VENTH(I)*WT(I)
      DLBTU(I)=DELH(I)*1.8*1000.0
      FENTH(I)=VENTH(I)-DLBTU(I)
C      WRITE(*,*) VENTH(I),DLBTU(I),FENTH(I)
   10 CONTINUE
C
C     MIXTURE ENTHALPIES = MOLE FRACTION*ENTHALPY OF PURE C
COMP.
C
      VMENTH=0.0
      FMENTH=0.0
      DO 20 J=1,NC
      VMENTH=VMENTH+YC(1,J)*VENTH(J)
      FMENTH=FMENTH+XC(1,J)*FENTH(J)
   20 CONTINUE
C
C
C
C      WRITE(*,*) 'ENTHALPY V/L',VMENTH,FMENTH
      RETURN
      END
```

2

VITA

Partha Roy

Candidate for the Degree of

Master of Science

Thesis: AN IMPROVED MODEL FOR PACKED COLUMN DISTILLATION

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