ABSTRACT

Title of Thesis:

ENHANCEMENT OF THE THERMOPHYSICAL CAPABILITY OF THE CHEMICAL ENGINEERING SIMULATION SYSTEM

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Thesis directed by:

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The CHESS (Chemical Engineering Smulation System) is a generalized steady-state, sequential-modular chemical process simulation program. In this thesis, the thermophysical data prediction capability of CHESS has been expanded by: incorporating more accurate thermodynamic phase-behavior models, by utilizing these models in generating a wider range of thermophysical properties, and providing an updated and expanded database for pure-component physical properties.

The overall performance of the simulation system's thermophysical package has been evaluated using the study of a subprocess consisting of various rotational equipment modules.

In this work, the Chao-Seader liquid phase activity coefficient model has been reinstalled in conjunction with the original Redlich-Kwong equation of state for the vapor phase. As an alternative, the Soave-Redlich-Kwong equation

of state has also been used as a vapor phase model with the Chao-Seader activity coefficient model to generate vapor-liquid equilibrium constants and other properties. The Peng-Robinson equation of state has also been included as an option to predict vapor and liquid phase behavior.

The data-library approach of the original version of CHESS has been reinstated. The library has also been updated to provide a expanded database of pure component properties. The overall property prediction procedure has been expanded to provide: liquid and vapor enthalpy departure functions, liquid and vapor entropy departure functions, vapor phase specific heat departure functions and liquid densities.

The limited results of the subprocess simulation indicate that no single model(s) can be used to represent all the thermophysical properties under the conditions normally encountered in natural gas processing, that is high pressure and low temperature. The Peng-Robinson model has been found to be more accurate in the prediction of most of the properties, such as equilibrium constants, specific heat departures and vapor entropy departures. However, the Redlich-Kwong/ Chao-Seader and the Soave-Redlich-Kwong/ Chao-Seader combinations have predicted enthalpy departures more accurately.

ENHANCEMENT OF THE THERMOPHYSICAL CAPABILITY OF THE CHEMICAL ENGINEERING SIMULATION SYSTEM

BY

JOYDEEP BANERJEE

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DEDICATION

Dedicated to the memory of my father,

Late Shri Bhabatosh Banerjee

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CHAPTER 1

INTRODUCTION

The application of digital computation for solving problems in the area of chemical engineering has grown significantly over the recent years. This progress has evolved in parallel with those made in computer hardware and software. The chemical engineering applications cover the entire spectrum of interest, ranging from fundamental research on molecular structures to real-time analysis and control of industrial processes. The area of process design, situated somewhat in the middle of this spectrum, has undergone vast changes in approach and methodology, necessitated largely by economic and environmental factors.

In computer-aided design of steady state chemical processes, processing entities are represented by a mathematical model that integrates the information on the qualitative behavior of the units, with quantitative relations, represented by equations, into a programmable module. A processing system is simulated by defining the interconnection of such modules through specified operating conditions and functional parameters. In such an inter-relationship, the modules can be thought of as stand-alone entities, requiring inputs to calculate outputs, or they may be made to interact with each other simultaneously, in which case the entire system is thought of as an aggregation of their individual mathematical models. Earlier simulators had adopted the first approach, whereas recent trends indicate a shift towards the second, or a combination of the two approaches. The 'Chemical Engineering Simulation System', known as CHESS, belongs to the first group of simulators.

CHESS was developed originally in the University of Houston (Motard and Lee, 1971). It has been used in various organizations, including NJIT. As newer processes came into perspective and as advancements in the scientific understanding of chemical engineering principles are being achieved, CHESS has undergone successive enhancements in scope here at NJIT. Such activities have encompassed all the components of the original system, such as computational algorithms, mathematical models for units and thermophysical predictive procedures.

The role of thermophysical property computation in chemical engineering simulation is of utmost importance. Key design decisions, such as equipment sizing, amounts of heat and work transformed in mechanical and thermal equipments, phase seperation strategy in single or multistage operations, are guided almost entirely by thermophysical property predictions. The accuracy of such decisions rely on the ability of thermophysical models to describe the complexity of natural phase behavior under widely varying conditions of temperature, pressure, composition etc. These thermophysical models may exibit any degree of sensitivity to one or many of the process parameters. The difficulty is furthered by the objectivity of numerical stability and computational convenience towards efficient simulation. Recently developed processes such as synthetic fuels, supercritical extraction, bio-conversion etc. have triggered the need for process simulators to be adept in handling processing conditions beyond the ordinary. Hence, much importance has been given in recent times to the enhancements of thermophysical property prediction in existing process simulators.

The primary motivation behind this work has been the necessity of incorporating current thermodynamic models into CHESS. In order to support these, the physical properties database of the original version has been expanded and updated. The second objective was to validate these models in conjunction with the rotational equipment modules.

The original-CHESS approach of grouping all the thermophysical models into one general module, had been discarded in the previous work at NJIT (Andreyuk, 1983). This modification has been followed in our work. However, we have restored the original approach of a system-resident databank of physical properties, keeping intact the earlier modification towards a time-consuming read-in procedure as an option. Existing data were updated and a major portion was appended.

In the original form, the thermodynamic prediction package of CHESS was limited. Although it had embodied models which were found to be the best at that time, thermodynamic research has outgrown these models. Similar revisions have taken place for pure-component properties also. In the original version, the RK/ Chao-Seader method for calculating equilibrium ratios. The enthalpy of both the liquid and vapor phases were calculated based on the Redlich-Kwong equation. We have introduced an extended form of the Chao-Seader activity coefficient model with Flory-Huggins size corrections, and have utilized it to predict liquid phase enthalpy and entropy departure functions and molal volumes. For the vapor phase, we have introduced the Soave modification of the Redlich-Kwong (SRK) equation of state as a replacement for the RK equation, with the liquid phase represented by the Chao-Seader correlations.

The Peng-Robinson equation of state has been introduced to represent both the vapor phase and the liquid phase behavior in an extensive manner. This equation is considered to be very successful in modelling various process environments.

The RK / SRK : Chao-Seader and the Peng-Robinson models, together with some others already incorporated in the previous extension of CHESS at NJIT (Andreyuk, 1983), will provide the users with a powerful thermophysical package.

In the area of simulating work-intensive equipments, the original version was quite limited. A generalized module was used to simulate both pumps and compressors. Gas expanders and Hydraulic Turbines were not included. Such restrictions were removed in the previous extension. For example, while the original version had assumed a constant polytropic coefficient of 1.26, the modified Compressor routine has used the Redlich-Kwong equation to evaluate specific heat departure functions at any given state. In this work, we have integrated the rotational equipment modules and the rest with the expanded thermophysical package.

Finally, the updated thermophysical capability of CHESS and the performance of the rotational equipment modules have been tested with the simulation study of a low temperature and high pressure process. In this way, we have substantiated the performance of both and some previously unnoticed errors have been removed. This study has also helped us in providing a guideline about selecting one thermodynamic model over another, in the specific case of the simulation of cryogenic processes.

CHAPTER 2

EXTENSION OF THE THERMOPHYSICAL SUPPORT OF CHESS

2.1 Importance of Thermodynamics in Process Simulation

The design of industrial chemical processes requires knowledge of the phase behavior of liquid and vapor mixtures, sometimes accompanied by the presence or formation of solids or ions. The phase behavior of a pure substance or that of a mixture is represented by certain thermophysical variables. We can characterize a substance by its physical constants and can predict its thermodynamic behavior by generalized equations. Many of the properties vary with process conditions or phase environments. In order for a simulation program to evaluate phase behavior accurately, a set of thermophysical models and associated data required should be provided. The correctness of the results obtained through simulation depends largely on the accuracy of these predictive procedures. In some modern chemical processes, a wide range of conditions are encountered. A present day simulation system would need to gather information extending over a range of -260 F to 1000 F and from near-atmospheric pressure to 10000 psia (Peng, Robinson, Ng 1978-79). Hence, the simulation system should have appropriate models to represent various thermophysical conditions, in order to be truly generic in nature.

In the following topics, we will substantiate the need for extending the thermophysical section of CHESS.

2.2 The Original-CHESS Approach

The original version of CHESS (Motard and Lee, 1971) incorporated a straightforward approach to the thermophysical models. It used the Redlich-Kwong equation (RK equation) for vapor phase and the Chao-Seader correlation for liquid phase computations. Pure-component data was provided for some 98 standard chemical components. The program-design methodology adopted in the original version of CHESS for the thermophysical properties was a complicated single subprogram named KZHT. This routine was used by the simulation system at different stages of computation via multiple entry points. Although it was execution-efficient, from a programming standpoint, it failed to provide even a minimum level of structured organization, making maintenance virtually impossible. From a thermodynamic point of view, it was inadequate in representing thermophysical states over wider ranges of conditions accurately.

2.3 The Previous Modification at NJIT

There has been a tremendous impetus for research in applied thermodynamics as processes grew in complexity and new processes were developed in the last decade. This was facilitated by the comming of age of the computer era and improvments in the analytical tools. Thus, it was necessary to update and improve the thermophysical support of CHESS (Andreyuk, 1983). In this previous modification of CHESS at NJIT, the following changes were performed :

- The KZHT approach was discarded in favor of a modularized method. In this method, the thermophysical models are seperated into individual modules, such that maintenance is easy. It also had incorporated an open-ended structure, where new modules could be added easily.
- The Virial equation of state was added to the set of vapor phase models.
- The Redlich-Kwong equation of state had been included in an enhanced fashion.
- The Wilson, the NRTL and the UNIQUAC liquid phase activity coefficient models were incorporatred.
- The original pure-component database (COMPID) was deleted in favor of a data-read-in procedure (CDATA).

2.4 Modifications Performed in This Work

The following modifications were performed in this work:

- The Soave-Redlich-Kwong equation of state has been introduced. It has been used as a vapor phase model with the Chao-Seader liquid phase correlation, and to generate vapor phase enthalpy and entropy departure functions.

- The Chao-Seader model has been reinstalled in a modified form. It has also been used for the determination of liquid phase enthalpy and entropy departure functions, and molal volumes.
- The Peng-Robinson equation of state has been included to predict for both the vapor phase and liquid phase behavior.
- The original CHESS module COMPID has been reinstalled. The database has been updated for the existing properties and many new properties have been added to it.
- The vapor phase specific heat departure functions have been evaluated by the Peng-Robinson, the SRK and the RK equation.

2.5 Equilibrium Constant Calculation Procedure

Chao-Seader Approach

In the Chao-Seader (1961) approach, followed in the original CHESS and retained in this version, the equilirium compositions in a vapor liquid (VLE) system is expressed as a ratio, which requires the value of the liquid phase pure-component fugacity coefficient. This ratio, termed as the equilibrium constant, is evaluated via models describing the phases. The method due to Chao and Seader uses the Redlich-Kwong equation for the vapor phase fugacity coefficient.

The Chao-Seader definition of the equilibrium ratio follows from fundamental thermodynamic relationships and is described as follows :

$$K_i = \frac{y_i}{x_i} = \frac{\gamma_i f^0_{i_L}}{\phi_{i_V}} \qquad (2.1)$$

where :

K_i = Equilibrium ratio of component i

y_i, x_i = Vapor and liquid phase composition of i

ϕ_{i_V} = Vapor phase fugacity coefficient of i

γ_i = Activity coefficient of i in liquid phase

$f^0_{i_L}$ = Liquid phase pure component fugacity

The original version of CHESS used the Redlich-Kwong equation of state to calculate the vapor phase fugacity coefficient. For the liquid phase, the Chao-Seader correlation for the fugacity ratio and Hildebrand's regular solution approach for the activity coefficients were implemented. The Yen and Wood's correlation was used for obtaining the liquid phase densities and hence, molal volumes. The Redlich-Kwong equation was also used for predicting the enthalpy departure functions of both the phases. In this work, the Chao-Seader approach has also been used, but with the SRK vapor phase model.

Again, in this modification of CHESS, we have included the Chao-Seader method in an extensive way. It has been used as an model for the liquid phase to predict liquid phase fugacity coefficients, enthalpy and entropy departures and liquid molal volumes. The Hildebrand activity coefficient model has been retained but the Flory-Huggins correction is applied uniformly. We have also used the Chao-Seader models to obtain liquid phase enthalpy and entropy departure functions.

<u>The Modular Thermodynamic Approach : Activity Coefficients</u>

The approach followed in Andreyuk's modification evaluates the liquid phase fugacity coefficient from an equation of state using system temperature and component vapor pressure. According to this method, the equilibrium ratio is expressed as following :

$$K_i = \frac{P_i^{o} \gamma_i \emptyset_i^{s} \{P.F\}}{P \emptyset_{i_V}} \qquad (2.2)$$

where :

P_i^{o} = saturation pressure of component i at T

P , T = system pressure and temperature

{P.F} = Poynting Factor

$$\text{Poynting Factor} = \exp \left[\int_{P_i^{o}}^{P} \{ V_L^{i} (T,P) / RT\} \, dP \right]$$

For a condensible component, this can be approximated by the following expression :

$$\text{Poynting Factor} = \exp[\, V_i^L \,(P - P_i^{\bullet}) \;/\; RT]$$

where :

V_i^L = liquid molar volume of component i

In VLE systems where temperature is much below the critical values of its components, a liquid is considered incompressible. The effect of pressure on the liquid phase fugacity is negligible unless the pressure is very high or the temperature is very low (Reid, Sherwood, Prausnitz: 1977). To account for the large difference between the system pressure and the component vapor pressures, especially in high-pressure environments, a correction factor is to be applied. This correlction is known as the Poynting Factor.

This pressure affected term is important for simulation of high-pressure systems. The original CHESS did not account for this. Successive modifications have included this correction in the equilibrium ratio calculations, while using the Virial equation and the RK equation as the vapor phase models.

Equation of State Approach : the Peng-Robinson Equation

The Peng-Robinson equation of state is applicable to both the liquid phase and the vapor phases in VLE calculations.

The equilibrium constants are evaluated from the basic definition, as shown below :

$$K_i = \hat{\phi}_{i_L} / \hat{\phi}_{i_V} = (\hat{f}_{i_L} / (x_i P)) / (\hat{f}_{i_V} / (y_i P))$$

$$= y_i / x_i \quad \text{at equilibrium.}$$

According to this method, which was implemented in this work, the fugacity coefficients are evaluated for both the liquid and the vapor phases, with the appropriate phase compositions.

2.6 Need for Incorporating Newer Equations of State in CHESS

In this topic, the need for the provision of new equations of state in the CHESS is discussed. The original CHESS had implemented only the RK equation of state with the Chao-Seader correlation in a limited manner. In contrast, let us first describe the improvements intended in this work. Then, we can proceed to a comparative discussion about the various equations.

The thermodynamic properties which will be predicted with the newly-included equations of state are :

- Fugacity coefficients of pure components (liquid) and mixtures (vapor),
- Enthalpy departure functions for vapor and liquid mixtures,

- Entropy departure functions for vapor and liquid mixtures,
- Departure functions for specific heats of pure component and mixtures of vapors, at constant pressure and at constant volume.

Problems With the RK Equation : Original Version of CHESS

CHESS in its original form was quite limited in its capability to predict thermodynamic properties. The Redlich-Kwong equation (RK equation) was used as the only model to represent vapor phase behaviour. Until the time CHESS was concieved, it was found to be the best, among the available generalized P-V-T correlations, for phase equilibrium prediction purposes. In CHESS, predictions were made for compressibility factors, specific volumes, fugacity coefficients and enthalpy departure functions of pure components or mixtures for both liquid and vapor phases using this model.

The RK equation gives large errors in predicting the VLE behaviour of multicomponent mixtures (Soave, 1972). This is due largely to the imperfections of the mixing rules which assume a molar arithmetic average for all mixture properties. The second drawback is in the assumption of temperature-independance of the inter-molecular attraction-force coefficient. This is manifested in its failure to predict mixture critical envelopes closely. The improper mixing rules yield widely errorsome results when polar species exist in a mixture. It was also demonstrated that agreement between experimental and predicted values for the vapor pressure is very poor. Thus, Soave presented a hypothesis that equations of state which predict saturation envelopes fairly closely, would work well with the prediction of mixture thermodynamic behaviour.

Soave Modified RK Equation (SRK equation)

In this work, the Soave-modified Redlich-Kwong equation (SRK equation) has been introduced into the set of P-V-T relationship models in the current versionof CHESS, which consisted ofthe Virial equation and the RK equation. Significant improvements in the prediction of thermophysical properties can be achieved utilizing this equation. It works extremely well with mixtures containing polar species. It also predicts vapor pressure values with a maximum deviation of 2 % (Soave,1979). The interaction parameters for polar-polar and polar-nonpolar pairs in systems having polar species have produced results which are much closer to experimental data. The correlation has temperature and composition dependent parameters by virtue of which the predicted values of thermophysical properties are very accurate. The idea of varying the coefficients in the RK equation for obtaining a better equation of state was first conceptualized by Soave (1972). Several other modifications based on his approach has been attempted since then but only a few has been as widely accepted, particularly in the hydrocarbon industry, as his model.

Another aspect of the SRK equation which is of tremendous use for the simulation of synthetic fuel processes or the LNG processes, is that it can predict vapor-liquid-solid equilibria (VLSE) conditions very accurately. Soave (1979) observed that the values of interaction parameters obtained from VLE data work well with equilibrium systems containing components in the solid state also. Although CHESS does not support systems containing solids presently, this feature should be considered for future improvements.

The Peng-Robinson Equation of State

One of the most challenging tests for a newly proposed equation of state is its capability to represent phase behaviour at or near the critical point. Two-constant equations (like the RK equation) fail to predict the critical compressibility factors accurately enough. This was observed in a study made by Redlich (1975). The three-constant equations (like the SRK), which include the critical compressibilty factor as a parameter have been found to be very successful in this respect. The most accurate among these is a further extension of the RK equation proposed by Peng and Robinson (1976).

The major shortcomming of the SRK equation is its failure to predict liquid volumes accurately. While vapor phase density predictions are fairly accurate, the estimated liquid density values exceed the experimental values in almost all cases. The deviations observed by Peng and Robinson were from 7% at reduced temperature below 0.65 to 27% in the vicinity of the critical points. It was found that the error for compounds with lower molecular weights (e.g Nitrogen, Methane) are tolerable but large errors occur for hydrocarbons having high molecular weights.

In its conception and structure, the Peng-Robinson equation is similar to the SRK equation. The temperature-dependence of the 'a' parameter (refer to Chapter 3) is described by a similar correlation in both of these, differing only in the values of the empirically-obtained numerical coefficients. This probably does not reflect difference between the approaches used. Soave used vapor pressure data at only two points for regression analysis: values at reduced temperatures of 0.7 and at the critical point. Peng and Robinson has made use of vapor pressure data over the entire range of practical interest, from the normal boiling point to the critical point. Improvements were observed for low-pressure systems involving natural gas condensates by Conrad and Gravier (1980). The authors also observed that the interaction parameters have a major influence on the prediced values of saturation pressures.

Under cryogenic conditions, the uncertainities associated with the predictions of enthalpy departures and VLE system K-values affect the process design significantly. In studies of such systems made by Klotz et.al (1983), the Peng-Robinson equation was found to be the most suitable model.

The values predicted for enthalpy departure functions in either of these equations have accuracies of the same order, but only the Peng-Robinson equation is known to give close estimates of vapor pressure. A few systems, having C_1--C_4 hydrocarbons paired with polar compounds, are presented in the original paper of Peng and Robinson,1976. The phase envelopes match the experimental P-T plots almost perfectly.

In many processes, the prediction of liquid-liquid equilibrium (LLE) systems is necessary. A variety of systems have been modelled successfully by Peng, Robinson and Ng (1978-1979) using their equation. These include VLE and LLE data prediction for three phase hydrocarbon systems containing water or other non-hydrocarbons, such as alcohols. Also included were VLSE systems with compositions defined by chemical equilibria such as systems where solid hydrates are formed. Predictions for unknown and undefined petroleum fractions containing C_7 and higher molecules were also found to be accurate. In various research projects undertaken recently at NJIT, systems containing immiscible liquid phases, VLSE systems and equilibrium systems having electrolytic components are being studied. The modified version of CHESS having the Peng-Robinson and the SRK equations of state models will be appropriate for the simulation study some of these systems. Further improvements should also include the Benedict-Webb-Rubin (BWR) equation of state.

The Virial Equation of State

In the previous extension of CHESS done at NJIT (Andreyuk, 1983), the Virial equation of state was implemented for predicting fugacity coefficients and vapor phase enthalpy departure functions. The Virial equation was developed from a statistical mechanics approach. The coefficients of the equation reflect interactions between two, three, four or more bodies (molecules) and are functions of temperature and composition. However, the Virial equation has some limitations. Erroneous results are obtained for phase conditions having vapor density figures above half the critical density. The Virial equation cannot handle systems with carboxylic acids. The most critical issue is the scarcity of data for the equation parameters. The Virial equation is universal in nature but not in the values of its coefficients. Each individual system is described by a unique set of parameters, the values of which are rarely reported in the literature. Different research groups adopt widely varying techniques for arriving at the values of the parameters, which may become meaningless unless the precise technique and its assumptions are evaluated. While some empirical correlations are available for the second Virial coefficients (B_{ij}) values, or correlations for the third, (C_{ijk}), are very rare. There are two widely accepted correlations for B_{ij}, one by Tsonopoulos, and the second by Hayden and O'Connell respectively (Prausnitz et al, 1980).

Although the Virial equation is very accurate for strongly interacting systems, it is accurate for low pressure applications only (Tassios,1980). It is expected thatfurther research would lead to correlations for higher coefficients in the Virial power series equation, which would enable us to use it for accurate predictions of phase behaviour in high pressure VLE enviornments. As mentioned before, CHESS has been modified for this equation already, but user-defined data for the coefficients of any specific component are required.

2.7 Need for the modified Chao-Seader Activity Coefficient Model

The Activity Coefficient Models of the Previous NJIT Version

In the previous extension of CHESS performed at NJIT (Andreyuk, 1983), three new models for predicting the activity coefficients were incorporated. These were the

Wilson equation, the NRTL equation and the UNIQUAC equation. These equations are more consistently reliable than other generalized equations proposed earlier (Reid, Sherwood and Prausnitz, 1977). They can reproduce highly non-ideal behavior fairly accurately. The theoretical assumptions made in these models are similar and they express the excess Gibb's free energy with two or more binary interaction parameters. The Wilson equation is excellent for strongly interacting binary mixtures, for example, solutions of alcohols and hydrocarbons. However, it is unable to predict for immiscible systems where the liquid phase splits into two phases. In LLE systems, the behaviour of only one of the liquid phases can be predicted with the Wilson equation, but the interplay of the phases cannot be determined. Again, unlike the UNIQUAC and the NRTL equations, the Wilson equation is not applicable to Vapor-Liquid-Liquid Equilibria (VLLE) calculations. Although the UNIQUAC equation involves complex computations, it has a sound theoretical basis. Again, the UNIQUAC parameters do not vary much with temperature. The UNIQUAC equation is based upon volume and surface fractions rather than mole fractions and hence, is applicable for solutions containing larger molecules such as polymers. The calculations based on such parameter-dependant equations are widely used in industry. They can easyly handle mixtures containing polar species, by using two or more parameters. However, the parameters for any of these models are obtained via regression analysis of experimental data and one has to use both plentiful and accurate data in order to obtain realistic results.

The Chao-Seader Method

The original version of CHESS used the Chao-Seader method for predicting activity coefficients of liquids, for both pure-components and mixtures. The Grayson-Streed modified empirical relationships were used, to make the model applicable to higher temperatures and pressures and with systems containing Hydrogen. The results obtained with this modification are quite accurate in general, especially at high pressure regions (Tassios, 1980).

In this extension of CHESS, we have redefined, generalized and increased the liquid-phase property prediction capacity of the Chao-Seader module. This was necessitated by the requirement of a model suitable for high pressure systems, which are frequently encountered in Hydraulic Turbines and other rotating equipments.

Although the Chao-Seader method, in general, works well for high-pressure systems, there may arise cases where erroneous results are obtained due to the implicit use of RK equation as the vapor phase model, as prescribed, for the Chao-Seader method (1961). Coward and Webb (1978) have found that spurious roots are present near the critical points of mixtures or high pressure systems. This amounts to more than one value predicted for the dew and bubble points and asymptotic nature of the phase envelope near the critical region, yielding no unique critical point. Thus, two or more states may be predicted for a single temperature and pressure combination. In this work, we have applied the SRK equation instead of the RK equation, and simulation results appear to be consistent with the RK equation, as will be shown in Chapter 5.

The Chao-Seader models originates in the 'regular solution theory' originally proposed by van der Waals and van Laar. The theory has been developed by Scatchard and Hildebrand (Henley and Seader, 1981). The principal assumption underlying the theory is that molecules are randomly dispersed in a solution, such that unequal molecular attractive forces between like and unlike pairs are counter-balanced by erratic movements due to thermal energy which tend to seperate them. This results in local compositions which are identical to the overall composition of the solution. Regular solutions have zero entropy of mixing and endothermic enthalpy of mixing in contrast to athermal solutions which have zero enthalpy of mixing. 'Regular Solution' theory assumes that excess Gibb's free energy is independent of temperature, while the 'Athermal Solution' theory assumes that mixing occurs at constant temperature. According to Reid, Sherwood and Prausnitz (1977), none of these assumptions are valid.

Using the regular solution theory, one arrives at the conclusion that the activity coefficient of a specie in a mixture is a function of its pure component properties only. Another important assumption is made in the definition of the 'solubility parameter' used by the model.

$$\text{Solubility Parameter:} \quad \delta_i = (\Delta U_i / V^{\circ}_{L_i})$$

$$= [(\Delta Hv_i - R T)/ V_{L_i}]^{1/2}$$

where :

V_{L_i} = Pure species liquid molal volume,

ΔU_i = Molar heat of vaporization from a saturated liquid to ideal gas state

ΔHv_i = Molal enthalpy of vaporization of pure liquid component , i.

The approximation that ΔU equals ΔHv, is acceptable only for temperatures much below the critical for most of the compounds.

The original version of CHESS did not include the Flory-Huggins correction for solutions where molecular sizes differ appreciably. In such systems, substantial athermal behaviour is expected. This situation arises when polymers are present in a solution. The Flory-Huggins correction applied on the Chao-Seader model improve predictions significantly, as observed by Henley and Seader (1981). They present a test result for n-Heptane - Tolune system at one atmospere pressure. The corrected equation reduces deviations in the predicted values of activity coefficients from 12% to 6% . In this work, we have applied this correction uniformly for all the included models. The following models derived from the Chao-Seader correlation are included in this work :

- Liquid phase activity coefficients.
- Liquid phase pure-component fugacity ratios.
- Liquid phase enthalpy departures.
- Liquid phase entropy departures.
- Liquid phase molal volumes.

A major discrepancy in the original CHESS was in the prediction of liquid phase enthalpies. These were calculated from the RK equation. This approach makes the liquid phase prediction inconsistent and error-prone, as the RK equation is not suitable for liquid phases. Again, liquid molal volumes were calculated using the Yen and Wood's correlation giving rise to another inconsistency and a possible source of error. In order to be consistent , we have incorporated the liquid molal volume correlation suggested by Chao-Seader's model. The enthalpy and entropy departure functions can be derived from fundamental relationships and we have adopted this strategy. Similar treatment was used by Henley and Seader (1981).

While the Chao-Seader method is generally expected to give better estimates, its applicability is limited to solutions having no polar components. Certain other restrictions exist.

In systems where polar components are present, especially in those having electrolytes, the regular solution assumption of segregation of molecules can not be expected to hold true. The Chao-Seader correlations are restricted to system conditions not exceeding 260 C and 1000 psia. In mixtures involving hydrocarbons, the reduced critical temperatures of any system component should not lie outside the range of 0.5 to 1.3. The reduced mixture critical pressure figures should be less than 0.8. This restriction is not applicable for Methane however. Systems having Methane and/or Hydrogen are accurately predicted for reduced mixture temperature below 0.93. However, predicted values are inaccurate above Methane mole-fraction concentrations of 0.3 and the mole-fraction of other dissolved gases should be lesser than 0.2. In any general system, the liquid phase aromatics' mole-fraction should not exceed 0.5 in the presence of paraffins and olefins.

2.8 Need for Updating the COMPID Thermophysical Database

In the previous research on CHESS (Andreyuk,1983), the original pure-component thermophysical data module, COMPID, was deleted from the system. The modifications were undertaken with a specific application in perspective and hence, all the required data on thermophysical properties of components were defined using a special input module.

In this work, we have restored the origial CHESS approach of creating a thermophysical database for 98 standard components defined by CHESS (Motard and Lee,1971). There is a provision for the input of alternate data sets or when the simulation involves non-standard components. The original database needed updating in most of its values, since more accurate data has been published later. Also, a set of property-data has been included for previously omitted properties.

Revision of Data

The values of many pure-component properties had to be updated. Previously, the Chao-Seader modified accentricity factors were stored. We have changed these to the data presented by Reid, Sherwood and Prausnitz (1977). We have retained the Chao-Seader modified Hildebrand solubility parameters and liquid molar volumes but have used correlated data for the Flory-Huggins' equation. The Hildebrand parameters are used for enthalpy and entropy departure functions for the liquid phases. The values of the critical constants and those for coefficients of ideal-vapor heat capacity are updated likewise in accordance with data obtained from Reid, Sherwood and Prausnitz's text (1977).

Enlargement of the Database

We have enlarged the database for additional physical properties' data which did not exist before. Some were required for the added computational modules, while others were provided for future applications. For the calculation of vapor pressures, we have used a six-parameter Antoine equation rather than the equations of state. Reid, Sherwood and Prausnitz (1977) have recommended this approach, as the reliability of the equations of state in vapor pressure predictions is low. The data provided in this modification to CHESS was extracted from Reid, Sherwood and Prausnitz's reference (1977), which include only the values of the first three coefficients for the library components.

We have included the Rackett parameters for estimation of saturated liquid density values. The original version assumed that liquid densities are constant and hence only unique values were stored. In reality however, the liquid density is a weak function of temperature and pressure and the Rackett equation is one of the best relationships to reflect this.

The data available for liquid specific heat coefficients is very limited. We have combined three sources in order to provide data for all the standard components. These will be described in the next chapter. The values of heats of vaporization at constant normal boiling points are also included.

CHESS now has an extensive support for enthalpy predictions. An interesting use of mixture enthalpy data would be to extrapolate VLE data to higher or lower temperatures by the use of Gibbs-Helmholtz equation in future work. This equation can be described as follows :

$$h = -T^2 [\partial(g/T)/ \partial(1/T)]_{P,X}$$

This relationship can be used to establish the validity of VLE data or to generate these under low-temperature conditions.

The enthalpy of phases are referred to the standard state of ideal gas conditions, for both liquids and vapors. A departure function is added to the ideal gas enthalpy at a particular temperature, to correct for pressure. For vapor components, the equations of state predict the departure values. For liquids, the derivative of the natural logarithm, of the system-pressure standard state pure component fugacity coefficient, with respect to temperature at constant composition and pressure, yields the enthalpy departure term (refer to Chapter 3 : Chao-Seader models). The fugacity coefficient is determined from correlations dependent on vapor pressure data, vapor phase corrections and liquid phase densities (Prausnitz, Anderson et al, 1980). The Chao-Seader models include this. Although, there is an order of uncertainity about the experimental data used for such correlations, good predictions are obtained, in general, using this approach (Prausnitz,1980). The original CHESS applied the idea of using the RK equation for estimating the liquid phase enthalpy. This method is inaccurate for a generalised situation and can be applied only for a specific component whose experimental data is to be analysed. We cannot use the SRK equation, as the temperature dependence of binary interaction parameters in the liquid phase is not accurately known (Prausnitz, Anderson et al, 1980). We have provided algorithms based on the equations of state to calculate departure functions and included updated values of zero-pressure ideal gas specific heat coefficients obtained from data collected by Prausnitz, Reid and Sherwood (1977).

The polytropic ratio (C_p/C_v) of a gas is required for evaluating the power requirements of a compressor. For isentropic compression paths, it is equal to the ratio of specific heats of the gas at constant pressure (C_p) and at constant volume (C_v). The departure functions in C_p and C_v and the difference between them can be estimated from basic thermodynamic identities utilizing an equation of state. We have utilized these with the newly-added equation of state modules for the rotating equipment routines, which are those for staged compression, hydaulic expansion, gas expansion and liquid pumping. A mention is appropriate here about the possibility of using these values for enthalpy estimation purposes. As described earlier, this approach is not accurate in general, according to Prausnitz et al (1980).

In the evaluation of (C_p / C_v) through the equations of state, one needs to know the critical temperature for a mixture accurately. Based on recommended made by Reid, Sherwood and Prausnitz (1977), we have chosen the Chueh Prausnitz method for this purpose. This method needs five pure-component parameters. These must be passed appropriately to the Chueh Prausnitz module, when non-standard components are used in a study.

Although the extension of the CHESS dataset was appropriate for the current work, these can be utilized for modules other than the rotating equipments and other thermophysical modules which may be introduced in future.

CHAPTER 3

THEORETICAL ASPECTS OF THE ADDED THERMOPHYSICAL MODULES

In this chapter, the thermodynamic basis of the various models implemented in this work is discussed. These will include the equations describing the models, equations of thermophysical properties derived from these models and principles involved in deriving them.

As a review, the various thermodynamic identities utilized in the derivations of the equations representing the changes of thermodynamic properties will be presented. We will also review the RK equation and the relationships arrived at through the use of it, since the SRK and the Peng-Robinson equations are related to it in principle.

3.1 General Expressions for Thermodynamic Properties

The thermodynamic state of a pure substance is described by a set of independant variables, temperature and pressure. Associated with each of these states is a set of characteristic properties. These are directly dependant on the independant variables only. Thus, the variations in such properties between two thermodynamic states are independant of the path chosen for the variation and are functions of the end-states alone. Furthermore, the properties of a mixture is determined by some aggregate of the individual properties of its constituents. Enthalpy, internal energy, entropy, fugacity coefficient and their derivatives are some important thermodynamic properties for describing chemical systems undergoing changes of material and energy contents in a processing environment.

In this section, the various thermodynamic identities needed to relate the properties to the state variables are summarized. These relations are obtained from the fundamental definition of either of the two free energy expressions (Gibbs and Helmholtz), in their integralform. The reference state would be that of an ideal gas under the same system conditions of temperature and pressure, thus yielding the departure functions for the respective properties. In conjunction with an equation of state or an activity coefficient model, these relations would be utilized in relating the respective properties to state variables, temperature (T) and pressure (P). The expressions would be presented in their final forms. The details are given in Reid, Sherwood and Prausnitz's text (1977) and Henley and Seader's text (1981), amongst several references. We have followed an uniform strategy in dealing with the phase condition calculations : the vapor and liquid phase models utilized in the VLE computations, are also used to generate other properties, for example, enthalpy and entropy departures, of the respective phases.

3.1.1 Various Methods of Calculating the Equilibrium Constants

Chao-Seader Approach

In this approach, followed in the original CHESS and retained in this version, the equilirium compositions in a vapor liquid (VLE) system is expressed as a ratio. This ratio, termed the equilibrium constant, is evaluated via models describing the phases. The values of the liquid phase pure- component fugacity coefficients and activity coefficients are expressed via the Chao-Seader correlation and the Hildebrand regular solution theory, respectively. The method due to Chao and Seader uses the Redlich- Kwong equation for the vapor phase fugacity coefficient. In this extension to CHESS, the Soave-Redlich_Kwong equation (SRK equation) has been implemented as an alternative vapor-phase model in conjunction with the Chao-Seader liquid phase models. The RK-Chao Seader approach has been retained unaltered, only the vapor-phase mixture fugacity coefficients are evaluated, alternatively, by the SRK equation. The Chao-Seader definition of the equilibrium ratio is described as follows :

$$K_i = \frac{y_i}{x_i} = \frac{\gamma_i f^0_{i_L}}{\emptyset_{i_V}} \qquad (3.1)$$

where :

K_i = Equilibrium ratio of component i

y_i, x_i = Vapor and liquid phase composition of i

ϕ_{i_V} = Vapor phase fugacity coefficient of i

γ_i = Activity coefficient ofi :liquidphase

$f^0_{i_L}$ = Liquid phase pure component fugacity

<u>The Activity Coefficient Approach</u>

According to this method, the equilibrium ratio is expressed as the following equation :

$$K_i = \frac{P^{\circ}_i \gamma_i \phi^{s}_i \{P.F\}}{P \phi_{i_V}} \qquad (3.2)$$

where :

P°_i = saturation pressure of component i at T

P , T = system pressure and temperature

{P.F} = Poynting Factor

$$\text{Poynting Factor} = \exp\left[\int_{P^{\circ}_i}^{P_i} \{ V_L (T,P)/ RT\} dP\right]$$

For a condensible component, the P.F can be approximated by the following expression :

$$\text{Poynting Factor} = \exp[V^{L}_i (P - P^{\circ}_i) / RT]$$

where :

V_i^L = liquid molar volume of component i

This approach, followed in Andreyuk's modification to CHESS, evaluates the liquid phase fugacity coefficient from vapor pressure, saturation-pressure fugacity coefficient and the Poynting effect. The fugacity coefficients for the vapor phase are evaluated by an equation of state : RK / Virial. The liquid phase activity coefficients are evaluated from a generalized correlation, such as, NRTL, Wilson or UNIQUAC.

Equation of State Approach : Peng-Robinson

The Peng-Robinson equation of state is applicable to both the liquid phase and the vapor phases in VLE calculations. The equilibrium constants are evaluated from the basic definition, as shown below :

$$K_i = \hat{\phi}_{i_L} / \hat{\phi}_{i_V} = (\hat{f}_{i_L} / (x_i P)) / (\hat{f}_{i_V} / (y_i P))$$
$$= y_i / x_i \quad \text{at equilibrium.} \qquad (3.3)$$

According to this method, which was implemented in this work, the fugacity coefficients are evaluated for both the liquid and the vapor phases, with the appropriate phase compositions and compressibility factors.

3.1.2 Fugacity Coefficients : for Vapors and Liquids

For a pure component vapor or liquid, the expression for the fugacity coefficient is given by :

$$\ln\left(\frac{f}{P}\right) = (Z - 1) + \int_{\infty}^{V} \{ P - RT/V \}\, dV - \ln Z \qquad (3.4)$$

where :

f = Fugacity of the component at temperature of T and pressure of P

f/P = Fugacity coefficient (or ratio)

Z = Compressibility Factor = (PV/RT)

V = Volume of the component at T and P

R = Universal Gas Constant.

For a component (i) in a mixture, vapor or liquid, the fugacity coefficient is expressed as the following :

$$RT \ln \hat{\phi}_i = - \int_{\infty}^{V_t} \left[\left(\frac{\partial P}{\partial N_i} \right)\Bigg|_{T, V_t, N_j} - \left(\frac{R\,T}{V_t} \right) \right] dV_t - RT \ln Z \qquad (3.5)$$

where :

$\hat{\phi}_i = \left(\frac{f_i}{P\, y_i} \right)$ = Fugacity Coefficient of component i

f_i = Fugacity of component i in the mixture

N_i = Total moles of i present in the mixture = $y_i N$

V_t = Total volume of the mixture = $\sum_i N_i V_i$

3.1.3 Enthalpy Departure Function : for Vapours and Liquids

In the integral form, the enthalpy departure function for a liquid or a vapor phase is given by :

$$H_f - H_v^0 = -\int_{\infty}^{V} \{ P - \left(\frac{\partial P}{\partial T}\right)\Big|_V \} dV + R T (Z - 1) \tag{3.6}$$

where :

H_f , H_v^0 = Enthalpies, of the real fluid (f : liquid or vapor : l or v) and zero-pressure ideal gasrespectively, bothat system P and T.

In the case of a mixture, the enthalpy departure is the sum of the enthalpy departures of the individual components.

$$H_f = \{ \sum_{i=1}^{n} [c_i H_{i_v}^{o}] \} + \{ H_f - H_v^{o} \} \tag{3.7}$$

where :

c_i = Fractional concentration of species i in f :l/v

H_f = Enthalpy of the 'f' phase, liquid or vapor

$H_f - H_v^0$ = Enthalpy Departure for the 'f' phase, to be obtained from eqn. (3.6), with mixture Z, V.

3.1.4 Entropy Departure Function : for Vapors and Liquids

The departure in entropy is related to the departure in enthalpy and the fugacity coefficient, as follows :

$$(S - S^0) / R = (H - H^0) / RT - \ln(f/ P^0)$$

where P^0 is the pressure in the ideal-gas reference state.

The corresponding final form of the integral expression is given as follows :

$$S - S^0 = \int_{\infty}^{V} \left[\left(\frac{\partial P}{\partial T} \right)\Big|_V - \left(\frac{R}{V} \right) \right] dV + R \ln Z \qquad (3.8)$$

In the case of a mixture, the total volume and the mixture compressibility factor are used for V and Z respectively.

3.1.5 Departure of Vapor Specific Heat at Constant Volume

The departure in vapor specific heat at constant volume is obtained from the following expression in differencial form :

$$\left(\frac{\partial C_V}{\partial V} \right)\Big|_T = T \left(\frac{\partial^2 P}{\partial T^2} \right)\Big|_V \qquad (3.9)$$

where :

C_V = Specific heat at constant volume.

In order to obtain the departure function, the above equation is integrated between an initial state at ideal gas conditions ($V^0 = R\,T\,/\,P$) and a final state at the system conditions ($V = Z\,R\,T/\,P$). Direct utilization of this identity requires an equation of state expressed appropriately in both the pressure-explicit and volume-explicit forms.

3.1.6 Difference Between the Vapor Specific Heats

The difference between vapor specific heats at constant pressure and at constant volume, for a real gas, is expressed as follows :

$$C_P - C_V = T \left(\frac{\partial P}{\partial T}\right)\Big|_V \left(\frac{\partial V}{\partial T}\right)\Big|_P$$

$$= - T \left(\frac{\partial P}{\partial T}\right)\Big|_V^2 \Big/ \left(\frac{\partial P}{\partial V}\right)\Big|_T \quad (3.10)$$

where :

C_P = Specific heat at constant pressure

For an ideal gas, this difference is a constant, equal to R, the Universal Gas Constant. The theoretical basis for ideal gas behavior is the kinetic theory of gases.

$$C_P^0 - C_V^0 = R \quad (3.11)$$

3.1.7 Departure of Vapor Specific Heat at Constant Pressure

The departure in specific heat at constant pressure is obtained from the departure in specific heat at constant volume and the difference between them, as presented in the following identity, obtained from equation (3.11) :

$$\left(\frac{C_P - C_P^0}{R}\right) = \left(\frac{C_V - C_V^0}{R}\right) + \left(\frac{C_P - C_V}{R}\right) - 1 \quad (3.12)$$

Thus, equations (3.9) and (3.10) are used in obtaining values for this departure function.

3.2 The Redlich-Kwong Equation of state

The Redlich-Kwong (RK) equation was the first major modification of the van der Waals equation of state for real gases, which gained wide applicability in the chemical industry. Other successful models developed recently, like the Soave-modified RK equation (SRK) and the Peng-Robinson equation, are guided by the RK methodology, although incorporating three parameters instead of two. In this section, the RK equation and the expressions derived from it are summarized.

The Equation

In the pressure -explicit form, the equation is expressed as :

$$P = \frac{R\,T}{V - b} - \frac{a\,T^{-0.5}}{V\,(V + b)}$$

where :

$$a = \frac{0.4274802\;R^{2}\;T_{c}^{2.5}}{P_{c}}$$

$$b = \frac{0.0866404\;R\;T_{c}}{P_{c}}$$

Mixture Combination Rules

The parameters 'a' and 'b' are defined for a mixture via the following mixing rules :

$$a_{mix} = \sum_{i=1}^{n} \sum_{j=1}^{n} \{ y_i y_j a_i^{0.5} a_j^{0.5} \}$$

$$b_{mix} = \sum_{i=1}^{n} y_i b_i$$

<u>The Compressibility Factor : for Vapor Phase Only</u>

The compressibility factor is obtained from the following Z-explicit, cubic equation form of RK equation :

$$Z^3 - Z^2 + (A - B^2 - B) Z - A B = 0$$

where :

$$A = a P / R^2 T^{2.5}$$

$$B = b P / R T$$

For mixtures, a_{mix} and b_{mix} are used in place of a and b.

<u>Fugacity Coefficients : for Vapor Phase Only</u>

For a pure component, the fugacity coefficient is expressed as :

$$\ln(\frac{f}{P}) = (Z - 1) - \ln(Z - \bar{B} P) - (\bar{A}^2 / \bar{B}) \ln(1 + \bar{B}P/ Z)$$

where :

$$\bar{A}^2 = (0.4274802 / P_c T_r^{2.5})$$

$$\bar{B} = (0.0866404 / P_c T_r)$$

$$T_r = T / T_c$$

For a component i in a mixture, the fugacity coefficient is obtained from the following equation :

$$\ln \hat{\phi}_i = \ln \left(\frac{f_i}{y_i P}\right) = \ln \left(\frac{V}{V - b_m}\right) + \left(\frac{b_i}{V - b_m}\right) - \ln Z_m$$

$$+ \left(\frac{a_m b_i}{b_m^2 R T^{1.5}}\right)\left[\ln\left(\frac{V + b_m}{V}\right) - \left(\frac{b_m}{V + b_m}\right)\right]$$

$$- \left\{\frac{2 \sum_{k=1}^{n} y_k a_{ik}}{b_m R T^{1.5}}\right\} \left\{\ln \left(\frac{V + b_m}{V}\right)\right\}$$

where :

$$a = (a_i a_k)^{1/2}$$

$a_m = a_{mix}$, $b_m = b_{mix}$, $Z_m = Z_{mix}$ = Mixture comp. factor

Enthalpy Departure Function : Vapor Phase Only

For a pure specie in the vapor phase, the departure in enthalpy is given by the following equation :

$$H - H^0 = R T(Z - 1) - (3 / 2)(a / b T^{1/2}) \ln\{ (V + b) / b \}$$

For a mixture containing n components, the sum of the departures in individual components is taken to be the overall departure. The expression is given below :

$$H - \sum_{i=1}^{n} y_i H_i^0 = RT (Z_m - 1) - (3/2)(A^2/B)\{ \ln(1 + BP/Z)\}$$

Entropy Departure Function : Vapor Phase Only

The entropy departure function for a pure component in the vapor phase is expressed as the following :

$$S - S^0 = R \ln[(V- b)/ V] - (a/ b T^{3/2})\ln[(V+ b)/ V] - RT \ln Z$$

For a mixture, the mixture 'a' and 'b' parameters as well as the mixture compressibility factor, 'Z' , is to be used in the above equation.

3.3 The Soave-Redlich-Kwong Equation of State

The Equation

In the pressure-explicit form, the equation of state is represented as follows :

$$P = \frac{RT}{(V - b)} - \frac{a(T)}{V(V + b)}$$

Parameter a(T) is a function of temperature and depends on the accentricity factor of a component. The parameters a and b are dimensionless as their values depend on the reduced properties of a component. The first accounts for the attractive forces between molecules and the second corrects for the molecular volumes of a real gas. For a pure substance, these are given by the following correlations :

$$a(T) = a_c\ \alpha(T)$$

$$b = 0.08664\ (P_r\ /\ T_r)$$

$$a_c = 0.42747\ (P_r\ /\ T_r^{2})$$

$$P_r = P\ /\ P_c = \text{Reduced Pressure}$$

$$T_r = T\ /\ T_c = \text{Reduced Temperature}$$

$$T_c = \text{Critical Temperature}$$

$$P_c = \text{Critical Pressure.}$$

The constants in a_c and b are the same as the RK equation. The temperature-dependant factor α was determined through regression analysis of vapor-liquid equilibrium (VLE) data. The correlation is given by the following equation :

$$\alpha(T) = \{\ 1 + m(\omega)\ [\ 1 - T_r^{0.5}\ ]\ \}^{2}$$

Thus, the value of α depends on the Pitzer accentricity factor, ω also, unlike the RK approach. However, there is a discrepancy among many published literature on the correlation for the term $m(\omega)$. According to the original article (Soave,1972), Reid, Sherwood and Prausnitz (1977) and Henley and Seader (1981), it is given by:

$$m(\omega) = 0.480 + 1.574\ \omega - 0.176\ (\omega^{2})$$

In another paper published more recently by Soave (1979), it is presented as follows :

$$m(\omega) = 0.47979 + 1.576\ \omega - 0.1925\ (\omega^{2}) + 0.025\ (\omega^{3})$$

The reason for this discrepancy lies in the method used to arrive at the correlation. The first form was correlated against non-polar components alone, whereas the second study had included systems with slightly polar species and also systems containing components in the solid phase. We have decided to implement the second correlation in view of its improved generality and since it was published more recently. A third version of the same equation is presented by Ferrel et al(1983) :

$$m(\omega) = 0.48508 + 1.55171\omega - 0.15613(\omega^2)$$

The regression criteria employed to arrive at this correlation were not mentioned in the paper.

The Mixture Combination Rules

As mentioned in the previous chapter, the success of the SRK equation in predicting VLE or vapor pressure data is due mainly to two aspects : the temperature dependance of one parameter and the accurate nature of mixing rules.

In order to predict accurately for a mixture, especially those containing polar components, Soave proposed a greatly improved set of mixture combination rules for the parameters in his equation. He introduced the concept of a binary interaction parameter for estimating 'a' in the already widespread notion of using a mole-fraction-weighted quadratic average. The following is the expression for the mixture 'a' parameter, denoted by 'A' :

$$a_{mix} = A = \sum_{i=1}^{n} \sum_{j=1}^{n} y_i \, y_j \, a_{ij}$$

where:

$$a_{ij} = a_i^{0.5} \, a_j^{0.5} \, (1 - K_{ij})$$

The value of K_{ij}, the 'interaction parameter' is nonzero for mixture-pairs (i,j) of which at least one is a polar compound. It is zero for the other pairs existing in the system. In the later case, a simple quadratic average is sufficient to reflect the mixing effect. Thus, interaction is significant for polar:polar and non-polar:polar pairs in the mixture. This binary interaction parameter was found to be adequate in predicting phases containing non-polars (Reid, Sherwood and Prausnitz, 1977). The values of the parameter for some commonly encountered hydrocarbon-polar pairs are given in Reid, Sherwood and Prausnitz's text (1977). The polar components for which data is available are: Nitrogen, Carbon Monoxide, Hydrogen Sulphide and Carbon Dioxide. No data is available for Water, which exibits a strong dipole moment and hence, polar behavior. We have supplied the available values to our program and assumed no interaction for other pairs, including those containing Water.

Better results can be obtained from a temperature-dependent correlation for K_{ij}. This was observed in a study of methanol-containing systems made by Ferrel et al(1983). A linear relationship between the interaction parameter and temperature was obtained. For a given system, one can arrive at such results provided accurate VLE data is available together with a regression program. Such procedures could be made an integral part of a simulation package. For the present, we will supply constant values, for the interaction pairs whose data is available.

For the second parameter in the equation of state, a simple mole-fraction average is found to suffice for mixtures (Soave,1972).

$$b_{mix} = B = \sum_{i=1}^{n} y_i b_i$$

However, in the article by Ferrel, it is mentioned that some research is currently under way to find an expression for b_{mix} having an interaction parameter. No significant improvement has yet been achieved.

The Compressibility Factor : for Vapor Phases Only

The compressibility factor, Z, is a measure of non-ideality for a vapor. The SRK equation written in the Z-explicit form is :

$$Z = \frac{P\,V}{R\,T} = \frac{V}{V - b} - \frac{\Omega_a}{\Omega_b} \cdot \frac{b}{V + b} \cdot F \quad (3.13)$$

where :

$$\Omega_a = 0.42747$$

$$\Omega_b = 0.08664$$

$$F = [\,1 + m(\omega).(\,1 - T_r^{\,0.5}\,)\,]^2 \,/\, T_r$$

Since the measurement and prediction of volume is associated with large errors, one can eliminate V from the above equation, using V = ZRT/P. Upon rearrangement, one obtains the following cubic equation for the compressibility factor:

$$Z^3 - Z^2 + Z\,[\,\bar{A} - \bar{B} - \bar{B}^2\,] - \bar{A}\,\bar{B} = 0$$

where :

$$\bar{A} = \frac{A\,P}{(R\,T)^2} \quad \text{and} \quad \bar{B} = \frac{B\,P}{R\,T}$$

$$A = a_{mix} \quad \text{and} \quad B = b_{mix}$$

A cubic equation has three roots that can have real, or imaginary values depending on the value of the coefficients. For a two phase system, under supercritical conditions, only one positive real root is obtained, the other two are imaginary. For two-phase subcritical conditions, all the roots are real, the largest being for the vapor phase and the smallest for the liquid phase. Thus, there is at least one real root, which would approach a value of zero for a liquid phase component and one for a vapor phase component. Since we will apply this module for the vapor phases only, an iterative procedure starting at a value of 1.00 for the vapor phase is adopted. A Newton's iterative algorithm is employed to solve for Z.

The Fugacity Coefficients : for Vapor Phases Only

The fugacity coefficient of a component 'i' in a mixture is derived from the definition and fundamental relationships given in equations (3.4) and (3.5). Expressing the SRK equation in terms of the total volume, one obtains the following :

$$P = \frac{N R T}{V_T - N b} - \frac{a N^2}{V_T (V_T + N b)} \qquad (3.14)$$

From equations (3.5) and (3.14) we obtain the fugacity coefficient :

$$\hat{\phi}_i = \exp \{(Z - 1) (B / \bar{B}) - \ln (Z - \bar{B}) - (\bar{A} / \bar{B}) \ln ((Z + \bar{B}) / Z)[2 (A / \bar{A})^{0.5} - (B / \bar{B})]\}$$

In the case of a pure component, the application of equation (3.4) yields the following relationship :

$$f_i^0 = \exp [(Z-1) - \ln(Z-b_i) - (a_i / b_i). \ln\{(Z + b_i)/Z \}$$

The Enthalpy Departure Function : for Vapor Phases Only

The enthalpy departure function of a real fluid is defined as the difference between its enthalpy and the enthalpy of ideal gas at the same temperature. When equation (3.13) is applied to equations (3.6) and (3.7), we obtain the following expression for the enthalpy departure of a mixture :

$$(H - H^0) = R\,T\,\{(Z - 1) - (1 / B).\ln((Z + B) / Z)$$

$$.\left(\sum_{i=1}^{n}\sum_{j=1}^{n} y_i\, y_j\,(1 - K_{ij})\,.(a_i\, a_j)^{0.5}\right.$$

$$.\,(1 - m_i/2\,(T_{r_i} / a_i) - m_j/2\,(T_{r_j} / a_j))\}$$

The Entropy Departure Function : for Vapor Phases Only

The entropy departure of a real fluid from that of an ideal gas at the same temperature is expressed in the fundamental equation given by (3.8). When this equation is applied to the SRK equation, we arrive at the following expression for entropy departure of a mixture :

$$(S - S^0) = R\,[\,\ln((V - B)/ V) - (\gamma / B)$$

$$.\,\ln((V+B)/ B) + \ln(V/ V_0)$$

where :

$$\gamma = -\left(\frac{1}{2}\right) \sum_{i=1}^{n} \sum_{j=1}^{n} y_i \, y_j \, (1 - K_{ij}) \, (0.42747/\ 0.08664)$$

$$.(B_i B_j)^{1/2} . (F_i F_j)^{1/2} . \{ (m_i / F_i^{1/2}) + (m_j / F_j^{1/2}) \}$$

and : $$F_i = [\, 1 + m_i \,.\, (1 - T_{r_i}^{1/2}) \,]^2 \,/\, T_{r_i}$$

and : $$V_0 = R\,T / P_0$$

We compute the volume, V, by an iterative procedure with the starting guess value of the ideal gas volume, V_0.

3.4 The Peng-Robinson Equation of State

The Equation

The pressure-explicit form of the Peng-Robinson equation is given by the following relation :

$$P = \frac{R\,T}{V - b} - \frac{a(T)}{V(V + b) + b(V - b)}$$

For pure substances, the parameters are expressed as follows :

$$a = a(T) = a(T_c) \,.\, \alpha(T_r)$$

$$a(T_c) = 0.45724 \, (R\,T_c^2) \,/\, P_c$$

$$\alpha(T_r) = [\, 1 + K(\omega)\, (\, 1 - T_r^{1/2}\,)\,]^2$$

$$b = 0.0778\, (\, R\, T_c\, /\, P_c\,)$$

$$K(\omega) = 0.37464 + 1.54226\, \omega - 0.26992\, \omega^2$$

Although these equations do not seem to reflect it, there is a considerable difference between the approaches taken in the Peng-Robinson and the Soave-Redlich-Kwong methods. While Soave used vapor pressure data only at the critical point and at $T_r = 0.7$ in order to arrive at his coefficients, Peng and Robinson regressed data over the entire range, starting at the normal boiling point and proceeding to the critical point. The justification of the Soave method lies in the definition of the Pitzer accentricity factor, which is a function of vapor pressure at reduced temperature of 0.7. Since Soave had proposed the dependance of the 'a' parameter on the accentricity factor, he had used the same conditions for consistency. The accentricity factor is used in both the correlations and both assumes that the parameter 'a' depends on it.

Mixture Combination Rules

In the case of a mixture, the parameters are to be evaluated according to the following mixing rules :

$$a_{mix} = A = \sum_{i=1}^{n} \sum_{j=1}^{n} y_i\, y_j\, a_{ij}$$

$$a_{ij} = (1 - \delta_{ij})\, a_i^{0.5}\, a_j^{0.5}$$

$$b_{mix} = B = \sum_{i=1}^{n} y_i\, b_i$$

Thus, a geometric molal average with an interaction parameter for the parameter 'a' and a mole-fraction average for the parameter 'b' is used. This approach apparently is the same as that adopted in SRK equation. However, Soave considered binary interaction significant only in the presence of polar species. Peng and Robinson have included all types of components in the consideration of interaction. In this extension of CHESS, we have included data for 19 components, which are C_1--C_{10} aliphatic hydrocarbons, Carbon Dioxide, Hydrogen Sulphide, Nitrogen, Cyclo-Hexane, Benzene, Toluene and Water. The values of the interaction parameters are shown in Table 3.1. The authors have successfully applied their equation to a variety of prediction purposes, including vapor pressures and liquid volumes. However, the success of a regression-oriented model depends largely on the regression objective function used. The regression-criterion chosen by Peng and Robinson was that of minimum deviation in bubble point pressure predictions, with regressions on the the interaction parameters and the correlation-parameters 'a' and 'b'of the equation of state.

Another important aspect of the Peng-Robinson methodology is that in certain situations, unary interaction is represented by 1 - 1 binary parameters. Thus, in the case of adiabatic flash calculations for systems where a water-soluble gas is present, components such as Methane, Water and Hydrogen Sulphide are assumed to interact with themselves. Moreover, the 1 - 1 interaction parameters are temperature-dependent relationships, having the form of polynomials in temperature. The coefficients are presented in Table 3.2. These 1 - 1 interacting pairs seem to be very realistic for polar molecules. The SRK model does not consider this aspect.

It can be conjured that better results in VLE predictions can be obtained through equations of state which takes into account multicomponent interaction. With the binary interaction parameter approach, where the effective interaction is assumed to be the sum of all the binary interactions, one assumes that interactions between molecules take place in pairs, unaffected by the presence of other molecules. For strongly interactive mixtures, this couldbeonlya poor of thephysicalsituation.

The Virial equation incorporates the idea of multicomponent-interactions, but it carries out an addition of the effects of unary, binary, ternary, etc. interactions, upto a number of terms equal to the number of components present in the system. Only an additive procedure,however, may not represent the phase behavior adequately.

TABLE 3.1

<u>Interaction Parameters for the Peng-Robinson Equation</u>

	N_2	CO_2	H_2S	C_7H_8	C_6H_6	Cy-C_6H_{12}	H_2O
Methane	0.036	0.100	0.085	0.040	0.040	0.035	0.500
Ethane	0.050	0.130	0.084	0.020	0.020	0.020	0.500
Propane	0.080	0.135	0.075	0.020	0.020	0.020	0.480
I-Butane	0.095	0.130	0.050	0.000	0.000	0.000	0.480
N-Butane	0.090	0.130	0.060	0.000	0.000	0.000	0.480
I-Pentane	0.095	0.125	0.060	0.000	0.000	0.000	0.480
N-Pentane	0.100	0.125	0.065	0.000	0.000	0.000	0.480
N-Hexane	0.100	0.125	0.060	0.000	0.000	0.000	0.480
N-Heptane	0.100	0.100	0.060	0.000	0.000	0.000	0.480
N-Octane	0.100	0.115	0.055	0.000	0.000	0.000	0.480
N-Nonane	0.100	0.110	0.050	0.000	0.000	0.000	0.480
N-Decane	0.100	0.110	0.045	0.010	0.010	0.010	0.000
Nitrogen	--	-0.02	0.180	0.180	0.160	0.100	0.000
CO_2	-0.02	--	0.100	0.090	0.075	0.100	0.000
H_2S	0.180	0.100	--	0.000	0.000	0.000	0.000
Toluene	0.180	0.090	0.000	--	0.000	0.000	0.000
Benzene	0.160	0.075	0.000	0.000	--	0.000	0.000
Cyclo-C_6H_{12}	0.100	0.100	0.000	0.000	0.000	--	0.000
Water	0.000	0.000	0.000	0.000	0.000	0.000	--

TABLE 3.2

Temperature-Dependant Factors for (1<-->1) Pair Interactions

$$\text{Interaction Parameter} = A + B\,T + C\,T^2$$

Units of T :: Degrees Kelvin.

Component	A	$B \times 10^2$	$C \times 10^5$
Methane	-1.5240	0.5328	-0.3982
Ethane	-0.9682	0.3384	-0.2354
Propane	-1.0380	0.3166	-0.2333
I- Butane	-0.9931	0.3166	-0.2333
N- Butane	-0.9246	0.3045	0.2276
Nitrogen	-2.2380	0.6700	-0.4686
CO_2	-0.5572	0.1879	-0.1274
H_2S	-0.3896	0.1565	-0.1142

The Compressibility Factor : for Vapors and Liquids

The Peng-Robinson equation, rearranged in the Z-explicit form, is :

$$Z = \frac{P\,V}{R\,T} = \frac{V}{V - b} - \frac{a}{V(V + b) + b(V - b)}$$

Eliminating volume and redefining the constants, one arrives at the following equation :

$$Z^3 - (1 - \bar{B})Z^2 + (\bar{A} - 3\bar{B}^2 - 2\bar{B})Z - (\bar{A} - \bar{B}^2 - \bar{B}^3) = 0$$

where :

$$\bar{A} = \frac{a_{mix}\,P}{(R\,T)^2} = \frac{A\,P}{(R\,T)^2}$$

$$\bar{B} = \frac{b_{mix}\,P}{(R\,T)} = \frac{B\,P}{(R\,T)}$$

The vapor phase compressibility factor is given by the largest positive real root and the liquid phase compressibility factor is given by the smallest positive real root, for a two-phase system. A Newton-Raphson procedure, with a starting value of 1 for the vapor phase and 0 for the liquid phase, yields the desired root. The universal critical compressibility factor predicted by this equation is 0.307.

The Fugacity Coefficients : for Vapors and Liquids

The fugacity coefficient for a component i in amixture, calculated by applying the Peng-Robinson equation to equations(3.4) and (3.5), is :

$$\ln \hat{\emptyset}_i = \ln \left(\frac{f_i}{y_i P}\right) = (b_i / B)(Z-1) - \ln(Z - \bar{B})$$

$$- (\bar{A} / \bar{B} / 2./\bar{2}) \left[\left(2 \sum_{j=1}^{n} y_j a_{ij}\right)/A - (b_i / B)\right]$$

$$. \ln\left[(Z + 2.414\bar{B}) / (Z - 0.414\bar{B})\right]$$

where :

$$\bar{A} = a_{mix} P / (R\,T)^2 = AP / (R\,T)^2$$

$$\bar{B} = b_{mix} P / (R\,T) = B\,P / (R\,T)$$

For a pure component, the fugacity coefficient expression has the following form :

$$\ln \emptyset = \ln(f/P) = (Z - 1) - \ln(Z - B^*) - (A^* / B^* / 2\sqrt{2})$$

$$. \ln\left[(Z + 2.414\,B^*) / (Z - 0.414\,B^*)\right]$$

where :

$$A^* = a_i P / (R\,T)^2$$

$$B^* = b_i P / (R\,T)$$

<u>The Entropy Departure : for Vapors and Liquids</u>

Starting from the basic thermodynamic identity in equation (3.8), we can establish that, for the Peng-Robinson equation, the entropy departure function is:

$$(S - S^0) = R \ln(Z - \bar{B}) + \frac{(\partial A / \partial T)}{2\sqrt{2}\,B} . \ln\left(\frac{Z + 2.414\,\bar{B}}{Z - 0.414\,\bar{B}}\right)$$

The derivative of the mixture 'a' parameter, A, with respect to temperature is given by the following expression :

$$\left[-2\sqrt{T} \right] \left(\frac{\partial A}{\partial T} \right) = \sum_{i=1}^{n} \sum_{j=1}^{n} \left[a_{ij}\, y_i\, y_j \left\{ \frac{K(\omega_i)}{(\alpha_i T_{C_i})^{0.5}} + \frac{K(\omega_j)}{(\alpha_j T_{C_j})^{0.5}} \right\} \right]$$

The derivations of these equations is presented in Appendix A.

<u>The Enthalpy Departure : for Vapors and Liquids</u>

From the thermodynamic identities (3.6) and (3.7) and the Peng-Robinson equation of state, we obtain the following expression for enthalpy departure for a mixture :

$$H - H^0 = \left\{ \frac{\left[T \left(\frac{\partial A}{\partial T} \right) - A \right]}{2\sqrt{2}\ B} \right\} \ln \left\{ \frac{Z + 2.414\ \bar{B}}{Z - 0.414\ \bar{B}} \right\} + R\,T(Z - 1)$$

The expression for the derivative was presented in the last section. The derivation of the enthalpy departure function is detailed in Appendix A.

3.5 Vapor Mixture Heat Capacity Functions

The heat capacity of a phase is a derivative thermodynamic property. Heat, unlike work, is a thermodynamic property of a substance since its association with changes of state is path-independant. The derivative of heat with respect to temperature along a specified path is also a thermodynamic property.

The derivative of enthalpy with respect to temperatue along a constant pressure path is termed as specific heat at constant pressure,C_p.It is characteristic of a substance as different substances exibit different heat requirement or release along such paths. The derivative of heat, rather internal energy with respect to temperature for a constant volume process is termed as specific heat at constant volume, C_v.

These pure component properties are extended to a mixture property with the additive molar assumption. These properties are related to each other. Their departure functions with respect to an ideal gas state can be predicted from basic thermodynamic relationships applied to an equation of state. Similarly, the difference between the two are predictable from thermodynamic identities. Again, all these are interrelated. The various relationships describing the evaluation of these properties from an pressure-explicit equation of state were presented in equations (3.9), (3.10) and (3.11).

Thus, starting with these equations and using an equation of state to express the derivatives, we can obtain the following for vapors :

(1) C_p values :

From $(C_p - C_p^0)$. C_p^0 is obtained for each component from zero-pressure heat content coefficients presented by Reid,Sherwood,Prausnitz('77)

$$C_p^0 = a + b T + c T^2 + d T^3$$

(2) C_v values :

From $(C_p - C_v)$ and C_p .

(3) Polytropic coefficients :

(C_p / C_v) , from the values obtained as above.

Let us present the expressions derived from the equations of state.

3.5.1 Soave-Redlich-Kwong Equation

Vapor Heat Capacity Departure at Constant Volume

Starting with the SRK equation of state and equation (3.6), we arrive at the following expression :

$$\frac{C_v - C_v^0}{R} = \frac{\Delta C_v}{R} = \frac{1}{2} \left(\frac{A_v^2}{B_v}\right) (MTA) \ln(1 + h_1)$$

where :

$$A_v^2 = [\, a_{mix}/(RT)^2 \,] = [\, A/(RT)^2 \,]$$

$$B_v = (\, b_{mix}/(RT) \,) = (\, B/(RT) \,)$$

$$h = (\, b / V) = (\, B_v P / Z \,)$$

$$MTA_1 = m(\, \omega_{mix} \,)\, T_{r_{mix}}^{1/2} \,/\, \alpha^{1/2}$$

$$\omega_{mix} = \sum_i y_i \omega_i$$

$$T_{r_{mix}} = T / T_{c_{mix}}$$

$T_{c_{mix}}$: obtained via the Chueh - Prausnitz correlation.

The derivation is presented in Appendix B.

Vapor Heat Capacity Difference

Applying the SRK equation to equation (3.10), we obtain the following expression :

$$\{ (C_p - C_v) / R \} =$$

$$\frac{\left(\frac{1+h}{1-h}\right) + 2\left(\frac{A_v^2}{B_v}\right)(MTA_2)\left(\frac{h}{b_{mix}}\right) + 4\left(\frac{A_v^2}{B_v}\right)^2 (MTA_2)^2 \left(\frac{h}{b_{mix}}\right)^2 \left(\frac{1+h}{1-h}\right)}{\left(\frac{1+h}{1-h}\right) - \left(\frac{A_v^2}{B_v}\right)\left(\frac{h}{b_{mix}}\right)\left(\frac{1-h}{1+h}\right)(2+h)}$$

where :

$$MTA_2 = m(\omega_{mix}) \;/\; \alpha^{1/2} \;/\; T$$

The derivation is presented in Appendix B.

Vapor Heat Capacity Departure at Constant Pressure

From the two expressions given above, we can obtain the departure function for C_p by direct substitution. It follows from equation (3.12) and is given below :

$$\frac{C_p - C_p^0}{R} = \frac{\Delta C_p}{R} =$$

$$\left[\frac{\left(\frac{1+h}{1-h}\right) + 2\left(\frac{A_v^2}{B_v}\right)(MTA_2)\left(\frac{h}{b_{mix}}\right) + 4\left(\frac{A_v^2}{B_v}\right)^2 (MTA_2)^2 \left(\frac{h}{b_{mix}}\right)^2 \left(\frac{1+h}{1-h}\right)}{\left(\frac{1+h}{1-h}\right) - \left(\frac{A_v^2}{B_v}\right)\left(\frac{h}{b_{mix}}\right)\left(\frac{1-h}{1+h}\right)(2+h)}\right]$$

$$+ \left[\left(\frac{1}{2}\right)\left(\frac{A_v^2}{B_v}\right)(MTA_1)\ln(1+h)\right] - 1$$

3.5.2 Peng-Robinson Equation

Vapor Heat-Capacity Departure at Constant Volume

Starting from the Peng-Robinson equation of state and equation (3.9) we arrive at the following expression of the departure function for C_v :

$$\frac{C_v - C_v^0}{R} = \frac{\Delta C_v}{R}$$

$$= \left(\frac{1}{5.656}\right)\left(\frac{A_v^2}{B_v}\right)(MTB_1)\ln\left[\frac{(1 + 2.414\,h)}{(1 - 0.414\,h)}\right]$$

where :

$$A_v^2 = a_{mix}/(RT)^2 = A/(RT)^2$$

$$B_v = b_{mix}/RT = B/RT$$

$$h = b/V = BP/Z$$

$$MTB_1 = K(\omega_{mix})\,T_{r_{mix}}^{1/2} / a_{mix}^{1/2}$$

The derivation is presented in Appendix B.

Vapor Heat Capacity Difference

When the Peng-Robinson equation is applied to the equation (3.10), we obtain the following expression for the difference between C_p and C_v :

$$\{C_p - C_v\} / R =$$

$$\left[\frac{\left(\frac{1+h}{1-h}\right) + \left(\frac{A_v^2}{B_v}\right)(MTB_2)\left\{\frac{(1+h)}{(1+2.414h)(1-0.414h)}\right\}}{\left(\frac{1+h}{1-h}\right) - \left(\frac{A_v^2}{B_v}\right)\left(\frac{h}{1.414}\right)\left\{\frac{(1-h^2)(2.828+h)}{[(1+2.414h)(1-0.414h)]^2}\right\}}\right]$$

$$\cdot \left[1 + \left(\frac{A_v^2}{B_v}\right)(MTB_2)\left\{\frac{(1-h)}{(1+2.214h)(1-0.414h)}\right\}\right]$$

where :

$$MTB_2 = MTB_1 \cdot b_{mix} = MTB_1 \cdot B$$

The derivation is presented in Appendix B.

Vapor Heat Capacity Departure at Constant Pressure

The heat capacity departure function is obtained directly from the two expressions presented above, as per equation (3.12). The final form is presented below :

$$\frac{\Delta C_p}{R} = \frac{C_p - C_p^0}{R} =$$

$$\left(\frac{1}{5.656}\right)\left(\frac{A_v^2}{B_v}\right)(MTB_1)\ \ln\left[\frac{(1 + 2.414\ h)}{(1 - 0.414\ h)}\right] - 1$$

$$+\left[\frac{\left(\frac{1+h}{1-h}\right) + \left(\frac{A_v^2}{B_v}\right)(MTB_2)\left\{\frac{(1+h)}{(1+2.414h)(1-0.414h)}\right\}}{\left(\frac{1+h}{1-h}\right) - \left(\frac{A_v^2}{B_v}\right)\left(\frac{h}{1.414}\right)\left\{\frac{(1-h^2)(2.828+h)}{[(1+2.414h)(1-0.414h)]^2}\right\}}\right]$$

$$\cdot\left[1 + \left(\frac{A_v^2}{B_v}\right)(MTB_2)\left\{\frac{(1-h)}{(1+2.214h)(1-0.414h)}\right\}\right]$$

3.5.3 Specific Heat Departures : Some Thermodynamic Issues

In order to calculate the heat capacity functions via the two equations of state described above, the SRK and the Peng-Robinson, we need to obtain certain physical properties of a vapor mixture. The equation of state parameters for the mixture would be available since the respective modules would have been invoked a priori. However, the accentricity factor and the critical temperature of the mixture are required to calculate the departure functions.

Based on suggestions made by Reid, Sherwood and Prausnitz (1977), we have used simple molal averaging to calculate the mixture accentric factor. The mixture critical temperatures are evaluated using the Chueh-Prausnitz method (Reid, Sherwood, Prausnitz, 1977). According to this method, the true critical temperature of a mixture depends on the surface fraction parameter, which is a function of the component critical volumes. The correlation makes use of certain binary interaction parameters for polar-nonpolar pairs. We have used the parameters which are available in Reid, Sherwood and Prausnitz's text(1977).

3.7 The RK/ SRK : Chao-Seader Liquid Phase Models

In this section, the Chao-Seader model for determining activity coefficients and the various thermodynamic expressions derived based on it will be presented.

Equilibrium Ratios : The Chao Seader-RK/ SRK Approach

In this method, the equilibrium ratios are calculated with the unsymmetric convention, as outlined previously, in the equations (2.2) and (3.2).

The activity coefficient is defined as the ratio of the activity in the liquid phase to the liquid phase concentration, x_i. The activity in the liquid phase is the ratio of the fugacity of a component in a mixture to its fugacity in some standard state. The standard state taken for computations in this work is the system conditions. The Chao-Seader correlation estimates the values of f^{o}_{iL}, the pure-component liquid phase fugacity coefficient.

The Chao-Seader activity coefficient model uses the RK equation of state for calculating vapor phase fugacity coefficients. The SRK equation of state has been supplied as an alternate vapor phase model. Scatchard and Hildebrand[s regular solution theory is used for predicting the liquid phase activity coefficients in conjunction with the RK vapor phase model. An extension of the Pitzer-Curl's correspon-ding state principle is used to determine the liquid phase fugacity ratios. We have included the Flory-Huggins modification of the regular solution theory to account for molecular size differences. The Grayson-Streed coefficients are used in this work in the determination of activity coefficients. This approach, originated by the original authors (Chao and Seader, 1961), has been successful particularly near critical conditions and higher pressures, practically for all hydrocarbon and light-gas containing systems. However, some limitations are applicable, which were discussed in Chapter 2, page 25.

Liquid Phase Component Fugacity Coefficient

The study made by Chao and Seader (1961) in developing their models involved a variety of equilibrium systems, usually hydrocarbons with light gases like Nitrogen and Hydrogen. The regression of the VLE data was performed in terms of reduced properties and accentricity factors, in order to obtain a correlation for the liquid-phase component fugacity ratios. For liquid conditions which are hypothetical, that is, when the system pressure is less than the saturation vapor pressure or when the temperature is greater than the critical temperature, extrapolated VLE data was used for the correlation coefficients. Although this could have been a source of serious error, the correlation is found to be very suitable for high pressure systems.

$$\log f^{0}_{i_L} = \log f^{(0)}_{i_L} + \omega_i \log f^{(1)}_{i_L}$$

where :

$$\log f^{(0)}_{i_L} = A_0 + A_1/T_{r_i} + A_2 T_{r_i} + A_3 T_{r_i}^2 + A_4 T_{r_i}^3 + (A_5 + A_6 T_{r_i} + A_7 T_{r_i}^2) P_{r_i} + (A_8 + A_9 T_{r_i}) P_{r_i}^2 - \log P_{r_i}$$

$$\log f_{i_L}^{(1)} = A_{10} + A_{11} T_{r_i} + A_{12}/T_{r_i} + A_{13} T_{r_i}^{3} + A_{14}(P_{r_i} - 0.6)$$

The values for the correlation coefficients A_{10} through A_{14} are taken from the original article. The Grayson Streed modified values for constants A_0 through A_9 are obtained fron Henley and Seader's text (1981). The revised values were obtained because Methane and Hydrogen were differentiated as 'simple fluids'. These were assumed to have an accentric factor of zero in order to reflect their behavior in hydrocarbon systems accurately.

The empirical equations presented above are applicable over a range of reduced temperatures of 0.5 to 1.3. Grayson and Streed have reset the reduced temperatures to 1 whenever the critical conditions were exceeded for a component. The same method was followed in the original CHESS. We had started without such restrictions, which gave rise to exponent overflows for values of $v_{iL}(1)$ under supercritical conditions. Hence the same method was reinstated.

<u>Liquid Phase Activity Coefficients</u>

The 'Regular Solution' theory is based on the assumption that liquids behave non-ideally due to the dissimilarities between the van der Waals' forces of attraction between the interacting molecules present in the solution. In contrast, an ideal solution theory assumes that intermolecular forces are equal and opposite, the species have molecules of uniform size and chemically, they are non-interactive. The key assumption in the regular solution theory is that the excess entropy of mixing is zero when mixing occurs at constant volume (Smith and van Ness, 1975). The molecules are assumed to be randomly dispersed, but unlike an ideal solution, unequal attractive and repulsive forces cause segregation of like molecules. The endothermic heat of mixing counterbalances this energy, yielding an entropy level identical with the ideal solution. An 'Ideal Solution' is described by Raoult's law.

For a multicomponent regular solution, the excess molal Gibb's free energy is given by :

$$g^E_{regular} = \sum_{i=1}^{n} (x_i V_{i_L}) [(1/2) \sum_{i=1}^{n} \sum_{j=1}^{n} \theta_i \theta_j (\delta_i - \delta_j)^2]$$

where :

V_{i_L} = Liquid molal volume of component 'i',

δ_i = SolubilityParameterof 'i'

= $[(\Delta H_V - R T)/ V_{i_L}]^{1/2}$

ΔH_V = Energy of Vaporization at a standard state, taken as 25 C and one atmosphere

θ_i = Additive volume fraction,

= $x_i V_{i_L} / \sum_i x_i V_{i_L}$

From the definition of excess molal free energy, it follows that :

$$\ln \gamma_i = \frac{\bar{g}_i^E}{R\,T} = \frac{V_{i_L}\,(\delta_i - \sum_j^n \theta_j \delta_j)}{R\,T}$$

$$\text{since: } \bar{g}_i^E = g^E - (R\,T)\left[\sum_{k=1} x_k \left\{ \partial(g^E/RT)\Big|_{T,P,x_r} / \partial x_k \right]\right.$$

In this modification of CHESS, the Flory-Huggins corrected form of the above equation is used. According to this approach, when the molecular size differences are appreciable, the solution behavior tends to be athermal rather than regular. This difference is reflected in the molal volume figures and such conditions are more realistic. The Flory-Huggins correction adds a term to the free energy representing the contribution of the size differences. It is given as follows :

$$g^E_{\text{correction}} = \sum_i^n \{ RT\; x_i \ln(\theta_i / x_i) \}$$

In order to represent the actual Gibb's free energy of the solution, the above correction is added to the regular solution contribution. Substituting the redefined free energy in the expression for the parrtial molal free energy of component 'i', yields the following final form for the equation for the activity coefficients :

$$\ln \gamma_{i_L} = 1 + \frac{V_{i_L} [\delta_i - \sum_j^n \theta_j \delta_j]^2}{R\,T} + \ln (V_{i_L} / V_L) - (V_{i_L} / V_L)$$

where :

$$V_L = \sum_i^n V_{i_L}$$

Henley and Seader (1981) recommends the use of this equation for the activity coefficient, which was not present in the original version of CHESS.

Vapor Phase Component Fugacity Coefficients : RK/SRK Eqns.

The Redlich-Kwong equation was used in the calculations of vapor phase fugacity coefficients while arriving at the Chao-Seader models (refer to sections 3.2). We have used the SRK equation instead (refer to section 3.3). The rationale behind this approach is that the SRK equation is structurally similar to the RK equation and was tested with similar equilibrium systems. It is evident from the results of our test cases that both of these equations are adequate in representing the vapor phase and they yield results that are close.

In a related study made with the use of Chao-Seader models, some computational problems were observed (Coward et al, 1978). The results for a Ethane(0.4) - Propane(0.4) - n-

Butane (0.2) system is presented. They showed that while the Benedict-Webb-Rubin equation of state creates a defined pressure-temperature envelope, the RK equation fails to do so. From the RK vapor phase model, a pair of dew and bubble points were obtained near the critical point of the mixture, resulting in a pair of divergent, asymptotic curves with no intersection and hence no critical state was reached. Such discontinuity is referred to as the 'spurious roots error'. Thus, the state of the system near the critical conditions becomes ambiguous and over extension of the correlation is to be avoided. Further research should investgate the performance of the SRK equation in this respect.

Various Liquid Phase Property Models Via Chao-Seader Models

Apart from the VLE calculations, our objective is to obtain the liquid-phase enthalpy and entropy departure functions and the liquid molar volumes based on the Chao-Seader activity coefficient and liquid phase fugacity coefficient correlations. The following topics would describe each of these in detail.

Enthalpy of Liquid Phase Mixtures

The liquid phase enthalpy relative to an ideal vapor condition is obtained from two terms : the partial molal excess enthalpy and the molal enthalpy departure. The vapor phase enthalpy is determined by a departure function evaluated by a equation of state, RK or SRK, as described in sections 3.2 and 3.3.

The partial molal excess enthalpy is determined from the differential form of the Gibb's integral equation. It represents the heat of mixing effect. The following relationship is used to obtain the excess enthalpy of species 'i' :

$$-\bar{H}_i^E = R T^2 \left\{ \frac{\partial \ln \gamma_{i_L}}{\partial T} \right\} \Bigg|_{P,x_i} = H_{i_L} - \bar{H}_{i_L}$$

The molal enthalpy departure represents the combined effects of pressure and the latent heat of vaporization. The following relationship is used to evaluate this term for a component 'i' in a mixture :

$$H_{i_V}^0 - H_{i_L} = R T^2 \left[\frac{\partial \ln f_{i_L}^0}{\partial T} \right] \Bigg|_P$$

The enthalpy of the liquid referred to an ideal gas condition is obtained from the two relations presented above. The following equation generates the departure function for the solution :

$$H_L - H_V^0 = \sum_{i=1}^{n} x_i \left[(H_{i_L} - H_{i_V}^0) + \bar{H}_i^E \right]$$

The ideal gas enthalpy, H_V^o , is obtained through data published in Reid, Sherwood and Prausnitz's book (1977). For the terms on the right hand side of the equation given above, the Chao-Seader correlations are applied to the respective equations given above. The following are the simplified results :

$$R\,T^2 \left(\frac{\partial \gamma_{i_L}}{\partial T}\right)\Bigg|_{P,x_i} = - v_{i_L} \left(\delta_i - \sum_{k=1}^{n} \Theta_k \, \delta_k^2 \right)$$

$$R\,T^2 \left(\frac{\partial \ln f^0_{i_L}}{\partial T}\right)\Bigg|_{P} = \left\{\frac{2.30258\, R\, T^2}{T_{c_i}}\right\}.\left\{ - \frac{A_1}{T_{r_i}}\right.$$

$$+ A_2 + T_{r_i} (2 A_3 + 3 A_4 T_{r_i}) + P_{r_i} (A_6 + 2 A_7 T_{r_i})$$

$$\left. + A_9 P_{r_i}^2 + \omega_i (A_{11} - A_{12} / T_{r_i}^2 + 3 A_{13} T_{r_i}^2) \right\}$$

The first of the two expressions above, representing the partial molal excess enthalpy, is always negative as regular solutions have endothermic heats of mixing.

Liquid Phase Entropy Departure

The liquid phase entropy departure function is expressed in a manner identical to the enthalpy departure function, as shown below :

$$S_L - S_V^0 = \sum_i^n x_i \left[(\Delta S)_{i_{dep}} + (\bar{S}^E_i) \right]$$

For the regular solutions, the second term, the excess entropy of mixing, is zero. Hence, we will have to evaluate only the first, the component entropy departure functions, in order to estimate the entropy departure for the solution.

The entropy departure, the enthalpy departure and fugacity coefficient are related through a basic thermodynamic identity :

$$[H - H^0]/RT = [S - S^0]/R - \ln[f/P]$$

In the case of a component 'i' in the liquid phase :

Fugacity coefficient, $f_{i_L} = F^{\circ}_{i_L} \; x_i \; \gamma_{i_L}$

Standard state pressure, P_0 = 1 atm.

Pure species Fugacity, $F^{\circ}_{i_L} = f^{\circ}_{i_L} \; P$

Thus: $f_{i_L} = f^{\circ}_{i_L} \; x_i \; \gamma_{i_L} \; P$

P = system pressure.

Hence, the expression for entropy departure can be presented in the following manner :

$$S - S^0 = [(H - H^0)/T] - R\left[\sum_{i=1}^{n} x_i \ln\{\gamma_i \, x_i \, f^0_i \, P\}\right]$$

Since the Chao-Seader models supply the values of the enthalpy departure, the pure species fugacity coefficient and the activity coefficients, we can estimate the entropy departure from the thermodynamic identity given above.

Liquid Phase Molal Volume

The liquid phase molal volume is obtained within the premise of the regular solution theory by summing species molal volumes and correcting for excess volume (Henley and Seader, 1981). The excess volume of mixing is proportional to the derivative of activity coefficient with respect to pressure. For regular solutions, activity coefficient can be assumed to be independent of pressure. Let us consider the identities involved in the following set of relationships :

$$V_L = \sum_{i=1}^{n} \left[x_i \left(V_{i_L} + \bar{V}^E_{i_L} \right) \right]$$

$$\bar{V}^E = R\,T \left(\frac{\partial \ln \gamma_{i_L}}{\partial P} \right) \Bigg|_{T, x_i} = 0$$

$$V_{i_L} = R\,T \left[\left(\frac{\partial \ln f^0_{i_L}}{\partial P} \right) \Bigg|_T + \left(\frac{1}{P} \right) \right]$$

$$= \left[2.30258\, R\,T / P_{c_i} \right] \left[A_5 + A_6 T_{r_i} + A_7 T_{r_i}^2 + 2 P_{r_i} \left(A_8 + A_9 T_{r_i} \right) + \omega_i A_{14} \right]$$

The equation is derived directly from the Chao-Seader model of pure component fugacity coefficients. Initially, we had started with this method for estimating molal volumes in the computation of activity coefficients. But it yielded computational problems. In the test case for rotating equipments, the simulation was carried out under high pressure and non-condensibles were present in the liquid phase. For light gases, there were exponent overflows in the computation of activity coefficients. It was observed that negative values were predicted for the volumes of the light gases. Hence, the modified Rackett approach was adopted for estimating molal volumes instead. However, under moderate conditions, comparable results were obtained from both these methods.

3.7 Pure Component Thermophysical Database

The original version of CHESS has a collection of thermophysical data for pure components, elements and compounds, in the form of a subprogram named 'COMPID'. A database was created for 98 standard components defined in CHESS. The data required for a simulation study is retrieved according to the identification numbers supplied by the user.

Although this standard component data library is limited compared to more recently published databanks (Prausnitz, Reid and Sherwood, 1977), it involves a well-selected group of substances frequently processed in the hydrocarbon and related industries. It has straight-chain hydrocarbons (C_1 - C_{20}), light gases(H_2, N_2, O_2, H_2S etc), unsaturated hydrocarbons, common solvents, cyclic and aromatic compounds and some polymer base compounds (Motard and Lee, 1971).

The use of non-standard compounds requires that the user provide for all the physical properties' data in the format and order the system specifies. The units of input data must be compatible with CHESS, where the constants are stored in °C, atmospheres, cc/gram moles and calories.

We have retained this approach of obtaining physical properties' data in this modification of CHESS. In order to include up-to-date information, a large set of new pure-component data was added and existing data had to be modified. The data values for critical constants and ideal-gas heat capacity coefficients were revised based on data obtained from Reid, Sherwood and Prausnitz's collection (1977). The values for Chao-Seader modified accentricity factors, Hildebrand solubility parameters and molal volumes, molecular weights, molal volumes at 25 C and liquid densities at 15 C were not modified over the years and were hence, kept unchanged in this version. However, any of such properties' data is liable to be updated as new data is published. Successive modifications have to consider this aspect first.

The Chao-Seader modified accentricity factors are equal to the Pitzer's accentricity factors up to the second significant digit for most of the components. As we needed to have the Pitzer's constants for the newly created modules, we have integrated this property data in a single set of Pitzer's accentricity factors.

In this extension of the data library, a few new constants were added. This was necessitated by the various modules introduced. We will discuss these and related thermodynamic issues under this topic.

Modified Rackett Parameters for Saturated Liquid Volumes

Based on recommendations made by Reid, Sherwood and Prausnitz (1977), Prausnitz and co-workers (1980), we have chosen the Spencer-Danner modified Rackett parameters to represent saturated liquids for volume calculations.

The Rackett equation, as it was first proposed, is expressed in the following manner :

$$1 / \rho_s = [R T_c / P_c] Z_c^{\{1 + (1 - T_r)^{2/7}\}}$$

where :

ρ_s = saturated liquid density

T_c , P_c = critical constants

$T_r = T / T_c$

Z_c = critical compressibility factor

Following the idea presented in this correlation, a total of ten correlations were published until 1972. Spencer and Danner(1972) had evaluated all of these with 64 Hydrocarbons and 47 other organic and inorganic compounds. They analyzed published data over a wide range of temperatures, from the triple-point to the critical points of components. Based on this study, a new correlation was proposed which has proved itself to be the best till date.

We have incorporated this model in our version of CHESS. The correlation is expressed as follows :

$$1 / \rho_s = [R T_c / \rho_c] Z_{RA}^{\{1 + (1 - T_r)^{2/7}\}}$$

where :

ρ_c = liquid density at the critical state

Z_{RA} = modified Rackett parameters evaluated from volumetric data

The authors published data for this parameter for a number of components which they analysed. Most of the standard components of the CHESS library are included in the list. For components for which no data is available, the authors have recommended the use of the critical compressibility factor instead. Errors are expected in the range of only 3 to 4 % in such cases. We have followed this and have obtained data from Reid, Sherwood and Prausnitz's text (1977).

Heats of Vaporization at Normal Boiling Points

This pure component property is frequently used in thermodynamic correlations. According to Reid, Sherwood and Prausnitz (1977), quite a few methods for estimation of this property exist that are generally accurate and convenient to use. The correlations are usually based upon critical constants and the normal boiling point. We have obtained data for all the standard components from the source mentioned above.

Antoine Vapor Pressure Coefficients

Vapor pressure correlations are generally based on the Clausius-Clapeyron equation which is a fundamental equation utilising the equality of chemical ponential, temperature and pressure in equilibrium phases. Although many correlations are available for predicting vapor pressures given temperature and in some cases, critical constants and normal boiling points, only a few has been tested over a wider range of applicability and hence, accepted (Reid, Sherwood and Prausnitz, 1977).

The Antione correlation is the most widely used and is very accurate within the temperature ranges in which the constants are evaluated. However, it is specified by Reid, Sherwood and Prausnitz (1977) that the equation should not be used above 1500 to 2000 mm Hg pressure, above which the presumed linear relationship between log of vapor pressure and the inverse of temperature fails in general.

The later versions of CHESS developed at NJIT have used a six constant form of the Antoine equation, expressed in the following manner :

$$\ln (P^{o}) = A(1) + \frac{A(2)}{T + A(3)} + A(4) \ln T + A(5)T + A(6)\,T^{2}$$

where:

P^{o} = saturation vapor pressure at temperature, T .

Units are : mm Hg and degrees Kelvin.

We have introduced the data for the first three coefficients for all the standard components. The data was obtained from Reid, Sherwood and Prausnitz's text. To obtain better accuracy over higher pressure ranges, one has to regress physical data to obtain values for all the coefficients. The above equation is a combination of some newer correlations mentioned in Reid, Sherwood and Prausnitz's text. It takes into account the non-linearity up to the second order as well as dependance of vapor pressure on the logarithm of temperture.

Coefficients of Specific Heats of Liquids

The specific heats of liquids is an important thermophysical data needed for simulation. The approach of using departure functions (Henley and Seader 1981) works well with equations of state which predict for the liquid phases accurately, such as the Peng-Robinson equation. However, departure functions predicted based on liquid-phase activity coefficient models are found to be erroneous frequently (Roche). In this modification, we have introduced coefficients for determining liquid specific heats for low temperatures (up to 325 K) and near-atmospheric pressures. The prediction of the liquid heat capacities is one of the most thoroughly investigated areas in chemical engineering. Unfortunately, it is also an area where not much published data, experimental in particular, is available.

The literature data, in general, is correlated against polynomials in absolute temperature. The difficulty that one has to face in assimilating whatever data is available is that of non-uniformity of the correlations and/or the different units used in different correlations. We have collected data from three sources, each of which was not compatible with the others. Hence, it was necessary to use internal conversion in the code to make the final value uniform with the units used in the rest of CHESS.

The first source of data is provided by Tamplin and Zuzic (1967). They have used a trinomial equation to express specific heat in calories per degrees celcius per gram -mole against temperature, which was in the units of degrees celcius instead of the usual practice of using absolute scale. They report that absolute deviation of predicted values from the experimental data is of the order of 0.01 to 0.1. A large number of the standard components of CHESS was included in this study.

For a few components, data was obtained from the collection made by Yaws. This source was found to be useful specially for inorganic components. The correlation is a four-constant, third-degree polynomial where specific heat has the unit of calories per degree Kelvin per gram and temperature was expressed in degrees Kelvin unit. Internal conversion to the molar unit was required.

For the rest of the components, it was necessary to generate our own data through a correlation. The Lyman-Danner correlation was chosen as the model. The accuracy is expected to be within 5 % (Reid, Sherwood and Prausnitz, 1977). This method predicts for the departure function, with respect to ideal-gas conditions and the parameters used are the association factors (a function of reduced normal boiling points, critical pressures and radii of gyration), the radii of gyration and the reduced temperatures. These properties were obtained from Reid, Sherwood and Prausnitz's text. We have used arbitraily chosen intervals between the freezing points and the normal boiling points of each component. We have obtained four coefficients for a trinomial equation for the specific heats in calories per gram-mole per degrees Kelvin versus temperatures in degrees Kelvin.

Future modifications of CHESS should attempt to create a uniform data-source for these constants. The Lyman-Danner procedure could be used for such purposes with a good degree of confidence.

Another important aspect should be noted here. A typical simulation program of today must have capability to obtain data for supercritical fluids. The only notable research in this respect was done by Peter (1949). He had produced charts for a few well-known components used in the hydrocarbon industry. It is required to arrive at a correlation based on his approach. The difficult part of this approach is to guess the point much beyond the critical conditions where the saturation-enthalpy curves meet. As a first trial, these may be assumed to be linear. The curve, however is parabolic in nature as is evident from Peter's charts. Such data is required for light gases like Ethylene, which exist in liquid phases beyond their critical states as dissolved gases, or for some other components which are found in the vapor phase above their saturation pressures.

Normal Boiling Points

This property is an useful data for many thermodynamic correlations. Initially we had used it for heats of vaporization using the Clausius-Clapeyron equation. But it was found to yield very inaccurate results under higer pressures. Thus, the original CHESS data-source of Hildebrand solubility parameters was implemented for the Chao-Seader models. However, this would be available for any possible use in the future.

The data was taken from Reid, Sherwood and Prausnitz's text (1977).

CHAPTER 4

SYSTEM ORGANIZATION AND COMPUTATIONAL ASPECTS

Simulation is the basic tool used by chemical engineers in process analysis and process synthesis. In the analysis of processes, a system is decomposed into a finite number of subsystems and each is studied to ascertain its effect on the entire system. In systhesis applications, subsystems are combined into systems, with the objective of arriving at the best process sequence. Apart from the complexities in the application of chemical engineering principles, a simulation program needs considerable attention in its computational aspects. A major part of these deals with the organizational aspects of the simulation system. In this chapter, a comprehensive review of CHESS is attempted. Illustration of some of the computational aspects of the simulator is presented.

4.1 System Organization and Simulation Strategy

The design issue of aggregating program-components into an organised process simulator is closely linked with a particular strategy adopted for solving a simulation problem. In this section, these aspects are presented.

4.1.1 Process Simulation Methodology

The most widely used approach in solving process flowsheeting problems is the 'sequential modular' approach. CHESS (the Chemical Engineering Simulation System) is based on this principle. In this approach, each process step is represented by a mathematical model. The mathematical model is a representation of one or more unit operations found in the process industries. These computational modules calculate the physical output(s) from a set of physical input(s). The unit modules are calculated sequentially, starting from known feed conditions. The calculation follows a specified unit-by-unit order. Iterative adjustments of selected recycle streams are performed together with iterations around portions of the process in order to accomodate design specifications. Network partitioning and tearing algorithms are used in conjunction with a variety of convergence algorithms to support them.

The inherent drawback of this method is that complete specifications of all equipment parameters and the conditions of the feed streams must be available at the time of unit module evaluation. For a design study, many of the equipment-conditions can be expected to be unknown. A user-iterated simulation study may be a solution for such difficulties, but that may not be desirable in a given situation. A solution strategy employed is to use system-defined control blocks to enforce convergence on design specifications, by manipulating specific design variables. The CHESS uses this method

Another approach to process simulation is associated with general non-linear equation solving algorithms. Some contemporary simulators have made use of this strategy, known as the 'simultaneous-modular' approach. The key idea in this is to solve simultaneously those equations which result from torn recycle streams together with those resulting from design specifications through only one level of iteration (Perkins, 1979). In this way, the interactions between stream variables and equipment parameters are taken into account so as to avoid conflicting iterations.

A summary of some other approaches in process simulation is appropriate at this point, before we describe CHESS in detail, so that a comparative view is obtained.

The 'equation-oriented' approach treats the entire flowsheet model as a large simultaneous equation-set that is solved by recently-developed sparse matrix solution algorithms (Clark and Reklaitis, 1984). Each unit is represented as a set(s) of equations. In the equation-oriented approach, the equations representing units are not grouped under seperate procedures calculating outputs given a set of inputs. In solving the flowsheet, the equations describing the units are assembled into an aggregate set and these are solved simultaneously, using iterative numerical techniques. Future investigation in the quasi-linearization aspects of the newly developed equation oriented modules is envisioned for obtaining a truly general solution scheme.

In the successive linearization approach, also known as the simultaneous-modular approach, the basis is the use of an already-existing set of sequential modular unit modules, but introducing an equation-oriented strategy. These are used to generate, automatically, the coefficients of linear or specially-simplified, non-linear models. The resulting approximate model of the flowsheet is iterated upon, until convergence in key recycle streams and design parameters is arrived at. The limitation of this strategy is that it has been tested on mostly linear or closely-linear systems so far (Clark and Reklaitis,1984). There are two inherently different methods in this approach. In one, an approximate equation-oriented model of the process is used alternately with the rigorous procedure-based model. Such a combinatorial strategy can perform either preliminary design calculations (the mass balance only) or rigorous design calculations (mass and energy balances). The same strategy is implemented in the state-of-the-art simulator program called ASPEN (Evans et al, 1979). In the preliminary-computation step, the sequential modular strategy is utilized to generate quasi-linear models for each unit. The detailed-design step works on these to solve for the non-linear flowsheet equations simultaneously. In a given application, either of the two modes can be invoked, but the second depends on the first implicitly. This approach has resulted in faster convergence for various example problems, as noted by Timer and coworkers (1984). In the second type of simultaneous-modular flowsheeting, a simple but rigorous strategy of solving simultaneously, all the torn recycle streams and design objectives, is achieved. An advantage of significant importance for system synthesis applications is that optimization studies can be done easily within the framework of these simulators. In future, such an extension should be considered for incorporation into CHESS.

In the 'non-sequential modular' simulators (HYSIM of Hyprotech), interactive use of the simultaneous modular approach is adopted, with a variable program structure.

In order to improve on design productivity, some commercial simulators are adopting a data-based approach. The emphasis in these is on data organization, where the simulator has access to non-process data such as project objectives, mechanical design specifications and process control goals. Such integrated systems are more meaningful in a real design environment. In one such system, CHESS was used as the host simulator (Tsubaki and Motard,1979). A reduction in the software overhead of up to 25% was achieved. In essence, a suitably programmed interface between project data base and CHESS data structures was established.

In another approach, a list-oriented data structure was used to facilitate flexibility in establishing topological variations efficiently. This also is a refinement of the sequential- modular approach (Thompson,1982). Such simulators are useful for instructional purposes.

4.1.2 Organization of CHESS

The internal control structure of the system is of a fixed nature. In fixed-structure simulators, usually adopting a sequential-modular simulation strategy, the executive program does not depend on the nature of the problem whose solution is sought for. In contrast, the executive program is tailored for a specific application purpose in variable-structured simulators. The executive module of CHESS determines the path of computation through the program, if not defined by the user, and matches streams to unit modules based on data supplied by the user. Although there is considerable storage overhead for loading all of the modules each time the program runs, a fixed-structure simulator is considered to be more efficient for shorter problems (Motard, 1975).

In either of these structures, the same modules may be used in different points of a flow network with differing process conditions. This is implemented by the use of an environment of subprograms. Thus, in CHESS, a particular network structure determines a specific subprogram-calling sequence.

The system is organized around two types of subprograms, the executive and the supportive modules. Table 4.1 presents the executive modules and their functions. Tables 4.2, 4.3 and 4.4 list all the supportive modules. The overall system linkage is explained in Figure 4.1.

The executive subprograms decide the computation sequences, control recycle calculations, initialize variables and perform input and output operations. The supportive programs can be broadly classified into three classes: the thermophysical modules, the equipment modules, and the control blocks.

The executive subprograms are driven by a main program segment. It allows for extension of any of the modules including itself. Additional modules can be added when wished, provided such changes are incorporated throughout the system in a consistent manner.

FIGURE 4.1

CHESS3 : Organizational Chart

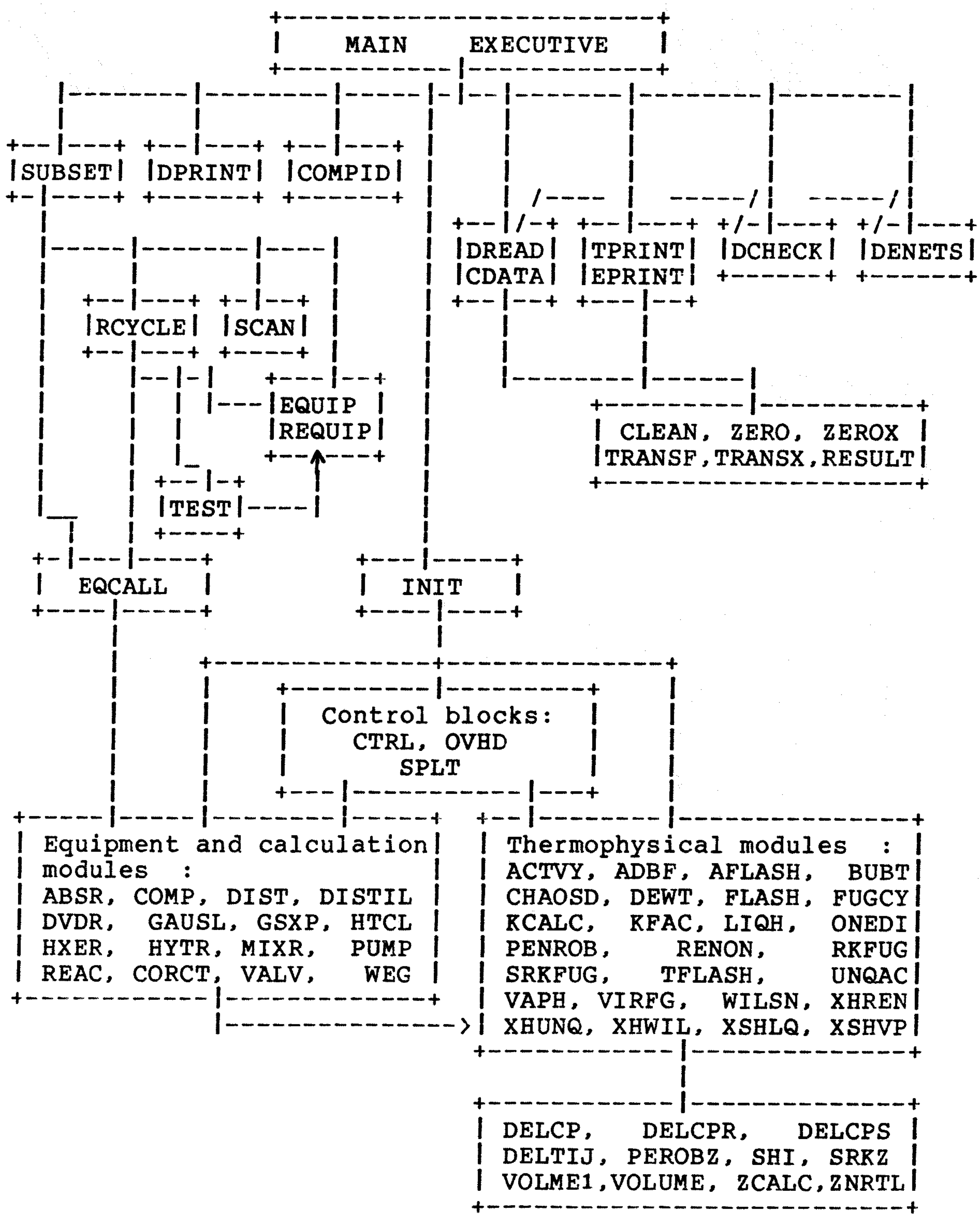

TABLE 4.1

Executive Modules of CHESS3

CDATA	-	Alternative input routine, collects user-defined pure components data
COMPID	-	Identifies standard chemical components and supplies their pure-component data
CLEAN	-	Initializes all COMMON block data structures with zero values
DCHECK	-	Performs consistency and closure tests on the network adjacency list
DENETS	-	Evaluates tearing scheme and prepares recycle loop calculation list
DPRINT	-	Prints the input data list
DREAD	-	Interprets and stores input data
EPRINT	-	Prints the summary of energy transfer between the system and surroundings
EQCALL	-	Invokes a specific equipment module
EQUIP/REQUIP	-	Transfers evaluated process data to EQPAR(I,NE), updates i/o stream matrix
INIT	-	Initializes known input streams with thermophysical data
RCYCLE	-	Controls recycle loop computations
RESULT	-	Prints out the final column profiles for the staged-contact processes
SCAN	-	Detects computational status: feed,

TABLE 4.1 (continued)

	unknown or unused streams and equipments
SUBSET	- Controls the path of computation through the process network
TEST	- Recycle loop convergence controller
TPRINT	- Prints intermediate and final results
TRANSF/TRANSX	- Transfers data from two-dimensional arrays to vectors for printing purposes
ZERO/ZEROX	- Initializes an array with zeros

TABLE 4.2

Thermophysical Modules of CHESS3

ACTVY	-	Invokes various activity coefficient modules
ADBF	-	Comprehensive equilibrium flash routine
AFLASH	-	Adiabatic flash module
BUBT	-	Predicts bubble point temperature
CHAOSD	-	Chao-Seader activity coefficient, enthalpy, entropy, volume, fugacity coefficient models for liquid phase
DELCP	-	Heat capacity departures by the RK eqn.
DELCPR	-	Heat capacity departure fuctions via the Peng-Robinson equation of state
DELCPS	-	Module for predicting heat capacity departure functions by the SRK equation
DEWT	-	Predicts dew point temperature
FLASH	-	Two phase VLE flash module
FUGCY	-	Selects a fugacity coefficient model
KCALC	-	Calculates equilibrium constants
KFAC	-	Calculates thermodynamic functions for distillation and absorption processes
LIQH	-	Calculates liquid phase enthalpy
ONEDI	-	Corrects for vapor phase dimerization
PENRCB	-	Peng-Robinson models for fugacity coefficient , enthalpy and entropy

TABLE 4.2 (continued)

	departure, compressibility factors (PEROBZ) and volumes(VOLME1) of liquid and vapor phases
RENON	- NRTL liquid phase activity coefficients
RKFUG	- Redlich-Kwong vapor phase models for fugacity coeff.s & enthalpy departure
SRKFUG	- Soave-Redlich-Kwong vapor and liquid phase models for fugacity coefficients, enthalpy and entropy departures, volume(VOLUME) and comp. factors(SRKZ)
TFLASH	- Isothermal flash module
UNQAC	- UNIQUAC activity coefficient model
VAPH	- Calculates vapor phase enthalpy
VIRFG	- Virial model for vapor phase fugacity
WILSN	- Wilson model for activity coefficients
XHREN	- Excess heat of liquid solutions by the NRTL model
XHUNQ	- Excess heat of liquid solutions by the UNIQUAC model
XHWIL	- Excess heat of liquid solutions by the Wilson model
XSHLQ	- Calling module : excess heat of liquids
XSHVP	- Calling module for vapor phase mixture enthalpy departure
ZCALC	- Compressibility factors via the RK eqn.

TABLE 4.3

Equipment and Computational Modules of CHESS3

ABSR	-	Simplified absorber/ stripper module
ABSR1/ABSR2	-	Rigorous absorber/ stripper module
COMP	-	Stagewige gas compression module
DIST	-	Simple distillation unit
DISTIL	-	Rigorous distillation procedures
DVDR	-	Single-phase stream divider
GAUSL	-	Gauss-Jordan matrix solution unit
GSXP	-	Gas expander power recovery module
HTCL	-	Fired heater/ bulk cooler module
HXER	-	Detailed heat exchanger module
HYTR	-	Hydraulic turbine power recovery unit
MATRIX	-	Part of rigorous stagewise procedure
MIXR	-	One/ Two phase stream mixing unit
PUMP	-	Pump routine
REAC	-	Simple reactor module
VALV	-	Constant enthalpy downstream pressure controller
CORECT	-	Convergence accelerator for MATRIX solving procedure of Gauss-Jordan
WEG	-	Iteration convergence accelerator with the Wegstein procedure
DVDR	-	One/ Two phase, single-inlet mulpiple-outlet stream divider

TABLE 4.4

Control Blocks of CHESS3

CTRL	- Component ratio, temperature and flowrate controller
OVHD	- Controlled condensation dividor for staged-column vapor overheads
SPLT	- Two-phase, single inlet-double outlet vaporization controller/ general two-phase stream divider

4.1.3 Computational Scheme

In the simulation of a typical chemical process environment, the intermediate stream conditions are not known a priori. This is coupled with the uncertainity of conditions that recycle streams will assume. Hence it is necessary to solve a set of non-linear simultaneous equations representing relationships between nodes of the process network. The nodes, which represent unit computation modules in an information flow graph, interact with the network through their own, singly defined properties.

The first step in this iterative technique is to 'partition' the specified network to identify those nodes which are not included in the recycle nets and simultaneously, to identify the recycle nets. In the next step, the identified recycle streams undergo a 'tearing process' which separates each into an assumed/ calculated stream, albeit one or two streams. The convergence algorithm then tries to make both sides of the tear stream agree. In this procedure, one can make use of various convergence acceleration and testing algorithms.

The network partitioning schemes follow algorithms that are rooted in graph-theoretic principles. The criteria of choosing one over another are diverse. The most important ones are those suitable to a particular application and execution time and storage requirements. The consideration that is most significant for chemical engineering simulators is that partition and tearing be kept to minimum. Thus, an optimal computational order results from the partition analysis. In CHESS, the 'Path Searching' algorithm is implemented (Motard, 1975). The shortest path between all nodes within a recycle net and the existence of any articulation points is detected.

The minimum number of tear streams often yields an undesirable computational order. Thus the result of the path searching algorithm needs to be tested against such problems.

Partitioning

Algebraically, a set of simultaneous equations can be solved by partitioning if at least one equation of the set defines the value of a single variable uniquely. The remaining equations are then solved sequentially. These may be represented as :

$$P(x_k) = 0$$

and

$$p_i(x_i) = 0$$

where: P is the set of p_i's and the second equation defines the value of x_i alone.

Tearing

Once the network is partitioned, every recycle net is a function of its tear streams. The simultaneous equations representing tear streams cannot be partitioned into a set which is solvable sequentially through successive substitution. The solution strategy which is most simplified, chooses a tearing variable and applies iteration computation. The choice of this variable is guided by some predefined selection criteria.

Algebraically, a recycle net can be represented as the following set of equations :

$$F(X) = 0 \tag{4.1}$$

where :

F is a set of N equations in the N sets of unknowns, X.

The set F is composed of two subsets. The first arises out of the torn recycle streams :

$$m_i(X) = x_i - n_i(X) = 0 \tag{4.2}$$

where x_i is an unknown in the recycle set.

The second subset occurs at each unspecified node, by virtue of unknown equipment parameters:

$$m_i(X) = s - q(X) = 0 \tag{4.3}$$

where s is the desired parameter and q is the estimated value.

Solution Procedure

In order to solve equation (4.1), various methods can be used. The methods of direct substitution and the Wegstein method are the most commonly used in process simulators. Recent developments indicate a trend towards the use of Broyden's method (Clark and Reklaitis ,1984). In this method, the Secant method is used with the Jacobian Matrix evaluated based on function values, or steps, generated during iteration.

CHESS uses the Wegstein's approach for convergence acceleration. This method can be described as follows :

$$f(x) = x$$

$$x_j^{i+1} = (1 - q_j^i) f_j^i(x^i) + q_j^i x_j^i$$

where :

$$q_j^i = \text{convergence parameter}$$

$$= S_j^i / (S_j^i - 1)$$

and

$$S_j^i = \frac{f_j^i(x_j^i) - f_j^{(i-1)}(x^{(i-1)})}{x_j^i - x_j^{(i-1)}}$$

Subscripts j refer to predicted values.

Unsubscripted values are the computed results.

i is the current iteration count.

Thus a straight line extrapolation is used between the predicted values of the ith and the (i-1)th iteration steps. In practice, it is necessary to specify the upper and the lower bounds for q . In CHESS, this is set from 0.5 to -10. The choice is based upon the objective of preventing interaction of successive refinements which results in over-extrapolation and consequent oscillatory convergence paths. In addition, an algebraic sign check is performed on two subsequent q values. The value of x is updated only if they have the same sign. Another important aspect is that CHESS applies Wegstein convergence only on the stream compositions for recycle calculations.

There are two ways to activate the tear-stream sequence scheme of CHESS. If the user does not specify a specific scheme, the network decomposition routine is invoked. The KE4 vector is used for this purpose, which will be discussed later.

In many problems, the user-supplied input stream conditions or equipment parameters may become the cause of oscillatory or divergent behaviour of computation. These problems are harder to debug and only the user can identify the cause. It should be noted though that an experienced process engineer may select additional tear streams and improve the overall computational effort because of a significant reduction in the number of computational steps.

4.2 Unit Computation and Information Flow

The area of steady state process simulation is primarily concerned with systems having components described in terms of lumped parameters. 'Lumped parameter' systems are represented by mathematical models describing the macroscopic material and energy conservation relationships between its components. The mathematical models are described in terms of algebraic equations, which can have various types : linear or non- linear, simultaneous or direct.

The implementation of a mathematical model and the associated algorithms for solving equations describing it is defined as a 'unit computational module' of a process simulator. A subsystem of the simulation model of a given process system may consist of an equipment node, a thermophysical model or a computational entity used by other subsystems. The thermophysical and computational modules of a process simulator work as supportive modules for the equipment or the executive modules. Each of the unit computation modules is unique in describing an operation at a given node of a process flow network. An information flow scheme represents the interrelationship between nodes and within a particular node sometimes, through descriptions of process variables associated and the computational scheme. This is uniquely defined for a particular process network and can be thought of as the paths in the network annotated with the process variables with the computational vectors describing them. The path itself is dependent on the order the system chooses for the computation to follow in completing the process flow network.

4.2.1 Unit Computation in CHESS

The unit computational modules in CHESS can be classified in three categories - the equipment modules, the thermophysical modules and the control blocks. These constitute an open-ended subsystem where users can accomodate additional modules. The capability of CHESS, or for that matter, any generalised simulator, in handling chemical reaction operations is limited. The basic reactor module in CHESS performs a stoichiometric material balance and adjusts for heats of reaction only. The users can specify up to fourteen additional modules in CHESS. These have to be coded in standard FORTRAN. They access and modify data primarily through the COMMON blocks. The appended modules must be compiled and then, linked with the system, after necessary changes are made in appropriate executive routines.

The equipment and control modules of original CHESS are outlined in the CHESS user's guide (Motard and Lee, 1971). The NJIT versions prior to this work is described in detail by Andreyuk (1983).

In this extension of CHESS, certain modules were added and some others were modified. ADBF, the equilibrium flash routine of CHESS2 was modified to supply additional mixture component information. The simple distillation module DIST of original CHESS was reinstalled. The COMPID module of original CHESS was used in creating an updated and extended database for standard component properties. CHESS2 (Andreyuk, 1983) used a special data-input subprogram, CDATA. We have reinstalled the DREAD routine of original CHESS in order to handle standard components. The DREAD routine was modified to reflect additions to the database. The the rotating equipment modules, HYTR, PUMP, GSXP and COMP were modified to accept the new equation of state modules.

Extension of the thermophysical module-set was the primary goal of this work. The secondary aspect was to verify the computational reliability of the rotating equipment modules. The added modules are presented with the source code in Appendix D.

The CHAOSD module deals with the RK/SRK : Chao-Seader correlation and the related models. The existing equation of state modules VIRFUG and RKFUG, for the Virial and RK equations of state respectively, are kept intact. The SRKFUG and its component modules define the Soave-Redlich-Kwong equation of state procedure. The PENROB and associated modules predict thermodynamic properties via the Peng-Robinson equation. The modular-approach actvity coefficient routines are kept intact, but access is via the alternative CDATA input procedure of CHESS2. These modules are : WILSN (Wilson model) RENON (NRTL model) and UNQAC (UNIQUAC model). The DELCPS and DELCPR modules predict specific heats at constant pressure and constant volume by using the SRK and the Peng-Robinson equations respectively.

During various tests, some difficulties were encountered with the flash routines, which were modified to handle the newer equations of state models. A brief account of the purpose of each computational modules were presented in Tables 4.2, 4.3 and 4.4.

In general, a control block is an unit computational module placed in the information-flow graph in order to influence one or more units. In each equipment unit controlled, one or more process parameters or stream flow rates/ compositions are adjusted to attain user-desired specifications. These can be thought of as iterative feedback/feedforward controllers trying to minimize discrepency functions. Some of the functions achieved by these blocks are - ratio or flow control, feedback or recycle rate control, and vaporization or condensation control in stagewise contact processes. The module CTRL is a generalized block controlling the component ratios, stream temperatures and and flow simultaneously. It adjusts the input stream pressure and temperature to meet the designated control objective. When used as a temperature controller in the isothermal flash routine, the technique of 'Damped Control of Temperature' is applied to avoid oscillations in convergence. If the approach is below 20 °C, a weighted average is used, as defined in the following :

$$T_{new} = \frac{T_{cal} + T_{old} \cdot i}{(i + 1)}$$

where :

T_{cal} = Guess value.

T_{old} = Calculated value in the 'i'th iteration.

T_{new} = Value for the (i+1) th. iteration.

In this method, when i=0, the control is equivalent to direct substitution, when i=1, the control is termed 'halving' and so on. When CTRL is used as a flow controller, the user must allocate any necessary make-up streams.

The block SPLT is used as a reboiler vaporization controller as well as a general two-phase splitter routine. The OVHD block controls the condensation process, whether partial or total, of the distillation modules.

Special mention is appropriate here about the ADBF and the DVDR modules of CHESS. These can represent an actual operation or can perform in other modes. For example, all the stream conditions are set by ADBF, while it is a generalized flash module. The DVDR module can perform specified stream splitting or it can work in conjunction with the CTRL block.

4.2.2 Flow of Information

The flow of information between CHESS modules follows the computational order evaluated by its executive routines or submitted directly by the user. The information flow scheme of a particular process being simulated may not have the desired material flow scheme. This is particularly evident for control block nodes.

In general, the flow of information between units is organised into three named COMMON blocks:STRMIN, STMOUT and STREAM. The block STRMIN contain inlet conditions for a stream input(s) to a computational module. The STMOUT block retains the output(s) stream properties after the computation is completed. The common block STREAM contains the properties and conditions of a stream used temporarily to evaluate thermodynamic conditions during execution. These blocks interface with the statically initialized or computed equipment parameter data, changing from node to node. The use of the common-blocked data structure of FORTRAN is applied ideally in this scheme.

The process or equipment units redefine the intensive and extensive properties of the streams. Apart from the above named three, there is an COMMON block called STMA which differentiates between the extensive and intensive properties of all the streams and stores them in two separate arrays. As unknown streams are converged on, the stream extensive property list, SEXTSV, and the stream intensive property list, SINTSV, matrices are updated. Thus, when the whole network is solved, one has, stored in these matrices, the final values of the conditions in each stream. The executive modules EQUIP and REQUIP performs this linkages, by moving the stream data from and to the general stream data bank and the localized equipment-oriented streams.

Descriptions of some components of a few of the COMMON blocks will be presented in Section 4.5.

4.3 Data Structure and Program Control

The data structure of CHESS is of a static nature, formed of arrays. Recently developed simulators like ASPEN (and the older FLOWTRAN) adopt a dynamic structuring strategy for both process data and network information. Although the later is better in storage and execution efficiency, it is more useful if a file-oriented or data-based approach is implemented in system design. In CHESS, the data management is based on principles commonly used years ago which avoids abstraction. For an application programmer, abstraction can be more of a hazard than a help. Thus, as a research tool, CHESS has a definite place through its ease of understanding and use.

Using only a few input variables, a CHESS programmer can exert control on quite a few execution criteria. For process synthesis applications, it is very useful as the simulation trend cannot be predicted even to a minor degree.

4.3.1 Data Structure

The nature of computational data in CHESS can be thought of as having two types - informative and referential. The referencing environment of global data through a blocked data structure was previously discussed.

The information about process entities, streams and computational nodes (unit operations), are also handled in arrays transmitted through data blocks. The network adjacency matrix is stored in a two-dimensional array, KPM(J,N). The stream numbers associated with an unit, its ID's and its node position in the network is stored in minor elements, with the node number N in the major for identification purposes. The data for the unit computational nodes are stored in another array, EQPAR(J,N). The minor elements contain defined values of process variables: pressure, temperature, etc, initiated by the user. The other elements of this array are completed as the computations converge on the specific node. Each unit module has a predefined order of arrangement of the parameters. These are described in detail by Motard and Lee (1971) and Andreyuk (1983).

The user-defined standard component identification numbers, pure component data and aggregate stream properties etc. are stored in separate common blocks. The executive routine controls the flow of information. The user-defined data (e.g CMPRO) are stored in common blocks separate from the data computed through node-to-node progress of execution (e.g STMA). Again, the thermophysical data associated with streams are stored in other seperate blocks (e.g ZDATA). The data contained in variable-data blocks convey calculated information back to executive modules (via EQUIP/REQUIP) which reassign values to the respective stream intensive and extensive arrays. Thus, the variable-data blocks are used as dummy blocks to pass information.

Each equipment is also associated with a set of arrays which create a local environment of up to four input and output streams with important stream properties (STRMIN and STMOUT). Thus, the data structure limits the equipments to these conditions.

4.3.2 Standard Component Properties' Database

The source listing of the module COMPID, presented in Appendix D, illustrates the standard components and their componential property library data. The components present in a process study are identified by the user. The system retrieves the pure component properties. The data is organized in vectors indexed by the component numbers.

If the user specifies non-standard components or alternatively, wishes to use his own data, the convention of COMPID with respect to units, order and number has to be followed. This can be found in the NSCOMP namelist in COMPID.

The storage scheme employed in COMPID is inefficient because it requires the entire database of 98 standard components to be present whereas the system will need a maximum of 10 components in a given study. An efficient method would be either using a read-in procedure (CDATA in CHESS2), or a providing an external data-based, linked-list data structure. The user has an option to use the CDATA input program of CHESS2 which is retained in this version. Although the storage scheme in COMPID is inefficient, it is easily maintainable and considerable reduction of input-data preparation load is provided by it. It should be noted that the storage liability for COMPID can be lessened when the computer architecture utilize an overlay/ segmentation structure on virtual memory.

4.3.3 User Defined Execution Parameters

Program control by external means is provided for in CHESS. These include choice of thermophysical models, directives for computational limits and error-handling features.

The thermodynamic calculations can be controlled not only by vapor and liquid phase models, but also through the decision of using enthalpy and entropy departure functions in either phase. The possible combinations these can provide help in describing a physical situation very closely.

The control over program execution limits is the most powerful tool a simulation study needs.In CHESS, the user can specify the maximum number of iterations trials and the tolerance limit for convergence, as well as execution (CPU) time. The simulator can be set up to run repeatedly without explicit system commands. The debugging aids provided are excellent. The user can get insights into sub-levels of iterative calculations to decide a new strategy. The stream summaries for recycle loops or the column profiles for stagewise contact modules can be chosen to be printed out. Another use of the debugging aids is in documenting the final values for an error free run.

The tolerance for convergence is the most significant control parameter provided. This value is maintained constant throughout the simulation. Internally, it is assigned to a default value of 0.001, which can be overridden by specific input data.

CHESS allows for another powerful feature. The user can bypass the system-evaluated partition and tear scheme by providing his own sequence. This can reduce the execution-time requirements considerably, especially if the physical nature of the problem suggests a best partition and indicates the critical tear streams. This is then user-specified through the KE2 (partition scheme), KE3 (tear streams) and KE4 (Wegstein convergence tear streams) vectors.

4.4 Input Data Specification

The input data in CHESS is read on a format free basis. The NAMELIST input convention of standard FORTRAN is utilized in CHESS.

The summary of the order and contents of input data is presented in TABLE - 4.5. The CHESS variables associated with the input data are identified in capital letters in this table. The descriptions of some important data objects are presented in TABLE - 4.6.

If a computational module is added, it has to be declared properly in the input as well as in the code. The requirements of such additions is presented in the next topic.

The unused elements of all input vectors must be filled in with zeros in order to maintain the integrity of the NAMELIST data structure.

TABLE 4.5

Arrangement and Specification of Input Data

Group	No.of Cards	Description
1	1	Header Card : TITLE Problem title in 20A4 format
2	3	.Thermophysical Control Card : NOCOMP,IDLL,IDLV,IDH,LDBUG,NDIM .Component Identification Card : NTCOMP(10) .Process Network Declaration Card: NOKPM,NOEQP,NOSEX,NOSIN,KUNITS
3	Max 50	Adjacency Data of Modules: KPM Node value, CHESS module name, Process ID,Inlet & Outlet stream(s)
4	1 + Max 50	Equipment Data Cards : .List of Unspecified Equipments: ENAME(50) Integers : One Card .Data for Specified Equipments(NE): EQPAR(J,NE):Total J 25,Total NE 50
5(a)	1 Max 100	Stream Condition Data Cards : .Stream Extensive Properties : . List of Unspecified Streams SNAME(100) Integers . Data for Specified Streams,J SEXTSV(13,J)

TABLE 4.5 (continued)

5(b)	1 Max 100	.Stream Intensive Properties : . List of Unspecified Streams SNAME(100) Integers . Data for Specified Streams,J SINTSV(10,J)
6	2	Coputational Parameter Cards : .Iteration and Print Control : LOOPS, NPFREQ, KTRACE, DERROR .Partition and Tear Control : KE2(50), KE3(10), KE4(10)

TABLE 4.6

Description of Input Data

Group	Variable	Description
2	NOCOMP	No. of chemical components present
	IDLL	Liquid phase model code, 0 -- 6
	IDLV	Vapor phase model code, 0 -- 6
	IDH	Enthalpy correction code, 0 -- 2
	LDBUG	System debug code, 0 -- 2
	NDIM	Indicates if a component dimerizes
	NTCOMP(10)	The component identification #s
	NOKPM	The number of computational modules
	NOEQP	The number of equipment units
	NOSEX	#Streams with known extensive prop.s
	NOSIN	#Streams with known intensive prop.s
	KUNITS	Input data physical units code
3	KPM(50,10)	Node(1 -- 50), Standard CHESS name, Given flowsheet name(A4), List of input stream numbers, List of output stream numbers [prefixed with aminus (-) sign for each]. Vapor products are listed first.
4	EQPAR(J,NE)	Parametersfor aspecified equipment node,NE. Outlined by Motard and Lee (1972) and Andreyuk (1983).

TABLE 4.6 (continued)

5(a)	SEXTSV(13,J)	Extensive properties of known stream, J. Stream #, stream enthalpy(optional), total molar flowrate, componetial flowrates.
5(b)	SINTSV(10,J)	Intensive properties of the corresponding streams. Stream no., stream flag (0--2), vapor fraction, temp., press., enthalpy.
6	LOOPS	Maximum number of recycle loop calculations allowed per run.
	NPFREQ	Iteration level when intermediate stream summaries are to be printed.
	KTRACE	Prints sequence of unit modules under program control if set > 0. When =1, prints sequence trace, when =2, prints all inlet states.
	DERROR	Tolerance in recycle computation : system default value = 0.0001
	KE2(50)	Ordered list of equipment numbers which are to be chosen for recycle computation (Optional)
	KE3(10)	Optional ordering oftearstreams
	KE4(10)	Stream #s which will be forced to converge with Wegstein procedure

4.5 'ADD' Modules and Key Variables

It is necessary for an appended module to communicate with the system data environment. This is accomplished via named COMMON blocks. The COMMON blocks required for a particular application is to be chosen from the set present in the source code of the MAIN calling program documented in Appendix D.

The key variables required to be known to the system are clarified in TABLE - 4.7 .These will identify the variables that are likely to be manipulated in an 'ADD' routine.

CHESS allows up to fourteen user-defined additional subprograms through these ADD modules.

TABLE 4.7

Some Key Variables

COMMON block	Variable	Definition
CONTL	NIN	No. of input streams
	NOUT	No. of output streams
	NOCOMP	Total no. of componts
	NE	Current module node no.
	NEN	Dummy module number
EQPA	EQPAR(25,50)	Parameters for the Equipment module
STRMIN/STMOUT	SINUM(4)/SONUM(4)	Stream nos. for inlet and outlet streams(1- 4)
	Others	Self explanatory
CMPRO	NC	Same as NOCOMP
	L(10)	Phasecondition ID #
ZDATA	CPL(10,4)/CPV(10,4)	Specific heat coeffs.
	ENP(10,10)	Ref. state sp.ht coeffs.
	ANT(6,10)	Antoine vp. pr. coeffs.
	ADEL(10)	Hildebrand solubility
	OMEGA(10)	Pitzer Acc. Factors
	AK(10,10)	EOS interaction paramtr.
	VOL(10)	Liquid molal vol.s
	TB(10)	Normal B.P s
	VC(10),PC(10),TC(10)	Critical Constants
	ZRA(10)	Rackett Parameters

4.6 Output Features

The input data is printed out in a well fashioned manner so that input errors can be easily detected.

The output capability is expanded in this work to enable systematic examination of the final thermodynamic profile of the calculated streams. This section of the output contain the major thermophysical properties and the stream intensive and extensive conditions.

The system prints the stream conditions at the initial state of the simulation and after the simulation is completed.

The summary of energy exchanges is printed for each energy-intensive equipment when the simulation terminates.

Apart from these, the user can choose to print iterated values for recycle loops or stagewise column profiles. This was discussed under Tables 4.5 and 4.6.

4.7 System Capacity and Constraints

The CHESS is limited in certain respects because of the staic organisation of its data structures. These are :

- It can handle a maximum of 100 streams.
- It can have at most 50 computational nodes.
- A stream can have a maximum of 10 components.
- An equipment node may have no more than four

input and output streams.

However, if the situation demandsit, such restrictions can be easily removed by redefining the upper bounds of the arrays.

CHESS has various thermodynamic limitations. Apart from the inherent restrictions on the applicability of each of the models, there are functional drawbacks. The limitations of the models were discussed previously.

Major changes are required to incorporate capability to handle solids and two-liquid phase systems. Significant progress has been recently achieved at NJIT regarding systems having liquid phase-splits. This will be included into CHESS at a later time.

CHAPTER 5

SIMULATION STUDY OF AN ILLUSTRATIVE SUBPROCESS

In this chapter, we shall present the formulation of and the results obtained from the simulation study of a simple subprocess, utilizing the extended capacity of the CHESS program.

As a validity check, we have tested the CHESS3 using example problems #1 and #3 of the standard CHESS example set. These problems were formulated by Motard and Lee (1971) and are discussed fully in the original user's manual. We have not considered the other CHESS examples, since they involve the testings of a particular control block, or ADD module linkage, or the use of debugging tools, rather than the thermophysical capabilities of the system.

The validation of the new thermophysical routines with the new unit operation modules was accomplished with a single comprehensive test case.

5.1 Formulation of the Test Problem

The test problem is a hypothetical subprocess used to exemplify various thermophysical models as well as the new unit operation modules : COMP (Compressor), HYTR (Hydraulic Turbine), GSXP (Gas Expander) and PUMP (Pump).

The subprocess assumes as input a vapor stream and a liquid stream comming in for a low-temperature process step. The feed vapor stream is compressed and the feed liquid stream is expanded through a hydraulic turbine. These are then mixed and sent to a single-stage adiabatic flash unit. The vapor product is routed through a gas-expander for power recovery, while the liquid product is pumped to a higher pressure.

The input streams contain Nitrogen and Carbon Dioxide in a mixture of paraffinic hydrocarbons, forming a 10-component system. Such streams are normally encountered in natural gas processing. Our objective is to purge Nitrogen completely and combine the rest of the material into a single liquid stream.

There are no recycle streams in the process. The primary issue associated with this sample case is to find out which thermophysical models are appropriate in representing the high-pressure, low-temperature processing environment. The secondary issue is to validate the performance of each of the rotational equipment modules.

The flowsheet of the subprocess is presented in Figure 5.1. The inlet stream conditions and equipment specifications are tabulated in Table 5.1. The information flow diagram for the CHESS3 simulation model is presented in Figure 5.2 .

The simulation results for various input combinations of thermophysical models and choices of enthalpy corrections are presented in Appendix C. The fully formatted output is presented for the first set only, the Peng-Robinson equation of state applied to both the vapor and the liquid phases. Only the relevent portions are supplied for the subsequent combinations, the SRK / Chao-Seader (SRK/CS) model, RK / Chao-Seader (RK/CS) model and lastly, the ideal gas-ideal liquid assumption. This is done to in order to eliminate the repetition of the printout of virtually the same input data (except for the thermodynamic-model codes : IDLL, IDLV and IDH) for the same test case.

FIGURE 5.1

Flowsheet of the Subprocess

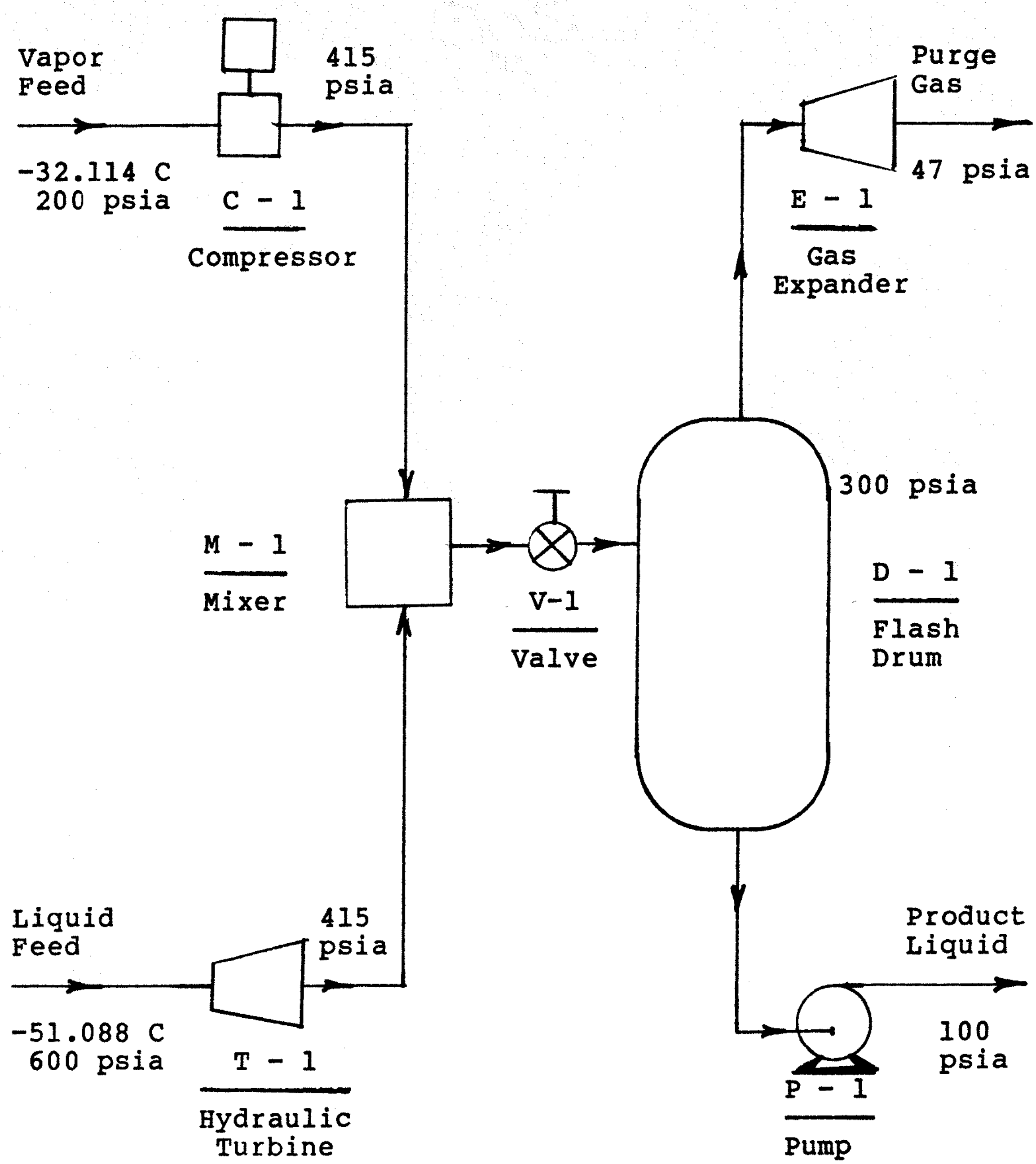

FIGURE 5.2

Information Flow Diagram

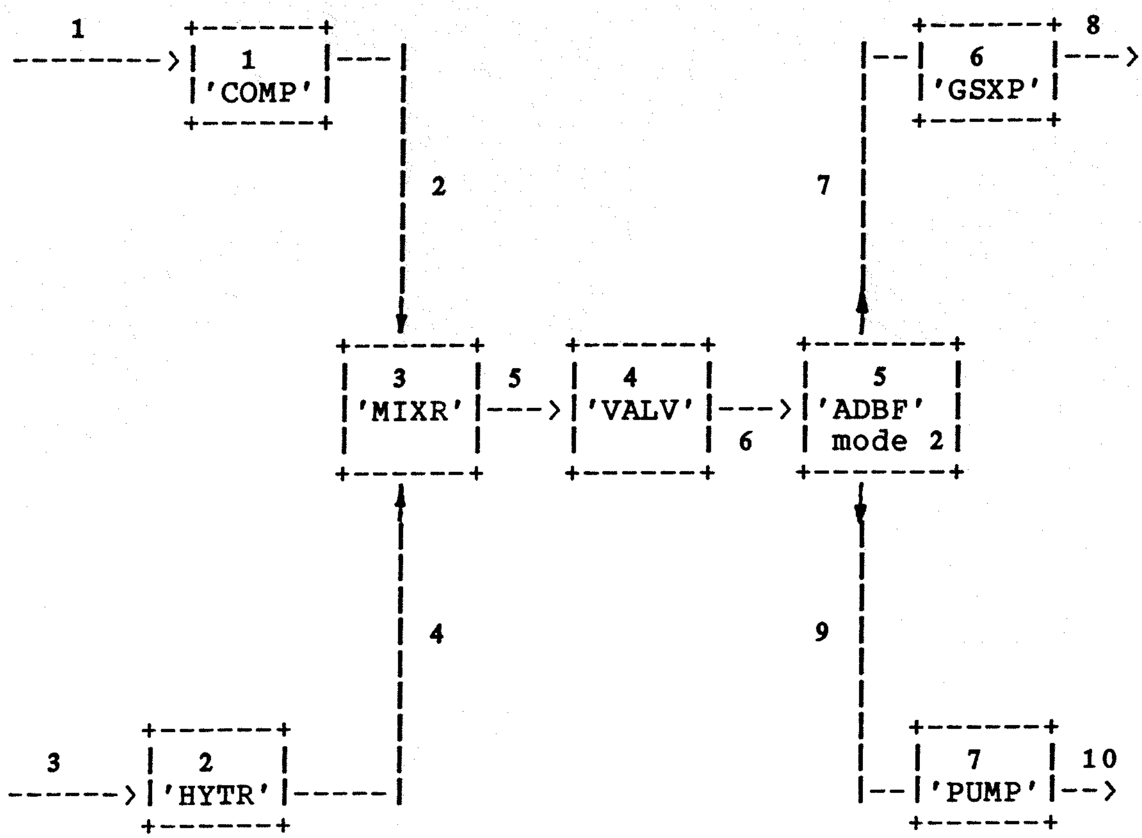

TABLE 5.1

Feed Conditions

Feed Stream		VAPOR	LIQUID
Vapor fraction		1.000	0.000
Pressure	(psia)	200.000	600.000
Temperature	(Deg. R)	433.866	400.000
Composition	(lb.mole/hr)		
Components			
CO_2		0.0205	0.0880
Nitrogen		0.1490	0.1490
Methane		28.4572	28.7860
Ethane		3.6273	20.1030
Propane		0.9263	24.9770
I-Butane		0.0384	2.8320
N-Butane		0.0896	10.2210
I-Pentane		0.0083	2.2240
N-Pentane		0.0061	2.3960
N-Heptane		0.0010	3.5890
Total		33.3236	95.3650

TABLE 5.1 (Continued)

Equipment Specifications

Unit ID	Unit operation	Inlet Pressure (atm)	Discharge Pressure (atm)	Temp. (Deg K)	Stages	Stage Efficiency
C - 1	Compressor	13.61	28.24	241.05	3	0.85
E - 1	Gas Expander	20.41	3.20	-	1	0.60
P - 1	Pump	20.41	34.02	-	1	0.75
T - 1	Hyd. Turbine	20.41	28.24	222.07	1	0.60
V - 1	Valve	28.24	20.41	-	-	-

5.2 Analysis of Results

In this section, the results obtained from simulating the test process will be discussed. The results are presented in a systematic manner in Appendix C in the form of the actual simulation outputs. In the following subsections, the issues pertinent to this work will be highlighted. These will include the performance of the newly included thermodynamic models in simulating the physical systems, the behavior of the rotational equipment modules and comparative evaluation of the interplay between them in terms of the simulated subsystem. We have restricted tabulation of the results already presented in Appendix C.

5.2.1 Correctness of Generated Thermodynamic Data

Fugacity and Activity Coefficients, Equilibrium Ratios

Let us consider Stream 6 (at the outlet of the expansion valve, V-1) for the analysis of the VLE data obtained through the various models.

The phase compositions and the adiabatic flash temperature predicted by the various VLE models are different. The temperature predicted by the Peng-Robinson equation is 222.526 K, compared to the values of 229.836 K and 230.926 K predicted by the RK/CS and SRK/CS combinations for the adiabatic expansion in the valve.

In order to compare the results, a common basis is required. Let us use the results of the Peng-Robinson adiabatic flash, to consider a seperate isothermal flash calculation, at 20.414 atm. and 222.526 K (total stream composition equal to Stream 6), for all the VLE data models.

The phase conditions predicted by the RK/CS, SRK/CS and the Peng-Robinson models are presented in Table 5.2. The values of the equilibrium ratios, liquid phase fugacity coefficients and vapor phase fugacity coefficients are presented in Tables 5.3, 5.4 and 5.5 respectively.

The data presented in Table 5.2 indicate the following :

- The SRK/CS and RK/CS predictions of vapor-liquid phase compositons and vapor fractions agree closely.
- The phase compositions predicted by the Peng-Robinson model are similar to the other two models, except for Nitrogen. Consequently, a higher value of vapor fraction is obtained by the Peng-Robinson models.

The data presented in Tables 5.3, 5.4 and 5.5 indicate the following :

- Similar component K-values are obtained via all the models, except for Nitrogen and Methane.
- The correct trend of lower K-values for higher molecular weight hydrocarbons has been predicted by all the models.
- Almost identical results for the RK/CS and SRK/CS indicate that, in this system, the controlling factor

for the K-values are the liquid phase fugacity coefficients.

- The vapor phase fugacity coefficients obtained by the various models agree reasonably. Results indicate a high degree of non-ideality for components other than N_2 and CH_4.This is the correct trend, since the other compo- nentshave very low vapor pressure values at 222.53 K and are actually in subcooled states.

Let us determine the relative accuracy of the models.

- The Chueh-Prausnitz estimate of mixture reduced temperature for the stream under study is 1.052. Again, the liquid-phase Methane mole fraction is 0.3099. Both of these figures violate the Chao-Seader restrictions.
- Chao-Seader method is sensitive to the presence of dissolved gases like Nitrogen and Carbon Dioxide.
- SRK equation is error-prone in systems containing Carbon Dioxide (Holland, 1981).
- The K-value predicted for Carbon Dioxide by the Peng-Robinson model lies between those for Methane and Ethane. This is to be expected in an actual situation in low-temperature processing (Roche). The SRK/CS and RK/CS K-values for Carbon Dioxide almost equal those for Methane. This does not seem to be likely.
- The K-values of Nitrogen are very sensitive to low temperatures computations and are known to exibit maxima in the K-vs-T plots (Roche). Hence, a high value is very

likely to be predicted.

Considering the above, one can infer that the obtained Peng-Robinson prediction of VLE data is accurate, at least qualitatively. However, the sensitivity of the Peng-Robinson model to low liquid concentrations should be studied thoroughly in future.

Compressibility Factors

Let us take up Stream 2 for comparison among the various models, since all the models are subjected to an identical thermodynamic state and stream compositions via a specified aftercooler-exit temperature and pressure at the outlet of the Compressor.

- The vapor mixture compressibility factors predicted for Stream 2 via the various equations of state are : 0.7837 by the Peng-Robinson equation, 0.8048 by the RK equation and 0.8038 via the SRK equation.
- As a rough estimate, let us make a comparison against pure-component compressibility factor charts evaluated by Nelson and Obert, as presented in Reid, Sherwood and Prausnitz's text (1977). The Chueh-Prausnitz method yields a mixture a value of 1.052 for the mixture reduced temperature. An estimate of the mixture reduced pressure of 0.63. The compressibility factor for Methane, the dominant component of Stream 2, at these reduced conditions is 0.79. Hence, we can

infer that all of our models have performed well in predicting vapor phase mixture compressibility factors.

Only the Peng-Robinson equation has been used to predict liquid phase mixture compressibility factors. Let us consider Stream 10. Its compressibility factor has been predicted as 0.123. This value could not be verified since data for compressibility factors of pure components are not given for liquid phase conditions.

TABLE 5.2

Stream Conditions : Isothermal Flash

	Feed Condition	Predicted Product Conditions					
Temperature, K	222.53	222.53		222.53		222.53	
Pressure, atm	20.414	20.414		20.414		20.414	
Vapor Fraction	-	0.2062		0.2062		0.2498	
Composition / Components	Composite Feed	RK/ Chao-Seader x_i	RK/ Chao-Seader y_i	SRK/ Chao-Seader x_i	SRK/ Chao-Seader y_i	Peng-Robinson x_i	Peng-Robinson y_i
CO_2	0.84E-3	1.00E-3	2.93E-4	1.00E-3	2.94E-4	1.12E-3	1.19E-3
Nitrogen	0.23E-2	2.36E-3	2.19E-3	2.36E-2	2.16E-3	0.5E-3	0.0841
Methane	0.4448	0.3098	0.9174	0.3099	0.9166	0.2629	0.8988
Ethane	0.1844	0.2186	0.0656	0.2185	0.0654	0.2457	0.0759
Propane	0.2013	0.2550	1.35E-2	0.2550	1.36E-2	0.2682	0.0142
i-Butane	2.23E-2	2.85E-2	5.27E-4	2.85E-2	5.35E-4	2.97E-2	4.7E-4
n-Butane	8.01E-2	0.1027	4.01E-4	0.1027	1.19E-3	0.1067	1.02E-3
i-Pentane	1.74E-2	2.23E-2	8.66E-5	2.23E-2	8.99E-5	2.31E-2	6.0E-5
n-Pentane	1.87E-2	2.40E-2	6.26E-5	2.40E-2	6.54E-5	2.49E-2	4.0E-5
n-Heptane	2.79E-2	3.60E-2	7.25E-6	3.58E-2	8.09E-6	3.72E-2	2.6E-6

TABLE 5.3

Equilibrium Constants : Isothermal Flash *

Temperature 222.53 K

Pressure 20.414 Atm

	RK/ Chao-Seader	SRK/ Chao-Seader	Peng-Robinson
CO_2	3.1949	3.2389	1.0631
Nitrogen	1.0171	1.0069	18.4606
Methane	3.2574	3.2557	3.7669
Ethane	0.3282	0.3294	0.3403
Propane	0.0581	0.0589	0.0585
i-Butane	0.0202	0.0206	0.0174
n-Butane	0.0125	0.0128	0.0105
i-Pentane	0.0043	0.0044	0.0029
n-Pentane	0.0029	0.0030	0.0019
n-Heptane	0.0002	0.0003	0.0007

NOTE-

* Compositions are presented in TABLE 5.2

TABLE 5.4

<u>Liquid Phase# Fugacity Coefficients : Isothermal Flash*</u>

Temperature 222.53 K

Pressure 20.414 Atm

	RK:Chao Seader	SRK:Chao Seader	Peng-Robinson
CO_2	0.25697	0.25697	0.86710
Nitrogen	1.01408	1.01408	18.24376
Methane	2.94961	2.94961	3.36366
Ethane	0.24528	0.24528	0.24777
Propane	0.03717	0.03717	0.03580
i-Butane	0.01141	0.01141	0.00926
n-Butane	0.00685	0.00685	0.00544
i-Pentane	0.00208	0.00208	0.00129
n-Pentane	0.00136	0.00136	0.00082
n-Heptane	0.00080	0.00080	0.00002

NOTES :

* - The SRK/RK : Chao-Seader values represent products of activity coefficients and liquid phase pure-component fugacity coefficients (eqn.s 2.1 or 3.1).
The Peng-Robinson values indicate the liquid-phasemixturefugacity coefficients.

\# - Compositions are presented in TABLE 5.2

TABLE 5.5

<u>Vapor Phase Fugacity Coefficients : Isothermal Flash</u> #

Temperature 222.53 K

Pressure 20.414 Atm

Components	RK-Chao Seader	SRK-Chao Seader	Peng-Robinson
CO_2	0.80430	0.79339	0.81586
Nitrogen	0.98323	0.99310	0.98826
Methane	0.90552	0.90597	0.89293
Ethane	0.74729	0.74459	0.72807
Propane	0.63956	0.63144	0.61246
i-Butane	0.56460	0.55326	0.53281
n-Butane	0.55025	0.53623	0.51644
i-Pentane	0.48739	0.46827	0.44768
n-Pentane	0.47612	0.45291	0.43249
n-Heptane	0.36243	0.32267	0.30344

NOTE :

Stream compositions are presented in TABLE 5.2.

Enthalpy Departure Functions

- Let us consider Stream 2, which has the same phase conditions: temperature, pressure and composition, as predicted by the various models. The RK estimate is -267.9 Cals/ Gm Mole as compared to -142.9 Cals/ Gm Mole predicted by the SRK equation and -104.4 Cals/ Gm Mole evaluated by the Peng-Robinson equation.
- As an approximate verification of these departure function values, let us consider the Yen-Alexander's charts (Reid, Sherwood, Prausnitz: 1977, Figure 5.5) as a reference. The mixture reduced pressure and reduced temperature of Stream 2 are 0.63 and 1.052 respectively. The Yen-Alexander charts predict -371.52 Cal/ Gm Mole as the enthalpy departure at this condition.
- Thus, the RK equation seems to have produced the closest values, while the SRK and the Peng-Robinson estimates do not seem to be accurate. However, all the predictions are much lower than expected.
- While the Yen-Alexander correlation is considered to be accurate, the values of the critical compressibility factors it uses conflict with RK/SRK/Peng-Robinson estimates.
- Again, we should consider that the enthalpy departure isotherms near the critical region are very sensitive to changes in pressure and exibit points of inflexion as well as steep maxima (Figures 5-2 to 5-5, Reid,

Sherwood, Prausnitz, 1977).

- Hence, a definitive conclusion can not be made regarding the accuracy of prediction, or applicability of any particular equation of state in these regions, as is the case in ous test problem.

The trends discussed above are for vapor stream enthalpy departure functions. Let us consider the liquid phase enthalpy departure predictions. In order to be consistent, let us compare the results of an isothermal flash on stream 4, with temperature, pressure and composition as determined by the Peng-Robinson equation, with the CS/RK or CS/SRK models.

- The Peng-Robinson equation has predicted a much lower value than the Chao-Seader method. The respective values are -546.7 and -2302.3 Cals /Gm Mole respectively. Referring to the Yen-Alexander's charts, the dominant components of Stream 4 : Methane, Ethane, Propane and n-Butane have pure-component enthalpy departure values of -276.4, -3664.8, -5092.1 and -6122.8 Cals/ Gm Moles respectively. Hence, as a rough estimate, if we assume an additive molar average by Kay's rule, the value for Stream 4 should be -2900 Cals/ Gm Mole.

Thus, the Chao-Seader model has a closer proximity to accuracy. Thus, we can propose that the RK/ Chao-Seader model be used for near-critical phase enthalpy estimates.

Let us discuss the applicability of the analytical approach of liquid phase enthalpy estimation.

- Analytical equations are frequently found to yield unsatisfactory results (Roche). However, specific heat data cannot be relied upon at higher pressures, because these are mostly generated under low pressure environments and limited ranges of temperature. Peter's chart extrapolations for supercritical phases are also errorsome. Thus, we have restricted the use of liquid specific heat data to near-atmospheric systems only.

Entropy Departure Functions

- The vapor phase entropy departure of Stream 2, which has an uniform state with respect to all the models has been predicted well through the SRK and the Peng-Robinson equations of state. The SRK and RK eqns. have predicted values of -0.4578 Cals/ Gm Mole. K and -7.465 Cals/Gm Mole. K, whereas the Peng-Robinson equation has estimated a value of -6.9271 Cals/ Gm Mole. K. Let us consider the Lee-Kesler Tables as a basis of comparison (Reid, Sherwood, Prausnitz, 1977). This method yields an aproximate value of -8.720 Cals/ Gm Mole. K as the entropy departure value for Stream 2. Thus, we can observe that the SRK and the Peng-Robinson equation is very accurate and the RK equation has failed to produce accurate values.

- However, for liquid streams, dissimilar results are obtained. For Stream 10, the Peng-Robinson estimate of entropy departure is -7.3126 Cals/ Gm Mole. K, whereas the RK/Chao-Seader estimate of -9.938 Cals/ Gm Mole. K. The Lee-Kesler tables predict an approximate value of -13.82 Cals/ Gm Mole. K. Thus, for liquid phases, the Peng- Robinson value is inacccurate. Again, we observe that although the Chao-Seader method has worked well for enthalpy departures, it is much inaccurate for entropy departures. Similarly, the RK and SRK equations can not be recommended for vapor phase entropy departure estimations. Though entropy as a state property is seldom used, one should be careful about selecting the right model when required.

Vapor Mixture Specific Heat Departure Functions

The vapor mixture specific heat departure functions for the inlet and outlet streams, 1 and 2, as predicted by the various equations of states are presented in Table 5.6. Let us compare the C_p values with the Lee-Kesler estimation method (Reid, Sherwood, Prausnitz, 1977). Considering the dominating components of Stream 1 : Methane, Ethane, Propane and i-Butane, we find that the individual departures in C_p are 0.2632, 0.6506, 5.7253 and 9.667 Cal/ Gm Mole. K respectively. A molar average of these would yield a value of 1.4487 Cals/ Gm Mole. K. Comparing this value with results obtained (Table 5.6), we observe that only the Peng-Robinson prediction has produced acceptable values. The SRK value is too large and the RK value is erroneous, since it is negative.

Again, for Stream 2, the SRK equation has predicted negative values of C_p departure and the difference between C_p and C_v. The RK equation predicts negative C_p departures for both the inlet and outlet conditions. However, the RK estimate is somewhat closer to the Peng-Robinson estimate for $(C_p - C_v)$ values. Thus only Peng-Robinson equation has produced the right values.

As there is no reference available in literature on the C_v and the $(C_p - C_v)$ values, we can't ascertain the accuracy of predictions with the eqns. However, the Peng-Robinson equation has predicted a C_p value of 8.4232 and a C_v value of 6.2937. This results in a polytropic ratio of 1.3384. Although this value is a bit high for heavy, polyatomic gases (1.1 - 1.2 usually), it is reasonably satisfactory for the light gases we have studied (1.2 - 1.4 usually). Hence, the Peng-Robinson equation can be relied upon as an accurate source of C_v values.

TABLE 5.6

<u>Specific Heat Departure Functions : Streams 1 and 2</u>

Unit : Calories/ Gram Mole/ ^{0}K

Equations of State	Departure Function Values: Stream # 1 [*]			Stream # 2 [*, +]		
	C_p	(C_p-C_p)	(C_p-C_v)	C_p	(C_p-C_p)	(C_p-C_v)
Peng-Robn.	8.2809	0.1423	2.1295	9.0681	0.1022	2.0894
SRK Eqn.	8.2809	4.2597	6.2469	8.9081	-2.6963	-0.7091
RK Eqn.	8.2809	-0.1725	2.6509	9.3296	-0.1876	2.7465

NOTES :

* : Stream states and compositions are given in Appendix C, same for all the models.

+ : Stream temperatures shown in Appendix C is at the aftercooler exit, actual temperature is higher than the compressor inlet stream, # 1.

5.2.2 Performance of Computational Modules

Rotational Equipment Modules

The performance of the rotational equipment modules have been determined largely by the behavior of different thermodynamic models. An overview of such results for each of the three thermophysical models are presented in Appendix C, where energy requirements are tabulated for each equipment.

For the Compressor (Unit 1), each of the equations of state have predicted for a single stage compression strategy. A stage-compression ratio of 2.075 is thus estimated uniformly. Based on our discussions of results obtained for specific heat departure functions under the previous topic, we can infer that only the Peng-Robinson esimate of 10.611 HP is the correct estimate of the compression power. Another result which should be discussed is the temperature at the exit of the Compressor. Its value, -54.6879 F , is lower than the inlet value of -25.7978 F. This anomaly is caused by the need of excessive cooling to be employed in the aftercooler of the compression stage. This was necessary because we tried to minimize the temperature difference between the two inlet streams of the Mixer (Unit 3), one of which is the vapor stream at the exit of the Compressor.

For the Hydraulic Turbine (Unit 2), all the models have predicted the same value of recoverable power, 1.698 HP. The reason for such results is that the Hydraulic Turbine module, HYTR, does not depend on any liquid phase model for estimating energy recovery. It calculates available energy differencial as the product of the specified pressure differential and the flowrate. One can also observe that outlet temperatures predicted by various models are different, though close in the values. This temperature is determined by an adiabatic flash, the target enthalpy of which is established from the specified fractional efficiency.

Results have disagreed considerably for the Gas Expander (Unit 6). The SRK model has predicted an outlet temperature of -214.05 F and a value of 11.096 HP for the recoverable power. The RK equation has predicted a value of -258.4 F for the exit temperature of the Gas Expander and a value of 13.726 HP for the recoverable power. The Peng-Robinson equation has predicted a temperature of -225.9 F at the exit of the Gas Expander and a value of 11.514 HP as the recoverable power. Hence, the RK equation has not performed well. The reason is that the RK equation is not suitable for calculating entropy departures at low temperatures, accuracy in the estimate of this property is requisite for the GSXP module. In our case, the RK-predicted exit condition is inside the two-phase envelope rather than in the superheated region. Thus, a large part of the high recoverable-energy value is contributed by latent heat of condensation. Since we have established earlier that the SRK and the Peng-Robinson equations are correct in predicting for the entropy departures, we can infer that the value of 11.096 or 11.514 HP, predicted by the SRK and the Peng-Robinson equations respectively, is the correct value of power recovery from Unit 6.

The power requirement of the Pump (Unit 7) have been predicted well by both the liquid phase models. While the Chao-Seader value is 3.785 and 3.784 HP (for the RK and the SRK combinations respectively), the Peng-Robinson equation has predicted a value of 4.22 HP.

Thus, in conclusion, we can say that the Peng-Robinson equation has been the most successful among all the models in predicting the behavior of the rotational equipments. Its use is recommended for simulating similar conditions of low temperatures and high pressures of actual cryogenic process plants.

Thermophysical Modules

In this section, a few important restrictions imposed on certain thermophysical modules will be discussed.

As discussed earlier, the RK equation has predicted a very low exit temperature for the Gas Expander unit. This had resulted in a thermodynamic state for the mixture where enthalpy departure values fluctuate widely over ranges of even 10 K temperature. Such behavior is confirmed by the grahical data presented in Reid, Sherwood and Prausnitz's text (1977), where isotherms in enthalpy departure functions exibit points of inflection and steep maxima. This results in the adiabatic flash calculations in AFLASH to get trapped in oscillations about a convergence. To prevent this, we have introduced a redefined stepsize of 5 K instead of 20 K, or the value estimated by the Wegstein's algorithm. This strategy has produced accurate convergence, whereas none was obtained before. In future modifications of CHESS, one should incorporate measures in all the modules which iterate on entropy or enthalpy values.

Secondly, as mentioned earlier, we have restricted the use of liquid specific heat coefficient data upto states of 1 Atm. pressure and 300 K temperature. This was necessitated by the occurance of large errors in low temperature and high pressure conditions.

CHAPTER 6

CONCLUSION

Based on the analysis of results obtained from the simulation of the test problems using modified CHESS, we can conclude that the newly-incorporated modules are operational. The integration of these models with the overall simulation system has been successful. The rotational equipment modules have represented actual operations fairly closely.

As for the relative performance of the various thermophysical models, the results indicate that some of them are more successful in predicting certain properties than the rest. The Chao-Seader model has performed very well in predicting liquid enthalpy departures, but is grossly inaccurate in estimating entropy departures. The assumption that the SRK equation could be a substitute for the RK equation in providing a vapor phase model for the Chao-Seader method, has been found to be correct. Except for specific heat departure functions, the SRK and the RK equations have produced similar results. Considering the overall performance in predictions of properties and phase behavior, the Peng-Robinson equation is found to be accurate in most occations, for both the liquid and the vapor phases, except for enthalpy departure functions.

Hence, it is recommended that future extensions would make it possible for an user to select a model for a specific phase, or an equipment, or a property, rather than an uniform model throughout.

The task remains for all these models to be tested under various other phase environments and processing conditions, in order to ascertain their capacity fully.

Further attention will be needed to update the equipment module set. A major improvement can be made if optimization algorithms are incorporated as a part of the system. Optimization techniques should be applied not only to determine lowest-investment processing strategies, but also to decide upon intra-unit configurations, such as heat-exchanger networks, compressor and gas-expander staging etc.

CHESS is still somewhat limited in the area of control blocks. Future work have to concentrate on the development of stream flow ratio control and composition control, whereby remotely situated modules can communicate information. The control modules of FLOWTRAN can be used as a guideline. Again, apart from component ratio and temperature, other stream properties such as enthalpy, should be considered as candidates for manipulation. In parallel, the convergence algorithms in control blocks in general and in particular equipment modules should be replaced with recently developed methods, such as the

Broyden's algorithm. Attention should also be given to update the distillation algorithms.

Some rethinking in organizational aspects is also necessary. Efforts should be made towards improving time and storage efficiency by incorporating dynamic storage facility and variable-sized load modules via the use of a preprocessor language. Such improvements will also make system more user-friendly and would reduce input coding time. A certain ammount of computer graphics should increase the marketibility of the package. There should also be an effort to produce microcomputer compatible, interactive versions. As such, a shift towards a databased organization may be made.

Future work should also yield the capability to handle solids and VLSE systems. It is recommended to update the physical properties' package periodically. CHESS also needs to have modules to handle unsteady state or batch processing as well as prediction procedures for dynamic behavior of steady state processes.

APPENDIX A

Enthalpy and Entropy Departure via Peng- Robinson Equation

A.1 The Entropy Departure Function

A.2 The Enthalpy Departure Function

A.1 Derivation of the Entropy Departure Function

The pressure-explicit form of the Peng-Robinson eqn. is given as follows :

$$P = \frac{R\,T}{V - b} - \frac{a(T)}{V(V + b) + b(V - b)} \qquad \text{(A-1)}$$

For a pure component :

$$a(T) = a(T_c) \cdot \alpha(T_r) = A \qquad \text{(A-2)}$$

$$a(T\,) = 0.45724\,(R\,T_c^{2})/\,P_c \qquad \text{(A-3)}$$

$$\alpha(T\,) = [\,1 + K(\omega)\,(\,1 - T^{1/2}\,)\,]^{2} \qquad \text{(A-4)}$$

$$b(T) = 0.0778\,(\,R\,T_c\,/\,P_c\,) = B \qquad \text{(A-5)}$$

$$K(\omega) = 0.37464 + 1.54226\,\omega - 0.26992\,\omega^{2} \qquad \text{(A-6)}$$

For a mixture :

$$a_{mix} = A = \sum_{i=1}^{n}\sum_{j=1}^{n} y_i\,y_j\,a_{ij} \qquad \text{(A-7)}$$

$$a_{ij} = (\,1 - \delta_{ij}\,)\,a_i^{1/2}\,a_j^{1/2} \qquad \text{(A-8)}$$

$$b_{mix} = B = \sum_{i=1}^{n} y_i\,b_i \qquad \text{(A-9)}$$

For the compressibility factor of a mixture :

$$Z^{3} - (1 - \bar{B})Z^{2} + (\bar{A} - 3\bar{B}^{2} - 2\bar{B})Z - (\bar{A} - \bar{B}^{2} - \bar{B}^{3}) = 0 \qquad \text{(A-10)}$$

where :

$$\bar{A} = \frac{a_{mix}\,P}{(R\,T)^2} = \frac{A\,P}{(R\,T)^2} \qquad \text{(A-11)}$$

$$\bar{B} = \frac{b_{mix}\,P}{(R\,T)} = \frac{B\,P}{(R\,T)} \qquad \text{(A-12)}$$

From (A-1) :

$$\left(\frac{\partial P}{\partial T}\right)_V = \frac{R}{V - B} - \frac{(\partial A/\partial T)}{V(V + B) + B(V - B)}$$

$$= \frac{R}{V - B} - \left(\frac{\partial A/\partial T}{2.828\,B}\right)\left(\frac{V - 0.414\,B}{V + 2.414\,B}\right) \qquad \text{(A-13)}$$

(by partial fractions)

From eqns. (3.8) and (A-13) :

$$S - S^{0} = \int_{\infty}^{V} \left[\left\{\frac{\partial P}{\partial T}\right\}_V - \left\{\frac{R}{V}\right\}\right] dV \qquad \text{(A-14)}$$

$$= R\ln(V-B) - R\ln(V) - \left(\frac{1}{2.828B}\right)\left(\frac{\partial A}{\partial T}\right)\ln\left(\frac{V - 0.414B}{V + 2.414B}\right) + R\ln\left(\frac{V}{V_0}\right)$$

$$= R\ln\left\{Z - \left(\frac{B\,P}{R\,T}\right)\right\} - \left(\frac{1}{2.828B}\right)\left(\frac{\partial A}{\partial T}\right)\ln\left(\frac{ZRT - 0.414\,BP}{ZRT + 2.414\,BP}\right)$$

$$[\ \text{as } (V/V_0) = (P\,V\,/\,R\,T) = Z\ ]$$

Thus :

$$(S - S^{0}) = R\ln(Z - \bar{B}) + \frac{(\partial A\,/\,\partial T)}{2\sqrt{2}\,B} \cdot \ln\left(\frac{Z + 2.414\,\bar{B}}{Z - 0.414\,\bar{B}}\right) \qquad \text{(A-15)}$$

where :

$$\bar{A} = a_{mix}\,P/\,(R\,T)^2 = A\,P/(R\,T)^2$$

$$\bar{B} = b_{mix}\,P/\,(R\,T) = B\,P/(R\,T)$$

The derivative of the 'a' parameter w.r.t temperature for the general case of a mixture is obtained as follows :

From eqn. (A-7) and (A-8) :

$$\frac{\partial A}{\partial T} = \frac{\partial}{\partial T}\left[\sum_{i=1}^{n}\sum_{j=1}^{n} x_i x_j (a_i a_j)^{1/2}(1-\delta_{ij})\right]$$

$$= \sum_{i=1}^{n}\sum_{j=1}^{n} (1-\delta_{ij})(1/2)(a_i a_j)^{-1/2}\left\{\frac{\partial}{\partial T}[a_i a_j]\right\}$$

Differentiating eqn. (A-4) w.r.t temperature :

$$(\partial a_i/\partial T) = a_{c_i}.2[1 + k(\omega_i)(1 - T_{r_i}^{1/2})]\{(-0.5)K(\omega_i)(T_{r_i}^{-1/2}/T_{c_i})\}$$

Again :

$$\frac{\partial}{\partial T}(a_i a_j) = a_i\left(\frac{\partial a_j}{\partial T}\right) + a_j\left(\frac{\partial a_i}{\partial T}\right)$$

Thus :

$$\left(\frac{\partial A}{\partial T}\right) = \sum_{i=1}^{n}\sum_{j=1}^{n}\left[a_{ij}\, y_i y_j \left\{\frac{K(\omega_i)}{(\alpha_i T_{C_i})^{0.5}} + \frac{K(\omega_j)}{(\alpha_j T_{C_j})^{0.5}}\right\}\right]/(-2\, T^{1/2}) \tag{A-16}$$

A.2 Derivation of the Enthalpy Departure Function

From equation (3.6) :

$$H - H^{o} = \int_{\infty}^{V}\left[T\left(\frac{\partial P}{\partial T}\right) - P\right]dV + RT(Z-1) \tag{A-17}$$

From equations (A-13) and (A-17) :

$$H - H^{\circ} = \int_{\infty}^{V} [-\{T(\partial A/\partial T) - A\}/\{V(V+B)+B(V-B)\}]\, dV$$

$$= \{A - T(\partial A/\partial T)\} \left(\frac{Z + 2.414\ \bar{B}}{Z - 0.414\ \bar{B}}\right)/(2.828\ B) + RT(Z-1)$$

The derivative term is obtained by and replaced with eqn. (A-16).

APPENDIX B

Vapour Mixture Heat Capacity Departure Functions

B.1 <u>Soave-Redlich-Kwong Equation</u>

B.1.1 Departure in C_v

B.1.2 Difference between C_p and C_v

B.1.3 Departure in C_p

B.2 <u>Peng Robinson Equation</u>

B.2.1 Departure in C_v

B.2.2 Difference between C_p and C_v

B.2.3 Departure in C_p

B.1 Soave - Redlich - Kwong Equation of State

B.1.1 Departure in Specific Heat at Constant Volume

The pressure- explicit form of the equation of state proposed by Soave is :

$$P = \frac{R\,T}{V - b} - \frac{a(T,\omega)}{V\,(V + b)}$$

Therefore :

$$\left(\frac{\partial P}{\partial T}\right)_V = \frac{R}{V - B} - \frac{(\partial A/\partial T)}{V(V + B)} \qquad \text{(B-1)}$$

where A and B represents the parameters for a pure component or a mixture, as the case may be.

Differentiating (B-1) w.r.t T and substituting in (3.9), we obtain :

$$\left(\frac{\partial C_v}{\partial V}\right)_T = T\left[\frac{\partial}{\partial T}\left\{\frac{R}{V - B} - \frac{(\partial A/\partial T)}{V\,(V + B)}\right\}\right] \qquad \text{(B-2)}$$

Let us derive the derivative of the parameter A for a mixture.

Let : $$A = A_{c_{mix}}\,\alpha_{mix} \qquad \text{(B-3)}$$

where A stands for the mixture parameter defined by the Peng- Robinson mixing rules.

Thus :

$$\left(\frac{\partial A}{\partial T}\right) = A_{c_{mix}}\left(\frac{\partial \alpha_{mix}}{\partial T}\right) \qquad \text{(B-4)}$$

We know :

$$\alpha_{mix} = [\, 1 - m(\omega_{mix})\, (T / T_{c_{mix}})^{1/2}\,]^{2} \qquad \text{(B-31)}$$

Hence :

$$(\partial A_{mix} / \partial T) = - \alpha_{mix}^{1/2} \; A_{c_{mix}}^{1/2} \; / \; m(\omega_{mix}) \; / \; T^{1/2} \; / \; T_{c_{mix}}^{1/2} \qquad \text{(B-5)}$$

From (B-2), (B-3), (B-4) and (B-5), we obtain :

$$\left(\frac{\partial C_V}{\partial V}\right) = - \left(\frac{A_c \, m(\omega_{mix}) \, \alpha_{mix}^{1/2} \, (T / T_c)^{-1/2}}{2\, V\, (V + B)}\right) \qquad \text{(B-6)}$$

Here, B refers to the mixture parameter. Integrating (B-6) over an isothermal path between states 1 and 2, we obtain :

$$C_{V_1} - C_{V_2} = \frac{A_{c_{mix}} \, m(\omega_{mix}) \, \alpha_{mix}^{1/2}}{2(\, T . T_{c_{mix}})^{1/2}} \int_{V_1}^{V_2} \frac{1}{V(V + B)} \, dV \qquad \text{(B-7)}$$

The integrand in (B-7) is the following :

$$\left(\frac{1}{B}\right) \ln\left[\frac{(V_2 + B) / V_2}{(V_1 + B) / V_1}\right]$$

If we define state 2 as that of the system(P, V, T) and state 1 as the ideal gas state (P-->0, V-->∞ ,T = T) :

$$\lim_{V_1 \to \infty} \left[\ln\left(\frac{V_1 + B}{V_1}\right) \right] = 0$$

Substituting in eqn.(B-7) and rearranging :

$$C_v - C_v^{\circ} = \frac{A \; m(\omega_{mix})(T_{r_{mix}} / \alpha_{mix})^{1/2}}{2 B R T} \ln\left(\frac{V + B}{V}\right) \quad \text{(B-8)}$$

Upon further rearrangement, we obtain the final form :

$$\frac{C_v - C_v^{\circ}}{R} = \frac{\Delta C_v}{R} = \frac{1}{2} \left(\frac{A_v^2}{B_v}\right) (MTA_1) \ln(1 + h) \quad \text{(B-9)}$$

where :

$$A_v^2 = (a_{mix} / R T)^2 = (A / R T)^2$$

$$B_v = (b_{mix} / R T) = (B / R T)$$

$$h = (b / V) = (B_v P / Z)$$

$$MTA_1 = m(\omega_{mix}) \, T_{r_{mix}}^{1/2} / \alpha^{1/2}$$

$$\omega_{mix} = \sum_i y_i \omega_i$$

$$T_{r_{mix}} = T / T_{c_{mix}}$$

B.1.2 Difference Between the Heat Capacities

Differentiating the SRK equation w.r.t volume at constant temperature, we obtain :

$$\left(\frac{\partial P}{\partial V}\right)_T = RT \left(\frac{1}{V - B}\right)^2 - \left(\frac{A}{B}\right) \left[\left(\frac{1}{V}\right)^2 - \left(\frac{1}{V + B}\right)^2 \right]$$

Substituting equations (B-3) and (B-31) in equation (B-1) and squaring both sides :

$$\left(\frac{\partial P}{\partial T}\right)^2 = \left(\frac{R}{V-B}\right)^2 - \left(\frac{2R\,A_C\, m(\omega_{mix})(\alpha/T_{r_{mix}})^{1/2}}{T_C\, V\,(V^2 - B^2)}\right) + \left(\frac{A_C^2\, m(\omega_{mix})^2\,(\alpha/T_{r_{mix}})^2}{T_C^2\, V^2\,(V+B)^2}\right)$$

Using these two equations for the thermodynamic identity in eqn.(3.10) and rearranging, we obtain the difference function as follows :

$$\{C_p - C_v / R\} =$$

$$\frac{\left(\frac{1+h}{1-h}\right) + 2\left(\frac{A_v}{B_v}\right)^2 (MTA_2)\left(\frac{h}{b_{mix}}\right) + 4\left(\frac{A_v}{B_v}\right)^2 (MTA_2)^2 \left(\frac{h}{b_{mix}}\right)^2 \left(\frac{1+h}{1-h}\right)}{\left(\frac{1+h}{1-h}\right) - \left(\frac{A_v}{B_v}\right)^2 \left(\frac{h}{b_{mix}}\right)\left(\frac{1-h}{1+h}\right)(2+h)} \tag{B-10}$$

where :

$$MTA_2 = m(\omega_{mix}) \;/\; \alpha^{1/2} \;/\; T$$

B.1.3 <u>Heat Capacity Departure at Constant Pressure</u>

Applying (B-9)and (B-10) to equation (3.11) ,we obtain the following function for departure in C_p :

$$\frac{C_p - C_p^0}{R} = \frac{\Delta C_p}{R} =$$

(Contd.)

$$= \frac{\left(\frac{1+h}{1-h}\right) + 2\left(\frac{A_v^2}{B_v}\right)(MTA_2)\left(\frac{h}{b_{mix}}\right) + 4\left(\frac{A_v^2}{B_v}\right)^2 (MTA_2)^2 \left(\frac{h}{b_{mix}}\right)^2 \left(\frac{1+h}{1-h}\right)}{\left(\frac{1+h}{1-h}\right) - \left(\frac{A_v^2}{B_v}\right)\left(\frac{h}{b_{mix}}\right)\left(\frac{1-h}{1+h}\right)(2+h)} \qquad \text{(B-11)}$$

$$\longrightarrow \quad + \frac{1}{2}\left(\frac{A_v^2}{B_v}\right)(MTA_1)\ln(1+h) - 1$$

B.2 Peng- Robinson Equation of State

B.2.1 Heat-Capacity Departure at Constant Volume

The pressure- explicit form of the Peng- Robinson equation of state is :

$$P = \frac{R\,T}{V - b} - \frac{a(T)}{V(V+b) + b(V-b)} \qquad \text{(B-12)}$$

Differentiating with respect to T at constant V :

$$\left(\frac{\partial P}{\partial T}\right)_V = \frac{R}{V - b} - \frac{[\partial a(T)/\partial T]}{V(V+b) + b(V-b)} \qquad \text{(B-13)}$$

The derivative of mixture 'a' parameter w.r.t T is :

$$\left(\frac{\partial A}{\partial T}\right) = A_{c_{mix}}\,[1 + K(\omega_{mix})(1 - T_{r_{mix}}^{1/2})][-K(\omega_{mix})T_{r_{mix}}^{-1/2}/T_{c_{mix}} \qquad \text{(B-14)}$$

Differentiating (B-13) and substituting (B-13) and (B-14) in (3.9), we obtain, upon rearrangement :

$$\left(\frac{\partial C_V}{\partial V}\right)_T = \frac{A_{mix}\,K(\omega_{mix})\,[\alpha_{mix} / T_{mix}\,T_{c_{mix}}]^{1/2}}{2\{V(V+B) + B(V-B)\}} \qquad \text{(B-15)}$$

Integrating (B-15) between states 1 and 2 over an isothermal path :

$$C_{V_1} - C_{V_2} = \frac{A_{c_{mix}} K(\omega_{mix}) \{\alpha_{mix} / (2 T_{c_{mix}} T)\}^{1/2}}{2.828\, B} \left[\ln\left(\frac{V - 0.414B}{V + 2.414B}\right)\right]\Bigg|_{V_1}^{V_2} \qquad \text{(B-16)}$$

If the state 1 is taken as the ideal gas state :

$$\lim_{V_1 \to \infty} \left\{ \ln \left[\left(\frac{V_1 - 0.414\, B}{V_1 + 2.414\, B}\right)\right]\right\} = 0 \qquad \text{(B-17)}$$

Substituting eqn. (B-17) in (B-16) and rearranging, we obtain the following final form of the departure function :

$$\frac{C_v - C_v^{o}}{R} = \frac{\Delta C_v}{R}$$

$$= \left(\frac{1}{5.656}\right) \left(\frac{A_v^{2}}{B_v}\right) (MTB_1) \ln\left[\frac{(1 + 2.414\, h)}{(1 - 0.414\, h)}\right] \qquad \text{(B-18)}$$

where :

$$A_v^{2} = a_{mix} / (RT)^2 = A / (RT)^2$$

$$B_v = b_{mix} / RT = B / RT$$

$$h = b / V = B P / Z$$

$$MTB_1 = K(\omega_{mix})\, T_{r_{mix}}^{1/2} / \alpha_{mix}^{1/2}$$

B.2.2 <u>Difference Between the Heat Capacities</u>

Differentiating eqn (B-12) w.r.t volume, V,at constant temperature, we arrive at the following expression :

$$\left(\frac{\partial P}{\partial V}\right)\Bigg|_T = - RT\left(\frac{1}{V - b}\right)^2 - \left[\frac{a(T)}{2.828\, b}\right]\left[\left(\frac{1}{V - 0.414b}\right)^2 - \left(\frac{1}{V - 2.414b}\right)^2\right] \qquad \text{(B-19)}$$

Squaring both sides of eqn. (B-13), then applying it together with eqn. (B-19) to equation (3.10),we arrive at the expression for the function yielding the difference in the specific heats at constant pressure (C_p), and that at constant volume (C_v). Upon rearrangement, we obtain the equation presented in the following :

$$\left[\frac{\left(\frac{1 + h}{1 - h}\right) + \left(\frac{A_v^2}{B_v}\right)(MTB_2)\left\{\frac{(1+h)}{(1+2.414h)(1-0.414h)}\right\}}{\left(\frac{1 + h}{1 - h}\right) - \left(\frac{A_v^2}{B_v}\right)\left(\frac{h}{1.414}\right)\left\{\frac{(1 - h^2)(2.828 + h)}{[(1+2.414h)(1-0.414h)]^2}\right\}}\right] . \rightarrow \qquad \text{(B-20)}$$

$$\rightarrow . \left[1 + \left(\frac{A_v^2}{B_v}\right)(MTB_2)\left\{\frac{(1-h)}{(1+2.214h)(1-0.414h)}\right\}\right]$$

where :

$$MTB_2 = MTB_1 \,.\, b_{mix} = MTB_1 \,.\, B$$

B.2.3 <u>Heat Capacity Departure at Constant Pressure</u>

Substituting equations (B-18) and (B-20) in equation (3.11),we obtain the following departure function for heat capacity at constant pressure :

$$\frac{\Delta C_p}{R} = \frac{C_p - C_p^{\circ}}{R} =$$

$$\left(\frac{1}{5.656}\right)\left(\frac{A_V^2}{B_V}\right)(MTB_1)\ln\left[\frac{(1 + 2.414\,h)}{(1 - 0.414\,h)}\right] - 1 + $$

$$\left[\frac{\left(\frac{1+h}{1-h}\right) + \left(\frac{A_V^2}{B_V}\right)(MTB_2)\left\{\frac{(1+h)}{(1+2.414h)(1-0.414h)}\right\}}{\left(\frac{1+h}{1-h}\right) - \left(\frac{A_V^2}{B_V}\right)\left(\frac{h}{1.414}\right)\left\{\frac{(1-h^2)(2.828+h)}{[(1+2.414h)(1-0.414h)]^2}\right\}}\right] \cdot \left[1 + \left(\frac{A_V^2}{B_V}\right)(MTB_2)\left\{\frac{(1-h)}{(1+2.214h)(1-0.414h)}\right\}\right]$$

APPENDIX C

OUTPUTS OBTAINED FROM THE SIMULATION STUDY : TEST CASE FOR ROTATIONAL EQUIPMENTS

THE OUTPUTS FROM THE PENG-ROBINSON EQUATION

```
*** ***  CHESS FLOW SHEET SIMULATION  *** ***
              VERSION  THREE
                JUNE 1985

 CHESS3 ... TEST CASE FOR ROTATIONAL EQUIPMENTS
     10        6        6        0        0        0

     49       46        2        3        4        5        6        7
      8       11

      7        6        2        4        1

BEGIN NETWORK READ
   1       COMP       U-1      1   -2    0    0    0    0    0
   2       HYTR       U-2      3   -4    0    0    0    0    0
   3       MIXR       U-3      2    4   -5    0    0    0    0
   4       VALV       U-4      5   -6    0    0    0    0    0
   5       ADBF       U-5      6   -7   -9    0    0    0    0
   6       GSXP       U-6      7   -8    0    0    0    0    0
   7       PUMP       U-7      9  -10    0    0    0    0    0
NETWORK COMPLETE

BEGIN EQUIPMENT DATA READ
      3        0        0        0        0        0        0        0
      0        0        0        0        0        0        0        0
      0        0        0        0        0        0        0        0
      0        0        0        0        0        0        0        0
      0        0        0        0        0        0        0        0
      0        0        0        0        0        0        0        0
      0        0

   1.0000      28.239      225.00      0.85000      3.0000      0.00000
  0.00000     0.00000     0.00000      0.00000     0.00000      0.00000
  0.00000     0.00000     0.00000      0.00000     0.00000      0.00000
  0.00000     0.00000     0.00000      0.00000     0.00000      0.00000
  0.00000

   2.0000      28.239     0.60000      0.00000     0.00000      0.00000
  0.00000     0.00000     0.00000      0.00000     0.00000      0.00000
  0.00000     0.00000     0.00000      0.00000     0.00000      0.00000
  0.00000     0.00000     0.00000      0.00000     0.00000      0.00000
  0.00000

   4.0000      20.414     0.00000      0.00000     0.00000      0.00000
  0.00000     0.00000     0.00000      0.00000     0.00000      0.00000
  0.00000     0.00000     0.00000      0.00000     0.00000      0.00000
  0.00000     0.00000     0.00000      0.00000     0.00000      0.00000
  0.00000

   5.0000      2.0000     0.00000      0.00000     0.00000      0.00000
  0.00000     0.00000     0.00000      0.00000     0.00000      0.00000
  0.00000     0.00000     0.00000      0.00000     0.00000      0.00000
  0.00000     0.00000     0.00000      0.00000     0.00000      0.00000
  0.00000

   6.0000      3.2023     0.60000      0.00000     0.00000      0.00000
  0.00000     0.00000     0.00000      0.00000     0.00000      0.00000
  0.00000     0.00000     0.00000      0.00000     0.00000      0.00000
  0.00000     0.00000     0.00000      0.00000     0.00000      0.00000
  0.00000

   7.0000      34.023     0.75000      0.00000     0.00000      0.00000
  0.00000     0.00000     0.00000      0.00000     0.00000      0.00000
```

```
   0.00000      0.00000      0.00000      0.00000      0.00000      0.00000
   0.00000      0.00000      0.00000      0.00000      0.00000      0.00000
   0.00000
 EQUIPMENT DATA COMPLETE

 BEGIN STREAM EXTENSIVE LIST READ
        2        4        5        6        7        8        9       10
        0        0        0        0        0        0        0        0
        0        0        0        0        0        0        0        0
        0        0        0        0        0        0        0        0
        0        0        0        0        0        0        0        0
        0        0        0        0        0        0        0        0
        0        0        0        0        0        0        0        0
        0        0        0        0        0        0        0        0
        0        0        0        0        0        0        0        0
        0        0        0        0        0        0        0        0
        0        0        0        0        0        0        0        0
        0        0        0        0        0        0        0        0
        0        0        0        0

   1.0000      0.00000      15129.       9.3070       67.646       12920.
   1646.8       420.54      17.434       40.678       3.7680       2.7690
   0.45400

   3.0000      0.00000      43296.       39.952       67.646       13069.
   9126.8       11340.      1285.7       4640.3       1009.7       1087.8
   1629.4
 STREAM EXTENSIVE LIST COMPLETE

 BEGIN STREAM INTENSIVE LIST READ
        2        4        5        6        7        9        0        0
        0        0        0        0        0        0        0        0
        0        0        0        0        0        0        0        0
        0        0        0        0        0        0        0        0
        0        0        0        0        0        0        0        0
        0        0        0        0        0        0        0        0
        0        0        0        0        0        0        0        0
        0        0        0        0        0        0        0        0
        0        0        0        0        0        0        0        0
        0        0        0        0        0        0        0        0
        0        0        0        0        0        0        0        0
        0        0        0        0        0        0        0        0
        0        0        0        0

   1.0000       1.0000       1.0000       241.05       13.609      0.00000
   0.00000      0.00000      0.00000      0.00000

   3.0000       1.0000      0.00000       222.07       40.827      0.00000
   0.00000      0.00000      0.00000      0.00000

   6.0000       2.0000      0.00000      0.00000      0.00000      0.00000
   0.00000      0.00000      0.00000      0.00000

   10.000       2.0000      0.00000      0.00000      0.00000      0.00000
   0.00000      0.00000      0.00000      0.00000
 STREAM INTENSIVE LIST COMPLETE

 BEGIN CALCULATION DATA READ
      20        5        0
   0.10000E-03

        0        0        0        0        0        0        0        0
        0        0        0        0        0        0        0        0
        0        0        0        0        0        0        0        0
        0        0        0        0        0        0        0        0
        0        0        0        0        0        0        0        0
```

0	0	0	0	0	0	0	0
0	0						
0	0	0	0	0	0	0	0
0	0						
0	0	0	0	0	0	0	0
0	0						

CALCULATION DATA COMPLETE

** DECOMPOSITION OF NET(S) WILL FOLLOW **

PRECURSOR LIST..

1	0	0	0	0	0	0
2	1	0	0	0	0	0
3	0	0	0	0	0	0
4	3	0	0	0	0	0
5	2	4	0	0	0	0
6	5	0	0	0	0	0
7	6	0	0	0	0	0
8	7	0	0	0	0	0
9	6	0	0	0	0	0
10	9	0	0	0	0	0

** THIS CASE HAS NO RECYCLE STREAM **

```
VAPOR-LIQUID EQUILIBRIUM DATA CODES:
    LIQUID =    6
    VAPOR =     6
    ENTHALPY = 0

VAPOR PHASE MODEL    : PENG-ROBINSON EQN.

LIQUID PHASE MOODEL  :PENG-ROBINSON EQN.

ENTHALPY CORRECTION : FOR BOTH PHASES.
```

CHESS3 ... TEST CASE FOR ROTATIONAL EQUIPMENTS

"PROCESS VECTORS"

...... EQUIPMENT			STREAM NUMBERS		
NUMBER	SUBROUTINE	NAME			
1	COMP	U-1	1	-2	0
2	HYTR	U-2	3	-4	0
3	MIXR	U-3	2	4	-5
4	VALV	U-4	5	-6	0
5	ADBF	U-5	6	-7	-9
6	GSXP	U-6	7	-8	0
7	PUMP	U-7	9	-10	0

CHESS3 ... TEST CASE FOR ROTATIONAL EQUIPMENTS

'STREAM CONNECTIONS'

STREAM	EQUIPMENT FROM	EQUIPMENT TO
1	0	1
2	1	3
3	0	2
4	2	3
5	3	4
6	4	5
7	5	6
8	6	0
9	5	7
10	7	0

CHESS3 ... TEST CASE FOR ROTATIONAL EQUIPMENTS

'OTHER SYSTEM VARIABLES'

NUMBER OF COMPONENTS	10
COMPONENT NUMBERS USED	49, 46, 2, 3, 4, 5, 6, 7, 8, 11,
TOLERANCE, 'DERROR'	0.0005
MAX. LOOPS IN RECYCLE CALC.	20

"INPUT DATA"

CHESS3 ... TEST CASE FOR ROTATIONAL EQUIPMENTS

STREAM NUMBER	1	2	3	4
EQUIP CONXION	FR 0 TO 1	FR 1 TO 3	FR 0 TO 2	FR 2 TO 3 FR
VAPOR FRACTION	1.0000	0.0000	0.0000	0.0000
TEMPERATURE, F	-25.7978	0.0000	-59.9618	0.0000
PRESSURE, PSIA	199.9979	0.0000	599.9934	0.0000
ENTHALPY, K.BTU	179.4818	0.0000	533.8254	0.0000

COMPOSITION, LB-MOLES/UNIT TIME

CO2	0.02052	0.00000	0.08808	0.00000
NITROGEN	0.14913	0.00000	0.14913	0.00000
METHANE	28.48314	0.00000	28.81215	0.00000
ETHANE	3.63050	0.00000	20.12111	0.00000
PROPANE	0.92711	0.00000	25.00037	0.00000
I-BUTANE	0.03843	0.00000	2.83448	0.00000
N-BUTANE	0.08968	0.00000	10.23009	0.00000
I-PENTANE	0.00831	0.00000	2.22600	0.00000
N-PENTANE	0.00610	0.00000	2.39818	0.00000
N-HEPTANE	0.00100	0.00000	3.59221	0.00000

TOTAL	33.35390	0.00000	95.45181	0.00000

STREAM NUMBER	5	6	7	8
EQUIP CONXION	FR 3 TO 4	FR 4 TO 5	FR 5 TO 6	FR 6 TO 0 FR
VAPOR FRACTION	0.0000	0.0000	0.0000	0.0000
TEMPERATURE, F	0.0000	0.0000	0.0000	0.0000
PRESSURE, PSIA	0.0000	0.0000	0.0000	0.0000
ENTHALPY, K.BTU	0.0000	0.0000	0.0000	0.0000

COMPOSITION, LB-MOLES/UNIT TIME

CO2	0.00000	0.00000	0.00000	0.00000
NITROGEN	0.00000	0.00000	0.00000	0.00000
METHANE	0.00000	0.00000	0.00000	0.00000
ETHANE	0.00000	0.00000	0.00000	0.00000
PROPANE	0.00000	0.00000	0.00000	0.00000
I-BUTANE	0.00000	0.00000	0.00000	0.00000
N-BUTANE	0.00000	0.00000	0.00000	0.00000
I-PENTANE	0.00000	0.00000	0.00000	0.00000
N-PENTANE	0.00000	0.00000	0.00000	0.00000
N-HEPTANE	0.00000	0.00000	0.00000	0.00000

TOTAL	0.00000	0.00000	0.00000	0.00000

STREAM NUMBER	9	10
EQUIP CONXION	FR 5 TO 7	FR 7 TO 0 FR
VAPOR FRACTION	0.0000	0.0000
TEMPERATURE, F	0.0000	0.0000
PRESSURE, PSIA	0.0000	0.0000
ENTHALPY, K.BTU	0.0000	0.0000

COMPOSITION, LB-MOLES/UNIT TIME

CO2	0.00000	0.00000
NITROGEN	0.00000	0.00000
METHANE	0.00000	0.00000
ETHANE	0.00000	0.00000
PROPANE	0.00000	0.00000
I-BUTANE	0.00000	0.00000
N-BUTANE	0.00000	0.00000
I-PENTANE	0.00000	0.00000
N-PENTANE	0.00000	0.00000
N-HEPTANE	0.00000	0.00000

TOTAL	0.00000	0.00000

FOLLOWING TABLES TRACE THE CHANGES IN THE THERMODYNAMIC PROPERTIES.

THE STREAM CONDITIONS AT THE OUTLET OF EACH EQUIPMENT NODE ARE TABULATED

IN CASES OF TWO-PHASE CONDITIONS, THE SECOND

PHASE CONDITIONS ARE REPORTED

SOME UNCALCULATED VALUES ARE REPORTED AS ZERO

UNITS ARE :GM.MOLE CALORIES OK ATM CC

ID = STANDARD COMPONENT IDENTIFICATION # OF CHESS
X, Y = LIQUID AND VAPOR COMPOSITIONS
FUG, GAMA= FUGACITY AND ACTIVITY COEFFICIENTS
K = EQUILIBRIUM RATIOS
VP= VAPOR PRESSURES VIA ANTOINE EQN.
VZ= COMP. FACTOR FOR COMPONENTS
M.VOL= MOLAL VOLUMES

****
STREAM NUMBER 2
****

TEMPERATURE : 225.000 PRESSURE : 28.2390 VAPOR FRACTION : 1.0000

ID	X	Y	FUG	GAMA	K	VP	VZ	M.VOL
49	0.00000	0.00062	0.00000	0.00000	0.00000	8.6173	0.0000	84.3288
46	0.00000	0.00447	0.00000	0.00000	0.00000	277.3489	0.0000	42.4503
2	0.00000	0.85397	0.00000	0.00000	0.00000	87.2802	0.0000	46.1448
3	0.00000	0.10885	0.00000	0.00000	0.00000	5.8046	0.0000	130.3393
4	0.00000	0.02780	0.00000	0.00000	0.00000	0.7580	0.0000	168.7855
5	0.00000	0.00115	0.00000	0.00000	0.00000	0.1844	0.0000	209.0497
6	0.00000	0.00269	0.00000	0.00000	0.00000	0.1041	0.0000	204.5101
7	0.00000	0.00025	0.00000	0.00000	0.00000	0.0124	0.0000	241.3936
8	0.00000	0.00018	0.00000	0.00000	0.00000	0.0305	0.0000	242.1529
11	0.00000	0.00003	0.00000	0.00000	0.00000	0.0003	0.0000	318.4167

TOTAL MOLAR FLOWRATE : 15129.00000
ENTHALPY : VAPOR -&- LIQUID 2797.5112000 0.0000000
ENTHALPY DEPARTURE :VAPOR -&- LIQUID -104.41481 0.00000
ENTROPY DEPARTURE :VAPOR -&- LIQUID -0.6116470 -6.9270887
VAP/LIQ/2ND PHASE MIX. COMPRESSIBILITY FACTOR : 0.783710

****
STREAM NUMBER 4
****

TEMPERATURE : 221.565 PRESSURE : 28.2390 VAPOR FRACTION : 0.0000

ID	X	Y	FUG	GAMA	K	VP	VZ	M.VOL
49	0.00092	0.00000	0.00000	0.00000	0.00000	7.1817	0.0000	83.9549
46	0.00156	0.00000	0.00000	0.00000	0.00000	267.3669	0.0000	42.4435
2	0.30165	0.00000	0.00000	0.00000	0.00000	82.5111	0.0000	46.1219
3	0.21080	0.00000	0.00000	0.00000	0.00000	5.2313	0.0000	129.7704
4	0.26192	0.00000	0.00000	0.00000	0.00000	0.6593	0.0000	168.0628
5	0.02970	0.00000	0.00000	0.00000	0.00000	0.1564	0.0000	208.2006
6	0.10718	0.00000	0.00000	0.00000	0.00000	0.0873	0.0000	203.6839
7	0.02332	0.00000	0.00000	0.00000	0.00000	0.0100	0.0000	240.4371
8	0.02512	0.00000	0.00000	0.00000	0.00000	0.0248	0.0000	241.1901
11	0.03763	0.00000	0.00000	0.00000	0.00000	0.0002	0.0000	317.1748

TOTAL MOLAR FLOWRATE : 43296.00000
ENTHALPY : VAPOR -&- LIQUID 0.0000000 3083.8850000
ENTHALPY DEPARTURE :VAPOR -&- LIQUID 0.00000 -534.65258
ENTROPY DEPARTURE :VAPOR -&- LIQUID -7.6318169 -7.6318169
VAP/LIQ/2ND PHASE MIX. COMPRESSIBILITY FACTOR : 0.101947

****
STREAM NUMBER 5
****

TEMPERATURE : 225.320 PRESSURE : 28.2390 VAPOR FRACTION : 0.1611

ID	X	Y	FUG	GAMA	K	VP	VZ	M.VOL
49	0.00086	0.00071	0.75842	0.67738	0.89314	8.7881	0.0000	41.5669
46	0.00114	0.01326	0.98845	12.49164	12.63754	278.4453	0.0000	42.5319
2	0.34074	0.90844	0.85926	2.48076	2.88708	87.8097	0.0000	46.3917
3	0.21956	0.06264	0.64957	0.20069	0.30896	5.8698	0.0000	64.9616
4	0.23967	0.01328	0.51296	0.03077	0.05999	0.7694	0.0000	179.8676
5	0.02656	0.00048	0.42433	0.00822	0.01938	0.1877	0.0000	222.4328
6	0.09539	0.00107	0.40640	0.00495	0.01218	0.1061	0.0000	217.5286
7	0.02065	0.00007	0.33451	0.00122	0.00364	0.0127	0.0000	256.4563
8	0.02222	0.00005	0.31908	0.00078	0.00246	0.0311	0.0000	257.3115
11	0.03321	0.00000	0.19687	0.00002	0.00012	0.0003	0.0000	337.9641

TOTAL MOLAR FLOWRATE : 58425.00000
ENTHALPY : VAPOR -&- LIQUID 2646.2861000 3079.4807000
ENTHALPY DEPARTURE :VAPOR -&- LIQUID -533.40551 -533.40551
ENTROPY DEPARTURE :VAPOR -&- LIQUID -7.4981556 -7.4981556
VAP/LIQ/2ND PHASE MIX. COMPRESSIBILITY FACTOR : 0.099084

****
STREAM NUMBER 6
****

TEMPERATURE : 222.526 PRESSURE : 20.4140 VAPOR FRACTION : 0.2499

ID	X	Y	FUG	GAMA	K	VP	VZ	M.VOL

49	0.00112	0.00108	0.81586	0.86710	1.06280	7.3906	0.0000	84.3696
46	0.00050	0.00841	0.98832	18.24341	18.45900	268.9143	0.0000	42.4510
2	0.26288	0.89879	0.89294	3.36363	3.76692	83.2442	0.0000	46.1472
3	0.24569	0.07590	0.72799	0.24777	0.34035	5.3177	0.0000	130.4012
4	0.26820	0.01423	0.61232	0.03580	0.05847	0.6740	0.0000	168.8621
5	0.02972	0.00047	0.53264	0.00926	0.01739	0.1606	0.0000	209.1425
6	0.10675	0.00102	0.51626	0.00544	0.01054	0.0897	0.0000	204.6002
7	0.02311	0.00006	0.44748	0.00129	0.00289	0.0103	0.0000	241.4980
8	0.02487	0.00004	0.43229	0.00082	0.00189	0.0256	0.0000	242.2577
11	0.03717	0.00000	0.30324	0.00002	0.00007	0.0002	0.0000	318.5522

TOTAL MOLAR FLOWRATE : 58425.00000
ENTHALPY : VAPOR -&- LIQUID 2645.2377000 3131.1689000
ENTHALPY DEPARTURE :VAPOR -&- LIQUID -551.38623 -551.38623
ENTROPY DEPARTURE :VAPOR -&- LIQUID -8.2840776 -8.2840776
VAP/LIQ/2ND PHASE MIX. COMPRESSIBILITY FACTOR : 0.074068

****
STREAM NUMBER 7
****

TEMPERATURE : 222.526 PRESSURE : 20.4140 VAPOR FRACTION : 1.0000

ID	X	Y	FUG	GAMA	K	VP	VZ	M.VOL
49	0.00000	0.00108	0.00000	0.00000	0.00000	7.3906	0.0000	84.0132
46	0.00000	0.00841	0.00000	0.00000	0.00000	268.9143	0.0000	42.4446
2	0.00000	0.89879	0.00000	0.00000	0.00000	83.2442	0.0000	46.1256
3	0.00000	0.07590	0.00000	0.00000	0.00000	5.3177	0.0000	129.8591
4	0.00000	0.01423	0.00000	0.00000	0.00000	0.6740	0.0000	168.1925
5	0.00000	0.00047	0.00000	0.00000	0.00000	0.1606	0.0000	208.3332
6	0.00000	0.00102	0.00000	0.00000	0.00000	0.0897	0.0000	203.8126
7	0.00000	0.00006	0.00000	0.00000	0.00000	0.0103	0.0000	240.5863
8	0.00000	0.00004	0.00000	0.00000	0.00000	0.0256	0.0000	241.3404
11	0.00000	0.00000	0.00000	0.00000	0.00000	0.0002	0.0000	317.3684

TOTAL MOLAR FLOWRATE : 14596.64000
ENTHALPY : VAPOR -&- LIQUID 2645.2392000 3131.1672000
ENTHALPY DEPARTURE :VAPOR -&- LIQUID -551.38623 -551.38623
ENTROPY DEPARTURE :VAPOR -&- LIQUID -8.2840700 -8.2840700
VAP/LIQ/2ND PHASE MIX. COMPRESSIBILITY FACTOR : 0.074068

****
STREAM NUMBER 9
****

TEMPERATURE : 222.526 PRESSURE : 20.4140 VAPOR FRACTION : 0.0000

ID	X	Y	FUG	GAMA	K	VP	VZ	M.VOL
49	0.00112	0.00000	0.00000	0.00000	0.00000	7.3906	0.0000	84.0132
46	0.00050	0.00000	0.00000	0.00000	0.00000	268.9143	0.0000	42.4446
2	0.26288	0.00000	0.00000	0.00000	0.00000	83.2442	0.0000	46.1256

3	0.24569	0.00000	0.00000	0.00000	0.00000	5.3177	0.0000	129.8591
4	0.26820	0.00000	0.00000	0.00000	0.00000	0.6740	0.0000	168.1925
5	0.02972	0.00000	0.00000	0.00000	0.00000	0.1606	0.0000	208.3332
6	0.10675	0.00000	0.00000	0.00000	0.00000	0.0897	0.0000	203.8126
7	0.02311	0.00000	0.00000	0.00000	0.00000	0.0103	0.0000	240.5863
8	0.02487	0.00000	0.00000	0.00000	0.00000	0.0256	0.0000	241.3404
11	0.03717	0.00000	0.00000	0.00000	0.00000	0.0002	0.0000	317.3684

```
TOTAL MOLAR FLOWRATE :          43828.35500
ENTHALPY  : VAPOR -&- LIQUID         2645.2392000        3131.1672000
ENTHALPY DEPARTURE  :VAPOR -&- LIQUID          -551.38623          -551.38623
ENTROPY  DEPARTURE  :VAPOR -&- LIQUID          -8.2840700          -8.2840700
VAP/LIQ/2ND PHASE MIX. COMPRESSIBILITY FACTOR :  0.074068
```

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****************************************
          STREAM  NUMBER   8
****************************************
```

TEMPERATURE : 129.863 PRESSURE : 3.2023 VAPOR FRACTION : 1.0000

ID	X	Y	FUG	GAMA	K	VP	VZ	M.VOL
49	0.00000	0.00108	0.00000	0.00000	0.00000	7.3906	0.0000	84.0132
46	0.00000	0.00841	0.00000	0.00000	0.00000	268.9143	0.0000	42.4446
2	0.00000	0.89878	0.00000	0.00000	0.00000	83.2442	0.0000	46.1256
3	0.00000	0.07590	0.00000	0.00000	0.00000	5.3177	0.0000	129.8591
4	0.00000	0.01423	0.00000	0.00000	0.00000	0.6740	0.0000	168.1925
5	0.00000	0.00047	0.00000	0.00000	0.00000	0.1606	0.0000	208.3332
6	0.00000	0.00102	0.00000	0.00000	0.00000	0.0897	0.0000	203.8126
7	0.00000	0.00006	0.00000	0.00000	0.00000	0.0103	0.0000	240.5863
8	0.00000	0.00004	0.00000	0.00000	0.00000	0.0256	0.0000	241.3404
11	0.00000	0.00000	0.00000	0.00000	0.00000	0.0002	0.0000	317.3684

```
TOTAL MOLAR FLOWRATE :          14596.64000
ENTHALPY  : VAPOR -&- LIQUID         2138.9807000          0.0000000
ENTHALPY DEPARTURE  :VAPOR -&- LIQUID          -24.28484             0.00000
ENTROPY  DEPARTURE  :VAPOR -&- LIQUID          -0.2058045          -8.2840700
VAP/LIQ/2ND PHASE MIX. COMPRESSIBILITY FACTOR :  0.911230
```

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****************************************
          STREAM  NUMBER  10
****************************************
```

TEMPERATURE : 222.093 PRESSURE : 34.0230 VAPOR FRACTION : 0.0000

ID	X	Y	FUG	GAMA	K	VP	VZ	M.VOL
49	0.00112	0.00000	0.00000	0.00000	0.00000	7.3906	0.0000	84.0132
46	0.00050	0.00000	0.00000	0.00000	0.00000	268.9143	0.0000	42.4446
2	0.26268	0.00000	0.00000	0.00000	0.00000	83.2442	0.0000	46.1256
3	0.24569	0.00000	0.00000	0.00000	0.00000	5.3177	0.0000	129.8591
4	0.26820	0.00000	0.00000	0.00000	0.00000	0.6740	0.0000	168.1925
5	0.02972	0.00000	0.00000	0.00000	0.00000	0.1606	0.0000	208.3332
6	0.10675	0.00000	0.00000	0.00000	0.00000	0.0897	0.0000	203.8126

7	0.02311	0.00000	0.00000	0.00000	0.00000	0.0103	0.0000	240.5863
8	0.02487	0.00000	0.00000	0.00000	0.00000	0.0256	0.0000	241.3404
11	0.03717	0.00000	0.00000	0.00000	0.00000	0.0002	0.0000	317.3684

TOTAL MOLAR FLOWRATE : 43828.35500
ENTHALPY : VAPOR -&- LIQUID 0.0000000 3146.6166000
ENTHALPY DEPARTURE :VAPOR -&- LIQUID 0.00000 -529.57519
ENTROPY DEPARTURE :VAPOR -&- LIQUID -7.3126326 -7.3126326
VAP/LIQ/2ND PHASE MIX. COMPRESSIBILITY FACTOR : 0.123004

*** SUBSET LOOP COMPLETE ***

FINAL RESULTS

CHESS3 ... TEST CASE FOR ROTATIONAL EQUIPMENTS

STREAM NUMBER	1	2	3	4	
EQUIP CONXION	FR 0 TO 1	FR 1 TO 3	FR 0 TO 2	FR 2 TO 3	FR
VAPOR FRACTION	1.0000	1.0000	0.0000	0.0000	
TEMPERATURE, F	-25.7978	-54.6879	-59.9618	-60.8703	
PRESSURE, PSIA	199.9979	415.0000	599.9934	415.0002	
ENTHALPY, K.BTU	179.4818	167.8440	533.8254	529.5044	
	COMPOSITION, LB-MOLES/UNIT TIME				
CO2	0.02052	0.02052	0.08808	0.08808	
NITROGEN	0.14913	0.14913	0.14913	0.14913	
METHANE	28.48314	28.48314	28.81215	28.81215	
ETHANE	3.63050	3.63050	20.12111	20.12111	
PROPANE	0.92711	0.92711	25.00037	25.00037	
I-BUTANE	0.03843	0.03843	2.83448	2.83448	
N-BUTANE	0.08968	0.08968	10.23009	10.23009	
I-PENTANE	0.00831	0.00831	2.22600	2.22600	
N-PENTANE	0.00610	0.00610	2.39818	2.39818	
N-HEPTANE	0.00100	0.00100	3.59221	3.59221	

TOTAL	33.35390	33.35390	95.45181	95.45181	

STREAM NUMBER	5	6	7	8	
EQUIP CONXION	FR 3 TO 4	FR 4 TO 5	FR 5 TO 6	FR 6 TO 0	FR
VAPOR FRACTION	0.1611	0.2498	1.0000	1.0000	
TEMPERATURE, F	-54.1116	-59.1410	-59.1410	-225.9336	
PRESSURE, PSIA	415.0000	300.0042	300.0042	47.0610	
ENTHALPY, K.BTU	697.3484	697.3481	153.1234	123.8179	
	COMPOSITION, LB-MOLES/UNIT TIME				
CO2	0.10860	0.10860	0.03844	0.03844	
NITROGEN	0.29826	0.29826	0.29826	0.29826	
METHANE	57.29530	57.29530	31.88199	31.88199	
ETHANE	23.75160	23.75160	2.69223	2.69223	
PROPANE	25.92747	25.92747	0.50487	0.50487	
I-BUTANE	2.87291	2.87291	0.01664	0.01664	
N-BUTANE	10.31976	10.31976	0.03624	0.03624	
I-PENTANE	2.23431	2.23431	0.00215	0.00215	
N-PENTANE	2.40429	2.40429	0.00151	0.00151	
N-HEPTANE	3.59321	3.59321	0.00009	0.00009	

TOTAL	128.80571	128.80571	32.18024	32.18024	

STREAM NUMBER	9	10	
EQUIP CONXION	FR 5 TO 7	FR 7 TO 0	FR
VAPOR FRACTION	0.0000	0.0000	
TEMPERATURE, F	-59.1410	-59.9213	
PRESSURE, PSIA	300.0042	500.0017	
ENTHALPY, K.BTU	544.2334	546.9187	

COMPOSITION, LB-MOLES/UNIT TIME

CO2	0.10860	0.10860
NITROGEN	0.04852	0.04852
METHANE	25.41331	25.41331
ETHANE	23.75160	23.75160
PROPANE	25.92746	25.92746
I-BUTANE	2.87291	2.87291
N-BUTANE	10.31974	10.31974
I-PENTANE	2.23431	2.23431
N-PENTANE	2.40429	2.40429
N-HEPTANE	3.59320	3.59320

TOTAL	96.62546	96.62546

```
CHESS3 ... TEST CASE FOR ROTATIONAL EQUIPMENTS


=============================
SUMMARY OF ENERGY REQUIREMENTS:
=============================


------------------------------------------------------

UNIT NUMBER =    1
COMPRESSOR
NUMBER OF STAGES =     1
COMPRESSION RATIO PER STAGE =    2.075
BREAK HORSEPOWER =       10.611
STAGE   DISCHARGE TEMP. ,DEG F  HEAT EXCH.DUTY: K-BTU
  1                     57.6                  34.694
------------------------------------------------------
------------------------------------------------------

UNIT NUMBER =    2
HYDRAULIC TURBINE
RECOVERABLE HORSEPOWER =        1.698
------------------------------------------------------
------------------------------------------------------

UNIT NUMBER =    6
GAS EXPANDER
RECOVERABLE HORSEPOWER =       11.514
------------------------------------------------------
------------------------------------------------------

UNIT NUMBER =    7
PUMP
BREAK HORSEPOWER =        4.220
------------------------------------------------------
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THE OUTPUTS FROM THE CHAO-SEADER : SRK MODEL

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*** ***  CHESS FLOW SHEET SIMULATION  *** ***
             VERSION  THREE
              JUNE 1985

 CHESS3 ... TEST CASE FOR ROTATIONAL EQUIPMENTS
     10         4         3         0         0         0

     49        46         2         3         4         5         6         7
      8        11

      7         6         2         4         1

BEGIN NETWORK READ
    1         COMP       U-1      1   -2    0    0    0    0    0
    2         HYTR       U-2      3   -4    0    0    0    0    0
    3         MIXR       U-3      2    4   -5    0    0    0    0
    4         VALV       U-4      5   -6    0    0    0    0    0
    5         ADBF       U-5      6   -7   -9    0    0    0    0
    6         GSXP       U-6      7   -8    0    0    0    0    0
    7         PUMP       U-7      9  -10    0    0    0    0    0
NETWORK COMPLETE

BEGIN EQUIPMENT DATA READ
      3         0         0         0         0         0         0         0
      0         0         0         0         0         0         0         0
      0         0         0         0         0         0         0         0
      0         0         0         0         0         0         0         0
      0         0         0         0         0         0         0         0
      0         0         0         0         0         0         0         0
      0         0

     1.0000        28.239        225.00        0.85000       3.0000       0.00000
     0.00000       0.00000       0.00000       0.00000       0.00000      0.00000
     0.00000       0.00000       0.00000       0.00000       0.00000      0.00000
     0.00000       0.00000       0.00000       0.00000       0.00000      0.00000
     0.00000

     2.0000        28.239        0.60000       0.00000       0.00000      0.00000
     0.00000       0.00000       0.00000       0.00000       0.00000      0.00000
     0.00000       0.00000       0.00000       0.00000       0.00000      0.00000
     0.00000       0.00000       0.00000       0.00000       0.00000      0.00000
     0.00000

     4.0000        20.414        0.00000       0.00000       0.00000      0.00000
     0.00000       0.00000       0.00000       0.00000       0.00000      0.00000
     0.00000       0.00000       0.00000       0.00000       0.00000      0.00000
     0.00000       0.00000       0.00000       0.00000       0.00000      0.00000
     0.00000

     5.0000        2.0000        0.00000       0.00000       0.00000      0.00000
     0.00000       0.00000       0.00000       0.00000       0.00000      0.00000
     0.00000       0.00000       0.00000       0.00000       0.00000      0.00000
     0.00000       0.00000       0.00000       0.00000       0.00000      0.00000
     0.00000

     6.0000        3.2023        0.60000       0.00000       0.00000      0.00000
     0.00000       0.00000       0.00000       0.00000       0.00000      0.00000
     0.00000       0.00000       0.00000       0.00000       0.00000      0.00000
     0.00000       0.00000       0.00000       0.00000       0.00000      0.00000
     0.00000

     7.0000        34.023        0.75000       0.00000       0.00000      0.00000
     0.00000       0.00000       0.00000       0.00000       0.00000      0.00000
```

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VAPOR-LIQUID EQUILIBRIUM DATA CODES:
    LIQUID =   4
    VAPOR =    3
    ENTHALPY = 0

LIQUID PHASE MODEL   : CHAO-SEADER EQN.

VAPOR PHASE MODEL    : SOAVE-REDLICH-KWONG EQN.

ENTHALPY CORRECTION : FOR BOTH PHASES.
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FOLLOWING TABLES TRACE THE CHANGES IN THE THERMODYNAMIC PROPERTIES.

THE STREAM CONDITIONS AT THE OUTLET OF EACH EQUIPMENT NODE ARE TABULATED

IN CASES OF TWO-PHASE CONDITIONS, THE SECOND

PHASE CONDITIONS ARE REPORTED

SOME UNCALCULATED VALUES ARE REPORTED AS ZERO

UNITS ARE :GM.MOLE CALORIES CK ATM CC

ID = STANDARD COMPONENT IDENTIFICATION # OF CHESS
X, Y = LIQUID AND VAPOR COMPOSITIONS
FUG, GAMA= FUGACITY AND ACTIVITY COEFFICIENTS
K = EQUILIBRIUM RATIOS
VP= VAPOR PRESSURES VIA ANTOINE EQN.
VZ= COMP. FACTOR FOR COMPONENTS
M.VOL= MOLAL VOLUMES

****
STREAM NUMBER 2
****

TEMPERATURE : 225.000 PRESSURE : 28.2390 VAPOR FRACTION : 1.0000

ID	X	Y	FUG	GAMA	K	VP	VZ	M.VOL
49	0.00000	0.00062	0.00000	0.00000	0.00000	8.6173	0.0000	84.3288
46	0.00000	0.00447	0.00000	0.00000	0.00000	277.3489	0.0000	42.4503
2	0.00000	0.85397	0.00000	0.00000	0.00000	87.2802	0.0000	46.1448
3	0.00000	0.10885	0.00000	0.00000	0.00000	5.8046	0.0000	130.3393
4	0.00000	0.02780	0.00000	0.00000	0.00000	0.7580	0.0000	168.7855
5	0.00000	0.00115	0.00000	0.00000	0.00000	0.1844	0.0000	209.0497
6	0.00000	0.00269	0.00000	0.00000	0.00000	0.1041	0.0000	204.5101
7	0.00000	0.00025	0.00000	0.00000	0.00000	0.0124	0.0000	241.3936
8	0.00000	0.00018	0.00000	0.00000	0.00000	0.0305	0.0000	242.1529
11	0.00000	0.00003	0.00000	0.00000	0.00000	0.0003	0.0000	318.4167

TOTAL MOLAR FLOWRATE : 15129.00000
ENTHALPY : VAPOR -&- LIQUID 2759.0117000 0.0000000
ENTHALPY DEPARTURE :VAPOR -&- LIQUID -142.91447 0.00000
ENTROPY DEPARTURE :VAPOR -&- LIQUID -0.4578047 -9.5337563
VAP/LIQ/2ND PHASE MIX. COMPRESSIBILITY FACTOR : 0.803780

****
STREAM NUMBER 4
****

TEMPERATURE : 220.848 PRESSURE : 28.2390 VAPOR FRACTION : 0.0000

ID	X	Y	FUG	GAMA	K	VP	VZ	M.VOL
49	0.00092	0.00000	0.00000	0.00000	0.00000	7.1817	0.0000	83.9549
46	0.00156	0.00000	0.00000	0.00000	0.00000	267.3669	0.0000	42.4435
2	0.30165	0.00000	0.00000	0.00000	0.00000	82.5111	0.0000	46.1219
3	0.21080	0.00000	0.00000	0.00000	0.00000	5.2313	0.0000	129.7704
4	0.26192	0.00000	0.00000	0.00000	0.00000	0.6593	0.0000	168.0828
5	0.02970	0.00000	0.00000	0.00000	0.00000	0.1564	0.0000	205.2006
6	0.10718	0.00000	0.00000	0.00000	0.00000	0.0873	0.0000	203.6839
7	0.02332	0.00000	0.00000	0.00000	0.00000	0.0100	0.0000	240.4371
8	0.02512	0.00000	0.00000	0.00000	0.00000	0.0248	0.0000	241.1901
11	0.03763	0.00000	0.00000	0.00000	0.00000	0.0002	0.0000	317.1748

TOTAL MOLAR FLOWRATE : 43296.00000
ENTHALPY : VAPOR -&- LIQUID 0.0000000 1305.7353000
ENTHALPY DEPARTURE :VAPOR -&- LIQUID 0.00000 -2303.47820
ENTROPY DEPARTURE :VAPOR -&- LIQUID -0.4578047 -9.5900469
VAP/LIQ/2ND PHASE MIX. COMPRESSIBILITY FACTOR : 0.803780

****
STREAM NUMBER 5
****

TEMPERATURE : 232.012 PRESSURE : 28.2390 VAPOR FRACTION : 0.1453

ID	X	Y	FUG	GAMA	K	VP	VZ	M.VOL
49	0.00092	0.00030	0.75094	0.26776	0.35656	13.0815	0.0000	41.5669
46	0.01564	0.01454	0.99726	1.00000	1.00274	301.6074	0.0000	42.5319
2	0.34767	0.89761	0.88713	2.47082	2.78519	99.2507	0.0000	46.3917
3	0.21238	0.06946	0.69367	0.24474	0.35282	7.3593	0.0000	64.9616
4	0.23183	0.01564	0.56464	0.04109	0.07277	1.0413	0.0000	179.8676
5	0.02569	0.00067	0.47894	0.01349	0.02817	0.2679	0.0000	222.4328
6	0.09227	0.00154	0.46068	0.00830	0.01802	0.1555	0.0000	217.5286
7	0.01998	0.00013	0.38888	0.00268	0.00690	0.0202	0.0000	256.4563
8	0.02150	0.00010	0.37304	0.00179	0.00480	0.0484	0.0000	257.3115
11	0.03213	0.00001	0.24465	0.00012	0.00050	0.0006	0.0000	337.9641

TOTAL MOLAR FLOWRATE : 58425.00000
ENTHALPY : VAPOR -&- LIQUID 2679.2937000 1512.4895000
ENTHALPY DEPARTURE :VAPOR -&- LIQUID -90.07259 -2166.84590
ENTROPY DEPARTURE :VAPOR -&- LIQUID -0.2698736 -6.7585056
VAP/LIQ/2ND PHASE MIX. COMPRESSIBILITY FACTOR : 0.879844

****
STREAM NUMBER 6
****

TEMPERATURE : 230.926 PRESSURE : 20.4140 VAPOR FRACTION : 0.2363

ID	X	Y	FUG	GAMA	K	VP	VZ	M.VOL

49	0.00110	0.00042	0.81369	0.34865	0.42848	12.2830	0.0000	39.6814
46	0.00958	0.00864	0.99594	1.00000	1.00408	297.8186	0.0000	42.4655
2	0.27150	0.88026	0.91627	3.31001	3.61248	97.3460	0.0000	46.1944
3	0.23978	0.08934	0.76843	0.31899	0.41513	7.1010	0.0000	61.9413
4	0.26175	0.01867	0.66303	0.05271	0.07949	0.9928	0.0000	170.4525
5	0.02900	0.00074	0.58912	0.01683	0.02857	0.2533	0.0000	211.0644
6	0.10418	0.00169	0.57305	0.01035	0.01805	0.1464	0.0000	206.4701
7	0.02256	0.00013	0.50743	0.00328	0.00647	0.0187	0.0000	243.6625
8	0.02427	0.00010	0.49255	0.00219	0.00444	0.0452	0.0000	244.4359
11	0.03627	0.00001	0.36339	0.00014	0.00039	0.0006	0.0000	321.3623

TOTAL MOLAR FLOWRATE : 58425.00000
ENTHALPY : VAPOR -&- LIQUID 2697.7580000 1364.2783000
ENTHALPY DEPARTURE :VAPOR -&- LIQUID -64.98239 -2411.48950
ENTROPY DEPARTURE :VAPOR -&- LIQUID -0.1899433 -7.5454512
VAP/LIQ/2ND PHASE MIX. COMPRESSIBILITY FACTOR : 0.912498

****
STREAM NUMBER 7
****

TEMPERATURE : 230.926 PRESSURE : 20.4140 VAPOR FRACTION : 1.0000

ID	X	Y	FUG	GAMA	K	VP	VZ	M.VOL
49	0.00000	0.00042	0.00000	0.00000	0.00000	12.2829	0.0000	39.5681
46	0.00000	0.00864	0.00000	0.00000	0.00000	297.8184	0.0000	42.4632
2	0.00000	0.88026	0.00000	0.00000	0.00000	97.3458	0.0000	46.1872
3	0.00000	0.08934	0.00000	0.00000	0.00000	7.1010	0.0000	61.7572
4	0.00000	0.01867	0.00000	0.00000	0.00000	0.9927	0.0000	170.1956
5	0.00000	0.00074	0.00000	0.00000	0.00000	0.2533	0.0000	210.7541
6	0.00000	0.00169	0.00000	0.00000	0.00000	0.1464	0.0000	206.1680
7	0.00000	0.00013	0.00000	0.00000	0.00000	0.0187	0.0000	243.3131
8	0.00000	0.00010	0.00000	0.00000	0.00000	0.0452	0.0000	244.0842
11	0.00000	0.00001	0.00000	0.00000	0.00000	0.0006	0.0000	320.9087

TOTAL MOLAR FLOWRATE : 13925.16000
ENTHALPY : VAPOR -&- LIQUID 2697.7578000 1364.2778000
ENTHALPY DEPARTURE :VAPOR -&- LIQUID -64.98260 -2411.48680
ENTROPY DEPARTURE :VAPOR -&- LIQUID -0.1899440 -7.5454388
VAP/LIQ/2ND PHASE MIX. COMPRESSIBILITY FACTOR : 0.912498

****
STREAM NUMBER 0
****

TEMPERATURE : 230.926 PRESSURE : 20.4140 VAPOR FRACTION : 0.0000

ID	X	Y	FUG	GAMA	K	VP	VZ	M.VOL
49	0.00110	0.00000	0.00000	0.00000	0.00000	12.2829	0.0000	39.5681
46	0.00958	0.00000	0.00000	0.00000	0.00000	297.8184	0.0000	42.4632
2	0.27150	0.00000	0.00000	0.00000	0.00000	97.3458	0.0000	46.1872

3	0.23978	0.00000	0.00000	0.00000	0.00000	7.1010	0.0000	61.7572
4	0.26175	0.00000	0.00000	0.00000	0.00000	0.9927	0.0000	170.1958
5	0.02900	0.00000	0.00000	0.00000	0.00000	0.2533	0.0000	210.7541
6	0.10418	0.00000	0.00000	0.00000	0.00000	0.1464	0.0000	206.1680
7	0.02256	0.00000	0.00000	0.00000	0.00000	0.0187	0.0000	243.3131
8	0.02427	0.00000	0.00000	0.00000	0.00000	0.0452	0.0000	244.0842
11	0.03627	0.00000	0.00000	0.00000	0.00000	0.0006	0.0000	320.9087

TOTAL MOLAR FLOWRATE : 44499.83500
ENTHALPY : VAPOR -&- LIQUID 2697.7578000 1364.2778000
ENTHALPY DEPARTURE :VAPOR -&- LIQUID -64.98260 -2411.48680
ENTROPY DEPARTURE :VAPOR -&- LIQUID -0.1899440 -7.5454383
VAP/LIQ/2ND PHASE MIX. COMPRESSIBILITY FACTOR : 0.912498

****
STREAM NUMBER 8
****

TEMPERATURE : 136.466 PRESSURE : 3.2023 VAPOR FRACTION : 1.0000

ID	X	Y	FUG	GAMA	K	VP	VZ	M.VOL
49	0.00000	0.00042	0.00000	0.00000	0.00000	12.2829	0.0000	39.5681
46	0.00000	0.00864	0.00000	0.00000	0.00000	297.8184	0.0000	42.4632
2	0.00000	0.88026	0.00000	0.00000	0.00000	97.3458	0.0000	46.1872
3	0.00000	0.08934	0.00000	0.00000	0.00000	7.1010	0.0000	61.7572
4	0.00000	0.01867	0.00000	0.00000	0.00000	0.9927	0.0000	170.1958
5	0.00000	0.00074	0.00000	0.00000	0.00000	0.2533	0.0000	210.7535
6	0.00000	0.00169	0.00000	0.00000	0.00000	0.1464	0.0000	206.1680
7	0.00000	0.00013	0.00000	0.00000	0.00000	0.0187	0.0000	243.3129
8	0.00000	0.00010	0.00000	0.00000	0.00000	0.0452	0.0000	244.0842
11	0.00000	0.00001	0.00000	0.00000	0.00000	0.0006	0.0000	320.9087

TOTAL MOLAR FLOWRATE : 13925.16000
ENTHALPY : VAPOR -&- LIQUID 2186.3720000 0.0000000
ENTHALPY DEPARTURE :VAPOR -&- LIQUID -35.85309 0.00000
ENTROPY DEPARTURE :VAPOR -&- LIQUID -0.1619433 -7.5454388
VAP/LIQ/2ND PHASE MIX. COMPRESSIBILITY FACTOR : 0.922442

****
STREAM NUMBER 10
****

TEMPERATURE : 209.600 PRESSURE : 34.0230 VAPOR FRACTION : 0.0000

ID	X	Y	FUG	GAMA	K	VP	VZ	M.VOL
49	0.00110	0.00000	0.00000	0.00000	0.00000	12.2829	0.0000	39.5681
46	0.00958	0.00000	0.00000	0.00000	0.00000	297.8184	0.0000	42.4632
2	0.27150	0.00000	0.00000	0.00000	0.00000	97.3458	0.0000	46.1872
3	0.23978	0.00000	0.00000	0.00000	0.00000	7.1010	0.0000	61.7572
4	0.26175	0.00000	0.00000	0.00000	0.00000	0.9927	0.0000	170.1958
5	0.02900	0.00000	0.00000	0.00000	0.00000	0.2533	0.0000	210.7535
6	0.10418	0.00000	0.00000	0.00000	0.00000	0.1464	0.0000	206.1680

7	0.02256	0.00000	0.00000	0.00000	0.00000	0.0187	0.0000	243.3129
8	0.02427	0.00000	0.00000	0.00000	0.00000	0.0452	0.0000	244.0842
11	0.03627	0.00000	0.00000	0.00000	0.00000	0.0006	0.0000	320.9087

TOTAL MOLAR FLOWRATE : 44499.83500
ENTHALPY : VAPOR -&- LIQUID 0.0000000 1377.9199000
ENTHALPY DEPARTURE :VAPOR -&- LIQUID 0.00000 -2114.99820
ENTROPY DEPARTURE :VAPOR -&- LIQUID -0.1619433 -9.9217310
VAP/LIQ/2ND PHASE MIX. COMPRESSIBILITY FACTOR : 0.922442

*** SUBSET LOOP COMPLETE ***

FINAL RESULTS

CHESS3 ... TEST CASE FOR ROTATIONAL EQUIPMENTS

STREAM NUMBER	1	2	3	4
EQUIP CONXION	FR 0 TO 1	FR 1 TO 3	FR 0 TO 2	FR 2 TO 3 FR
VAPOR FRACTION	1.0000	1.0000	0.0000	0.0000
TEMPERATURE, F	-25.7978	-54.6879	-59.9618	-62.1620
PRESSURE, PSIA	199.9979	415.0000	599.9934	415.0002
ENTHALPY, K.BTU	178.7560	165.5341	228.5163	224.1954
	COMPOSITION, LB-MOLES/UNIT TIME			
CO2	0.02052	0.02052	0.08808	0.08808
NITROGEN	0.14913	0.14913	0.14913	0.14913
METHANE	28.48314	28.48314	28.81215	28.81215
ETHANE	3.63050	3.63050	20.12111	20.12111
PROPANE	0.92711	0.92711	25.00037	25.00037
I-BUTANE	0.03843	0.03843	2.83448	2.83448
N-BUTANE	0.08968	0.08968	10.23009	10.23009
I-PENTANE	0.00831	0.00831	2.22600	2.22600
N-PENTANE	0.00610	0.00610	2.39818	2.39818
N-HEPTANE	0.00100	0.00100	3.59221	3.59221

TOTAL	33.35390	33.35390	95.45181	95.45181

STREAM NUMBER	5	6	7	8
EQUIP CONXION	FR 3 TO 4	FR 4 TO 5	FR 5 TO 6	FR 6 TO 0 FR
VAPOR FRACTION	0.1453	0.2383	1.0000	1.0000
TEMPERATURE, F	-42.0668	-44.0215	-44.0215	-214.0486
PRESSURE, PSIA	415.0000	300.0042	300.0042	47.0610
ENTHALPY, K.BTU	389.7292	389.7292	148.9796	120.7391
	COMPOSITION, LB-MOLES/UNIT TIME			
CO2	0.10860	0.10860	0.01456	0.01456
NITROGEN	0.29826	0.29826	0.29826	0.29826
METHANE	57.29530	57.29530	30.40161	30.40161
ETHANE	23.75160	23.75160	3.08541	3.08541
PROPANE	25.92747	25.92747	0.64495	0.64495
I-BUTANE	2.87291	2.87291	0.02568	0.02568
N-BUTANE	10.31976	10.31976	0.05830	0.05830
I-PENTANE	2.23431	2.23431	0.00452	0.00452
N-PENTANE	2.40429	2.40429	0.00334	0.00334
N-HEPTANE	3.59321	3.59321	0.00044	0.00044

TOTAL	128.80571	128.80571	30.69987	30.69987

STREAM NUMBER	9	10	
EQUIP CONXION	FR 5 TO 7	FR 7 TO 0	FR
VAPOR FRACTION	0.0000	0.0000	
TEMPERATURE, F	-44.0215	-82.4079	
PRESSURE, PSIA	300.0042	500.0017	
ENTHALPY, K.BTU	240.7603	243.1678	

COMPOSITION, LB-MOLES/UNIT TIME

CO2	0.10860	0.10860
NITROGEN	0.94928	0.94928
METHANE	26.89369	26.89369
ETHANE	23.75160	23.75160
PROPANE	25.92746	25.92746
I-BUTANE	2.87291	2.87291
N-BUTANE	10.31974	10.31974
I-PENTANE	2.23431	2.23431
N-PENTANE	2.40429	2.40429
N-HEPTANE	3.59321	3.59321

TOTAL	98.10583	98.10583

```
CHESS3 ... TEST CASE FOR ROTATIONAL EQUIPMENTS

==============================
SUMMARY OF ENERGY REQUIREMENTS:
==============================

------------------------------------------------------------
UNIT NUMBER =    1
COMPRESSOR
NUMBER OF STAGES =     1
COMPRESSION RATIO PER STAGE =   2.075
BREAK HORSEPOWER =       10.421
STAGE   DISCHARGE TEMP. ,DEG F   HEAT EXCH.DUTY: K-BTU
  1                   40.6                      30.826
------------------------------------------------------------
------------------------------------------------------------
UNIT NUMBER =    2
HYDRAULIC TURBINE
RECOVERABLE HORSEPOWER =        1.698
------------------------------------------------------------
------------------------------------------------------------
UNIT NUMBER =    6
GAS EXPANDER
RECOVERABLE HORSEPOWER =       11.096
------------------------------------------------------------
------------------------------------------------------------
UNIT NUMBER =    7
PUMP
BREAK HORSEPOWER =        3.784
------------------------------------------------------------
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THE OUTPUTS FROM THE CHAO-SEADER : RK MODEL

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 *** ***  CHESS FLOW SHEET SIMULATION  *** ***
              VERSION  THREE
                JUNE 1985

  CHESS3 ... TEST CASE FOR ROTATIONAL EQUIPMENTS
      10          4          2          0          0          0

      49         46          2          3          4          5          6          7
       8         11

       7          6          2          4          1

BEGIN NETWORK READ
   1       COMP     U-1     1   -2    0    0    0    0    0
   2       HYTR     U-2     3   -4    0    0    0    0    0
   3       MIXR     U-3     2    4   -5    0    0    0    0
   4       VALV     U-4     5   -6    0    0    0    0    0
   5       ADBF     U-5     6   -7   -9    0    0    0    0
   6       GSXP     U-6     7   -8    0    0    0    0    0
   7       PUMP     U-7     9  -10    0    0    0    0    0
NETWORK COMPLETE

BEGIN EQUIPMENT DATA READ
       3          0          0          0          0          0          0          0
       0          0          0          0          0          0          0          0
       0          0          0          0          0          0          0          0
       0          0          0          0          0          0          0          0
       0          0          0          0          0          0          0          0
       0          0          0          0          0          0          0          0
       0          0

     1.0000      28.239      225.00      0.85000      3.0000      0.00000
    0.00000     0.00000     0.00000      0.00000     0.00000      0.00000
    0.00000     0.00000     0.00000      0.00000     0.00000      0.00000
    0.00000     0.00000     0.00000      0.00000     0.00000      0.00000
    0.00000

     2.0000      28.239     0.60000      0.00000     0.00000      0.00000
    0.00000     0.00000     0.00000      0.00000     0.00000      0.00000
    0.00000     0.00000     0.00000      0.00000     0.00000      0.00000
    0.00000     0.00000     0.00000      0.00000     0.00000      0.00000
    0.00000

     4.0000      20.414     0.00000      0.00000     0.00000      0.00000
    0.00000     0.00000     0.00000      0.00000     0.00000      0.00000
    0.00000     0.00000     0.00000      0.00000     0.00000      0.00000
    0.00000     0.00000     0.00000      0.00000     0.00000      0.00000
    0.00000

     5.0000      2.0000     0.00000      0.00000     0.00000      0.00000
    0.00000     0.00000     0.00000      0.00000     0.00000      0.00000
    0.00000     0.00000     0.00000      0.00000     0.00000      0.00000
    0.00000     0.00000     0.00000      0.00000     0.00000      0.00000
    0.00000

     6.0000      3.2023     0.60000      0.00000     0.00000      0.00000
    0.00000     0.00000     0.00000      0.00000     0.00000      0.00000
    0.00000     0.00000     0.00000      0.00000     0.00000      0.00000
    0.00000     0.00000     0.00000      0.00000     0.00000      0.00000
    0.00000

     7.0000      34.023     0.75000      0.00000     0.00000      0.00000
    0.00000     0.00000     0.00000      0.00000     0.00000      0.00000
```

```
VAPOR-LIQUID EQUILIBRIUM DATA CODES:
    LIQUID =   4
    VAPOR =    2
    ENTHALPY = 0

LIQUID PHASE MODEL   : CHAO-SEADER EQN.

VAPOR PHASE MODEL    : REDLICH-KWONG EQN.

ENTHALPY CORRECTION  : FOR BOTH PHASES.
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FOLLOWING TABLES TRACE THE CHANGES IN THE THERMODYNAMIC PROPERTIES.

THE STREAM CONDITIONS AT THE OUTLET OF EACH EQUIPMENT NODE ARE TABULATED

IN CASES OF TWO-PHASE CONDITIONS, THE SECOND

PHASE CONDITIONS ARE REPORTED

SOME UNCALCULATED VALUES ARE REPORTED AS ZERO

UNITS ARE :GM.MOLE CALORIES OK ATM CC

ID = STANDARD COMPONENT IDENTIFICATION # OF CHESS
X, Y = LIQUID AND VAPOR COMPOSITIONS
FUG, GAMA= FUGACITY AND ACTIVITY COEFFICIENTS
K = EQUILIBRIUM RATIOS
VP= VAPOR PRESSURES VIA ANTOINE EQN.
VZ= COMP. FACTOR FOR COMPONENTS
M.VOL= MOLAL VOLUMES

****
STREAM NUMBER 2
****

TEMPERATURE : 225.000 PRESSURE : 28.2390 VAPOR FRACTION : 1.0000

ID	X	Y	FUG	GAMA	K	VP	VZ	M.VOL
49	0.00000	0.00062	0.00000	0.00000	0.00000	8.6173	1.0000	84.3288
46	0.00000	0.00447	0.00000	0.00000	0.00000	277.3489	1.0000	42.4503
2	0.00000	0.85397	0.00000	0.00000	0.00000	87.2802	1.0000	46.1448
3	0.00000	0.10885	0.00000	0.00000	0.00000	5.8046	1.0000	130.3393
4	0.00000	0.02780	0.00000	0.00000	0.00000	0.7580	1.0000	168.7655
5	0.00000	0.00115	0.00000	0.00000	0.00000	0.1844	1.0000	209.0497
6	0.00000	0.00269	0.00000	0.00000	0.00000	0.1041	1.0000	234.5101
7	0.00000	0.00025	0.00000	0.00000	0.00000	0.0124	1.0000	241.3936
8	0.00000	0.00018	0.00000	0.00000	0.00000	0.0305	1.0000	242.1529
11	0.00000	0.00003	0.00000	0.00000	0.00000	0.0003	1.0000	318.4167

TOTAL MOLAR FLOWRATE : 15129.00000
ENTHALPY : VAPOR -&- LIQUID 2634.0612000 0.0000000
ENTHALPY DEPARTURE :VAPOR -&- LIQUID -267.86499 0.00000
ENTROPY DEPARTURE :VAPOR -&- LIQUID -7.4649525 -9.5337563
VAP/LIQ/2ND PHASE MIX. COMPRESSIBILITY FACTOR : 0.804796

****
STREAM NUMBER 4
****

TEMPERATURE : 220.948 PRESSURE : 28.2390 VAPOR FRACTION : 0.0000

ID	X	Y	FUG	GAMA	K	VP	VZ	M.VOL
49	0.00092	0.00000	0.00000	0.00000	0.00000	7.1817	1.0000	83.9549
46	0.00156	0.00000	0.00000	0.00000	0.00000	267.3669	1.0000	42.4435
2	0.30185	0.00000	0.00000	0.00000	0.00000	82.5111	1.0000	46.1219
3	0.21080	0.00000	0.00000	0.00000	0.00000	5.2313	1.0000	129.7704
4	0.26192	0.00000	0.00000	0.00000	0.00000	0.6593	1.0000	168.0828
5	0.02970	0.00000	0.00000	0.00000	0.00000	0.1564	1.0000	208.2006
6	0.10718	0.00000	0.00000	0.00000	0.00000	0.0873	1.0000	203.6639
7	0.02332	0.00000	0.00000	0.00000	0.00000	0.0100	1.0000	240.4371
8	0.02512	0.00000	0.00000	0.00000	0.00000	0.0248	1.0000	241.1901
11	0.03763	0.00000	0.00000	0.00000	0.00000	0.0002	1.0000	317.1748

TOTAL MOLAR FLOWRATE : 43296.00000
ENTHALPY : VAPOR -&- LIQUID 0.0000000 1305.7353000
ENTHALPY DEPARTURE :VAPOR -&- LIQUID 0.00000 -2303.47820
ENTROPY DEPARTURE :VAPOR -&- LIQUID -7.4649525 -9.5900469
VAP/LIQ/2ND PHASE MIX. COMPRESSIBILITY FACTOR : 0.804796

****
STREAM NUMBER 5
****

TEMPERATURE : 230.883 PRESSURE : 28.2390 VAPOR FRACTION : 0.1401

ID	X	Y	FUG	GAMA	K	VP	VZ	M.VOL
49	0.00091	0.00029	0.75953	0.25751	0.33904	12.2525	1.0000	41.5669
46	0.01598	0.01514	0.98254	1.00000	1.01777	297.6702	1.0000	42.5319
2	0.35143	0.90043	0.88443	2.43460	2.75272	97.2717	1.0000	46.3917
3	0.21101	0.06707	0.69293	0.23665	0.34152	7.0910	1.0000	64.9616
4	0.23034	0.01480	0.56911	0.03929	0.06903	0.9909	1.0000	179.8676
5	0.02552	0.00063	0.48642	0.01283	0.02638	0.2527	1.0000	222.4325
6	0.09168	0.00143	0.47060	0.00787	0.01673	0.1461	1.0000	217.5286
7	0.01985	0.00012	0.40393	0.00253	0.00626	0.0187	1.0000	256.4563
8	0.02136	0.00009	0.39212	0.00168	0.00429	0.0450	1.0000	257.3115
11	0.03192	0.00001	0.27823	0.00011	0.00041	0.0006	1.0000	337.9641

TOTAL MOLAR FLOWRATE : 58425.00000
ENTHALPY : VAPOR -&- LIQUID 2573.9140000 1498.3305000
ENTHALPY DEPARTURE :VAPOR -&- LIQUID -181.65636 -2161.43280
ENTROPY DEPARTURE :VAPOR -&- LIQUID -7.1847095 -6.7553120
VAP/LIQ/2ND PHASE MIX. COMPRESSIBILITY FACTOR : 0.876312

****
STREAM NUMBER 6
****

TEMPERATURE : 229.836 PRESSURE : 20.4140 VAPOR FRACTION : 0.2348

ID	X	Y	FUG	GAMA	K	VP	VZ	M.VOL

49	0.00109	0.00040	0.82059	0.33561	0.40899	11.5235	1.0000	39.5635
46	0.00963	0.00881	0.93557	1.00000	1.01464	294.0264	1.0000	42.4631
2	0.27462	0.88404	0.91436	3.26266	3.56824	95.4525	1.0000	46.1669
3	0.23866	0.08649	0.76794	0.30868	0.40196	6.8483	1.0000	61.7497
4	0.26053	0.01777	0.66683	0.05044	0.07565	0.9458	1.0000	170.1657
5	0.02887	0.00070	0.59567	0.01603	0.02690	0.2393	1.0000	210.7419
6	0.10370	0.00158	0.58183	0.00982	0.01688	0.1377	1.0000	206.1562
7	0.02245	0.00012	0.52132	0.00310	0.00594	0.0174	1.0000	243.2993
8	0.02416	0.00009	0.51036	0.00206	0.00403	0.0421	1.0000	244.0704
11	0.03611	0.00001	0.39872	0.00013	0.00033	0.0005	1.0000	320.8906

TOTAL MOLAR FLOWRATE : 58425.00000
ENTHALPY : VAPOR -&- LIQUID 2624.6708000 1350.6262000
ENTHALPY DEPARTURE :VAPOR -&- LIQUID -129.75816 -2406.30150
ENTROPY DEPARTURE :VAPOR -&- LIQUID -6.3819580 -7.5506163
VAP/LIQ/2ND PHASE MIX. COMPRESSIBILITY FACTOR : 0.909762

****
STREAM NUMBER 7
****

TEMPERATURE : 229.836 PRESSURE : 20.4140 VAPOR FRACTION : 1.0000

ID	X	Y	FUG	GAMA	K	VP	VZ	M.VOL
49	0.00000	0.00040	0.00000	0.00000	0.00000	11.5235	1.0000	39.4467
46	0.00000	0.00881	0.00000	0.00000	0.00000	294.0266	1.0000	42.4609
2	0.00000	0.88404	0.00000	0.00000	0.00000	95.4527	1.0000	46.1797
3	0.00000	0.08649	0.00000	0.00000	0.00000	6.8483	1.0000	61.5596
4	0.00000	0.01777	0.00000	0.00000	0.00000	0.9458	1.0000	169.9375
5	0.00000	0.00070	0.00000	0.00000	0.00000	0.2393	1.0000	210.4419
6	0.00000	0.00158	0.00000	0.00000	0.00000	0.1377	1.0000	205.8643
7	0.00000	0.00012	0.00000	0.00000	0.00000	0.0174	1.0000	242.9614
8	0.00000	0.00009	0.00000	0.00000	0.00000	0.0421	1.0000	243.7303
11	0.00000	0.00001	0.00000	0.00000	0.00000	0.0005	1.0000	320.4519

TOTAL MOLAR FLOWRATE : 13716.37800
ENTHALPY : VAPOR -&- LIQUID 2624.6716000 1350.6276000
ENTHALPY DEPARTURE :VAPOR -&- LIQUID -129.75826 -2406.30100
ENTROPY DEPARTURE :VAPOR -&- LIQUID -6.3819580 -7.5506105
VAP/LIQ/2ND PHASE MIX. COMPRESSIBILITY FACTOR : 0.909762

****
STREAM NUMBER 9
****

TEMPERATURE : 229.836 PRESSURE : 20.4140 VAPOR FRACTION : 0.0000

ID	X	Y	FUG	GAMA	K	VP	VZ	M.VOL
49	0.00109	0.00000	0.00000	0.00000	0.00000	11.5235	1.0000	39.4467
46	0.00963	0.00000	0.00000	0.00000	0.00000	294.0266	1.0000	42.4609
2	0.27462	0.00000	0.00000	0.00000	0.00000	95.4527	1.0000	46.1797

3	0.23866	0.00000	0.00000	0.00000	0.00000	6.8483	1.0000	61.5596
4	0.26053	0.00000	0.00000	0.00000	0.00000	0.9458	1.0000	169.9375
5	0.02867	0.00000	0.00000	0.00000	0.00000	0.2393	1.0000	210.4419
6	0.10370	0.00000	0.00000	0.00000	0.00000	0.1377	1.0000	205.8643
7	0.02245	0.00000	0.00000	0.00000	0.00000	0.0174	1.0000	242.9614
8	0.02416	0.00000	0.00000	0.00000	0.00000	0.0421	1.0000	243.7303
11	0.03611	0.00000	0.00000	0.00000	0.00000	0.0005	1.0000	320.4519

TOTAL MOLAR FLOWRATE : 44706.61700
ENTHALPY : VAPOR -&- LIQUID 2624.6716000 1350.6276000
ENTHALPY DEPARTURE :VAPOR -&- LIQUID -129.75826 -2406.30100
ENTROPY DEPARTURE :VAPOR -&- LIQUID -6.3819580 -7.5506105
VAP/LIQ/2ND PHASE MIX. COMPRESSIBILITY FACTOR : 0.909762

****
STREAM NUMBER 9
****

TEMPERATURE : 111.803 PRESSURE : 3.2023 VAPOR FRACTION : 1.0000

ID	X	Y	FUG	GAMA	K	VP	VZ	M.VOL
49	0.00000	0.00040	0.00000	0.00000	0.00000	11.5235	1.0000	39.4467
46	0.00000	0.00881	0.00000	0.00000	0.00000	294.0266	1.0000	42.4609
2	0.00000	0.88434	0.00000	0.00000	0.00000	95.4527	1.0000	46.1797
3	0.00000	0.08649	0.00000	0.00000	0.00000	6.8483	1.0000	61.5597
4	0.00000	0.01777	0.00000	0.00000	0.00000	0.9458	1.0000	169.9375
5	0.00000	0.00070	0.00000	0.00000	0.00000	0.2393	1.0000	210.4419
6	0.00000	0.00158	0.00000	0.00000	0.00000	0.1377	1.0000	205.8643
7	0.00000	0.00012	0.00000	0.00000	0.00000	0.0174	1.0000	242.9614
8	0.00000	0.00009	0.00000	0.00000	0.00000	0.0421	1.0000	243.7307
11	0.00000	0.00001	0.00000	0.00000	0.00000	0.0005	1.0000	320.4519

TOTAL MOLAR FLOWRATE : 13718.37800
ENTHALPY : VAPOR -&- LIQUID 1982.5373000 0.0000000
ENTHALPY DEPARTURE :VAPOR -&- LIQUID -84.81599 0.00000
ENTROPY DEPARTURE :VAPOR -&- LIQUID -2.8055820 -7.5506105
VAP/LIQ/2ND PHASE MIX. COMPRESSIBILITY FACTOR : 0.855825

****
STREAM NUMBER 10
****

TEMPERATURE : 208.433 PRESSURE : 34.0230 VAPOR FRACTION : 0.0000

ID	X	Y	FUG	GAMA	K	VP	VZ	M.VOL
49	0.00109	0.00000	0.00000	0.00000	0.00000	11.5235	1.0000	39.4467
46	0.00963	0.00000	0.00000	0.00000	0.00000	294.0266	1.0000	42.4609
2	0.27482	0.00000	0.00000	0.00000	0.00000	95.4527	1.0000	46.1797
3	0.23866	0.00000	0.00000	0.00000	0.00000	6.8483	1.0000	61.5597
4	0.26053	0.00000	0.00000	0.00000	0.00000	0.9458	1.0000	169.9375
5	0.02867	0.00000	0.00000	0.00000	0.00000	0.2393	1.0000	210.4419
6	0.10370	0.00000	0.00000	0.00000	0.00000	0.1377	1.0000	205.8643

7	0.02245	0.00000	0.00000	0.00000	0.00000	0.0174	1.0000	242.9614
8	0.02416	0.00000	0.00000	0.00000	0.00000	0.0421	1.0000	243.7307
11	0.03611	0.00000	0.00000	0.00000	0.00000	0.0005	1.0000	320.4519

```
TOTAL MOLAR FLOWRATE :          44706.61700
ENTHALPY   : VAPOR -&- LIQUID             0.0000000        1364.2094000
ENTHALPY DEPARTURE  :VAPOR -&- LIQUID              0.00000          -2109.33710
ENTROPY  DEPARTURE  :VAPOR -&- LIQUID          -2.8055820           -9.9385748
VAP/LIQ/2ND PHASE MIX. COMPRESSIBILITY FACTOR :  0.855825

***  SUBSET LOOP COMPLETE  ***
```

FINAL RESULTS

CHESS3 ... TEST CASE FOR ROTATIONAL EQUIPMENTS

STREAM NUMBER	1	2	3	4	
EQUIP CONXION	FR 0 TO 1	FR 1 TO 3	FR 0 TO 2	FR 2 TO 3	FR
VAPOR FRACTION	1.0000	1.0000	0.0000	0.0000	
TEMPERATURE, F	-25.7978	-54.6879	-59.9618	-62.1620	
PRESSURE, PSIA	199.9979	415.0000	599.9934	415.0002	
ENTHALPY, K.BTU	175.7751	158.0374	228.5163	224.1954	
COMPOSITION, LB-MOLES/UNIT TIME					
CO2	0.02052	0.02052	0.08808	0.08808	
NITROGEN	0.14913	0.14913	0.14913	0.14913	
METHANE	28.48314	28.48314	28.81215	28.81215	
ETHANE	3.63050	3.63050	20.12111	20.12111	
PROPANE	0.92711	0.92711	25.00037	25.00037	
I-BUTANE	0.03843	0.03843	2.83448	2.83448	
N-BUTANE	0.08968	0.08968	10.23009	10.23009	
I-PENTANE	0.00831	0.00831	2.22600	2.22600	
N-PENTANE	0.00610	0.00610	2.39818	2.39818	
N-HEPTANE	0.00100	0.00100	3.59221	3.59221	

TOTAL	33.35390	33.35390	95.45181	95.45181	

STREAM NUMBER	5	6	7	8	
EQUIP CONXION	FR 3 TO 4	FR 4 TO 5	FR 5 TO 6	FR 6 TO 0	FR
VAPOR FRACTION	0.1401	0.2348	1.0000	1.0000	
TEMPERATURE, F	-44.0981	-45.9834	-45.9834	-258.4431	
PRESSURE, PSIA	415.0000	300.0042	300.0042	47.0610	
ENTHALPY, K.BTU	382.2327	382.2324	142.7912	107.8568	
COMPOSITION, LB-MOLES/UNIT TIME					
CO2	0.10860	0.10860	0.01363	0.01363	
NITROGEN	0.29826	0.29826	0.29826	0.29826	
METHANE	57.29530	57.29530	29.94574	29.94574	
ETHANE	23.75160	23.75160	2.92959	2.92959	
PROPANE	25.92747	25.92747	0.60184	0.60184	
I-BUTANE	2.87291	2.87291	0.02372	0.02372	
N-BUTANE	10.31976	10.31976	0.05345	0.05345	
I-PENTANE	2.23431	2.23431	0.00408	0.00408	
N-PENTANE	2.40429	2.40429	0.00298	0.00298	
N-HEPTANE	3.59321	3.59321	0.00037	0.00037	

TOTAL	128.80571	128.80571	30.24399	30.24399	

STREAM NUMBER	9	10	
EQUIP CONXION	FR 5 TO 7	FR 7 TO 0	FR
VAPOR FRACTION	0.0000	0.0000	
TEMPERATURE, F	-45.9834	-84.5091	
PRESSURE, PSIA	300.0042	500.0017	
ENTHALPY, K.BTU	239.4590	241.8670	

COMPOSITION, LB-MOLES/UNIT TIME

CO2	0.10860	0.10860
NITROGEN	0.95798	0.95798
METHANE	27.34956	27.34956
ETHANE	23.75160	23.75160
PROPANE	25.92746	25.92746
I-BUTANE	2.87291	2.87291
N-BUTANE	10.31975	10.31975
I-PENTANE	2.23431	2.23431
N-PENTANE	2.40429	2.40429
N-HEPTANE	3.59320	3.59320

TOTAL	98.56171	98.56171

```
CHESS3 ... TEST CASE FOR ROTATIONAL EQUIPMENTS


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SUMMARY OF ENERGY REQUIREMENTS:
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-------------------------------------------------------

UNIT NUMBER =    1
COMPRESSOR
NUMBER OF STAGES =     1
COMPRESSION RATIO PER STAGE =    2.075
BREAK HORSEPOWER =        10.909
STAGE   DISCHARGE TEMP. ,DEG F  HEAT EXCH.DUTY: K-BTU
  1                    85.5                       48.079
-------------------------------------------------------
-------------------------------------------------------

UNIT NUMBER =    2
HYDRAULIC TURBINE
RECOVERABLE HORSEPOWER =        1.698
-------------------------------------------------------
-------------------------------------------------------

UNIT NUMBER =    6
GAS EXPANDER
RECOVERABLE HORSEPOWER =       13.726
-------------------------------------------------------
-------------------------------------------------------

UNIT NUMBER =    7
PUMP
BREAK HORSEPOWER =        3.785
-------------------------------------------------------
```

THE OUTPUTS FROM THE IDEAL MODELS

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*** ***  CHESS FLOW SHEET SIMULATION  *** ***
                VERSION  THREE
                  JUNE 1985

   CHESS3 ... TEST CASE FOR ROTATIONAL EQUIPMENTS
       10          0          0          2          0          0

       49         46          2          3          4          5          6          7
        8         11

        7          6          2          4          1

  BEGIN NETWORK READ
     1        COMP       U-1      1   -2    0    0    0    0    0
     2        HYTR       U-2      3   -4    0    0    0    0    0
     3        MIXR       U-3      2    4   -5    0    0    0    0
     4        VALV       U-4      5   -6    0    0    0    0    0
     5        ADBF       U-5      6   -7   -9    0    0    0    0
     6        GSXP       U-6      7   -8    0    0    0    0    0
     7        PUMP       U-7      9  -10    0    0    0    0    0
  NETWORK COMPLETE

  BEGIN EQUIPMENT DATA READ
        3          0          0          0          0          0          0          0
        0          0          0          0          0          0          0          0
        0          0          0          0          0          0          0          0
        0          0          0          0          0          0          0          0
        0          0          0          0          0          0          0          0
        0          0          0          0          0          0          0          0
        0          0

     1.0000       28.239       225.00      0.85000       3.0000      0.00000
    0.00000      0.00000      0.00000      0.00000      0.00000      0.00000
    0.00000      0.00000      0.00000      0.00000      0.00000      0.00000
    0.00000      0.00000      0.00000      0.00000      0.00000      0.00000
    0.00000

     2.0000       28.239      0.60000      0.00000      0.00000      0.00000
    0.00000      0.00000      0.00000      0.00000      0.00000      0.00000
    0.00000      0.00000      0.00000      0.00000      0.00000      0.00000
    0.00000      0.00000      0.00000      0.00000      0.00000      0.00000
    0.00000

     4.0000       20.414      0.00000      0.00000      0.00000      0.00000
    0.00000      0.00000      0.00000      0.00000      0.00000      0.00000
    0.00000      0.00000      0.00000      0.00000      0.00000      0.00000
    0.00000      0.00000      0.00000      0.00000      0.00000      0.00000
    0.00000

     5.0000       2.0000      0.00000      0.00000      0.00000      0.00000
    0.00000      0.00000      0.00000      0.00000      0.00000      0.00000
    0.00000      0.00000      0.00000      0.00000      0.00000      0.00000
    0.00000      0.00000      0.00000      0.00000      0.00000      0.00000
    0.00000

     6.0000       3.2023      0.60000      0.00000      0.00000      0.00000
    0.00000      0.00000      0.00000      0.00000      0.00000      0.00000
    0.00000      0.00000      0.00000      0.00000      0.00000      0.00000
    0.00000      0.00000      0.00000      0.00000      0.00000      0.00000
    0.00000

     7.0000       34.023      0.75000      0.00000      0.00000      0.00000
    0.00000      0.00000      0.00000      0.00000      0.00000      0.00000
```

```
VAPOR-LIQUID EQUILIBRIUM DATA CODES:
    LIQUID =    0
    VAPOR =     0
    ENTHALPY = 2

IDEAL GAS AND IDEAL LIQUID STATE MODELS

ENTHALPY CORRECTIONS ARE NOT CALCULATED
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FOLLOWING TABLES TRACE THE CHANGES IN THE THERMODYNAMIC PROPERTIES.

THE STREAM CONDITIONS AT THE OUTLET OF EACH EQUIPMENT NODE ARE TABULATED

IN CASES OF TWO-PHASE CONDITIONS, THE SECOND

PHASE CONDITIONS ARE REPORTED

SOME UNCALCULATED VALUES ARE REPORTED AS ZERO

UNITS ARE   :GM.MOLE  CALORIES  OK  ATM  CC

ID = STANDARD COMPONENT IDENTIFICATION # OF CHESS
X, Y = LIQUID AND VAPOR COMPOSITIONS
FUG, GAMA= FUGACITY AND ACTIVITY COEFFICIENTS
K = EQUILIBRIUM RATIOS
VP= VAPOR PRESSURES VIA ANTOINE EQN.
VZ= COMP. FACTOR FOR COMPONENTS
M.VOL= MOLAL VOLUMES


****************************************
          STREAM  NUMBER   2
****************************************

TEMPERATURE : 225.000 PRESSURE : 28.2390  VAPOR FRACTION : 1.0000
```

ID	X	Y	FUG	GAMA	K	VP	VZ	M.VOL
49	0.00000	0.00062	0.00000	0.00000	0.00000	8.6173	0.0000	84.3288
46	0.00000	0.00447	0.00000	0.00000	0.00000	277.3489	0.0000	42.4503
2	0.00000	0.85397	0.00000	0.00000	0.00000	87.2802	0.0000	46.1448
3	0.00000	0.10885	0.00000	0.00000	0.00000	5.8046	0.0000	130.3393
4	0.00000	0.02780	0.00000	0.00000	0.00000	0.7580	0.0000	168.7855
5	0.00000	0.00115	0.00000	0.00000	0.00000	0.1844	0.0000	209.0497
6	0.00000	0.00269	0.00000	0.00000	0.00000	0.1041	0.0000	234.5101
7	0.00000	0.00025	0.00000	0.00000	0.00000	0.0124	0.0000	241.3936
8	0.00000	0.00018	0.00000	0.00000	0.00000	0.0305	0.0000	242.1529
11	0.00000	0.00003	0.00000	0.00000	0.00000	0.0003	0.0000	318.4167

```
TOTAL MOLAR FLOWRATE :          15129.00000
ENTHALPY   : VAPOR -&- LIQUID        2901.9262000          0.0000000
ENTHALPY DEPARTURE   :VAPOR -&- LIQUID             0.00000            0.00000
ENTROPY  DEPARTURE   :VAPOR -&- LIQUID          0.0000000          0.0000000
VAP/LIQ/2ND PHASE MIX. COMPRESSIBILITY FACTOR :   1.000000


****************************************
          STREAM  NUMBER   4
****************************************

TEMPERATURE : 220.085 PRESSURE : 28.2390  VAPOR FRACTION : 0.0000
```

ID	X	Y	FUG	GAMA	K	VP	VZ	M.VOL
49	0.00092	0.00000	0.00000	0.00000	0.00000	7.1817	0.0000	83.9549
46	0.00156	0.00000	0.00000	0.00000	0.00000	267.3669	0.0000	42.4435
2	0.30165	0.00000	0.00000	0.00000	0.00000	82.5111	0.0000	46.1219
3	0.21060	0.00000	0.00000	0.00000	0.00000	5.2313	0.0000	129.7704
4	0.26192	0.00000	0.00000	0.00000	0.00000	0.6593	0.0000	168.0828
5	0.02970	0.00000	0.00000	0.00000	0.00000	0.1564	0.0000	208.2006
6	0.10718	0.00000	0.00000	0.00000	0.00000	0.0873	0.0000	203.6839
7	0.02332	0.00000	0.00000	0.00000	0.00000	0.0130	0.0000	240.4371
8	0.02512	0.00000	0.00000	0.00000	0.00000	0.0248	0.0000	241.1901
11	0.03763	0.00000	0.00000	0.00000	0.00000	0.0002	0.0000	317.1748

TOTAL MOLAR FLOWRATE : 43296.00000
ENTHALPY : VAPOR -&- LIQUID 0.0000000 3599.9321000
ENTHALPY DEPARTURE :VAPOR -&- LIQUID 0.00000 0.00000
ENTROPY DEPARTURE :VAPOR -&- LIQUID 0.0000000 0.0000000
VAP/LIQ/2ND PHASE MIX. COMPRESSIBILITY FACTOR : 1.000000

****

STREAM NUMBER 5

****

TEMPERATURE : 220.965 PRESSURE : 28.2390 VAPOR FRACTION : 0.1567

ID	X	Y	FUG	GAMA	K	VP	VZ	M.VOL
49	0.00096	0.00022	1.00000	1.00000	0.23712	6.6961	0.0000	41.5669
46	0.00158	0.01415	1.00000	1.00000	9.33556	263.6267	0.0000	42.5319
2	0.34392	0.94291	1.00000	1.00000	2.85946	80.7482	0.0000	46.3917
3	0.21831	0.03726	1.00000	1.00000	0.17799	5.0262	0.0000	64.9616
4	0.23831	0.00506	1.00000	1.00000	0.02213	0.6249	0.0000	179.8676
5	0.02641	0.00013	1.00000	1.00000	0.00520	0.1468	0.0000	222.4328
6	0.09485	0.00026	1.00000	1.00000	0.00289	0.0815	0.0000	217.5286
7	0.02054	0.00001	1.00000	1.00000	0.00032	0.0092	0.0000	256.4563
8	0.02210	0.00002	1.00000	1.00000	0.00081	0.0230	0.0000	257.3115
11	0.03303	0.00000	1.00000	1.00000	0.00001	0.0002	0.0000	337.9641

TOTAL MOLAR FLOWRATE : 58425.00000
ENTHALPY : VAPOR -&- LIQUID 2686.4770000 3555.3085000
ENTHALPY DEPARTURE :VAPOR -&- LIQUID 0.00000 0.00000
ENTROPY DEPARTURE :VAPOR -&- LIQUID 0.0000000 0.0000000
VAP/LIQ/2ND PHASE MIX. COMPRESSIBILITY FACTOR : 1.000000

****

STREAM NUMBER 6

****

TEMPERATURE : 220.964 PRESSURE : 20.4140 VAPOR FRACTION : 0.2623

ID	X	Y	FUG	GAMA	K	VP	VZ	M.VOL

49	0.00114	0.00035	1.00000	1.00000	0.32799	6.6956	0.0000	83.8134
46	0.00068	0.00824	1.00000	1.00000	12.91382	263.6228	0.0000	42.4409
2	0.25041	0.92550	1.00000	1.00000	3.95544	80.7463	0.0000	46.1130
3	0.24978	0.05746	1.00000	1.00000	0.24620	5.0260	0.0000	129.5551
4	0.27267	0.00780	1.00000	1.00000	0.03061	0.6248	0.0000	167.8168
5	0.03021	0.00020	1.00000	1.00000	0.00719	0.1468	0.0000	207.8791
6	0.10853	0.00040	1.00000	1.00000	0.00399	0.0815	0.0000	203.3710
7	0.02350	0.00001	1.00000	1.00000	0.00045	0.0092	0.0000	240.0748
8	0.02528	0.00003	1.00000	1.00000	0.00112	0.0230	0.0000	240.8256
11	0.03779	0.00000	1.00000	1.00000	0.00001	0.0002	0.0000	316.7043

TOTAL MOLAR FLOWRATE : 58425.00000
ENTHALPY : VAPOR -&- LIQUID 2688.1188000 3679.0754000
ENTHALPY DEPARTURE :VAPOR -&- LIQUID 0.00000 0.00000
ENTROPY DEPARTURE :VAPOR -&- LIQUID 0.0000000 0.0000000
VAP/LIQ/2ND PHASE MIX. COMPRESSIBILITY FACTOR : 1.000000

****
STREAM NUMBER 7
****

TEMPERATURE : 220.964 PRESSURE : 20.4140 VAPOR FRACTION : 1.0000

ID	X	Y	FUG	GAMA	K	VP	VZ	M.VOL
49	0.00000	0.00035	0.00000	0.00000	0.00000	6.6956	0.0000	83.8132
46	0.00000	0.00824	0.00000	0.00000	0.00000	263.6228	0.0000	42.4409
2	0.00000	0.92550	0.00000	0.00000	0.00000	80.7463	0.0000	46.1130
3	0.00000	0.05746	0.00000	0.00000	0.00000	5.0260	0.0000	129.5547
4	0.00000	0.00780	0.00000	0.00000	0.00000	0.6248	0.0000	167.8166
5	0.00000	0.00020	0.00000	0.00000	0.00000	0.1468	0.0000	207.8786
6	0.00000	0.00040	0.00000	0.00000	0.00000	0.0815	0.0000	203.3705
7	0.00000	0.00001	0.00000	0.00000	0.00000	0.0092	0.0000	240.0745
8	0.00000	0.00003	0.00000	0.00000	0.00000	0.0230	0.0000	240.8253
11	0.00000	0.00000	0.00000	0.00000	0.00000	0.0002	0.0000	316.7039

TOTAL MOLAR FLOWRATE : 15323.23400
ENTHALPY : VAPOR -&- LIQUID 2688.1186000 3679.0751000
ENTHALPY DEPARTURE :VAPOR -&- LIQUID 0.00000 0.00000
ENTROPY DEPARTURE :VAPOR -&- LIQUID 0.0000000 0.0000000
VAP/LIQ/2ND PHASE MIX. COMPRESSIBILITY FACTOR : 1.000000

****
STREAM NUMBER 9
****

TEMPERATURE : 220.964 PRESSURE : 20.4140 VAPOR FRACTION : 0.0000

ID	X	Y	FUG	GAMA	K	VP	VZ	M.VOL
49	0.00114	0.00000	0.00000	0.00000	0.00000	6.6956	0.0000	83.8132
46	0.00068	0.00000	0.00000	0.00000	0.00000	263.6228	0.0000	42.4409
2	0.25041	0.00000	0.00000	0.00000	0.00000	80.7463	0.0000	46.1130

3	0.24978	0.00000	0.00000	0.00000	0.00000	5.0260	0.0000	129.5547
4	0.27267	0.00000	0.00000	0.00000	0.00000	0.6248	0.0000	167.8166
5	0.03021	0.00000	0.00000	0.00000	0.00000	0.1468	0.0000	207.8786
6	0.10853	0.00000	0.00000	0.00000	0.00000	0.0815	0.0000	203.3705
7	0.02350	0.00000	0.00000	0.00000	0.00000	0.0092	0.0000	240.0745
8	0.02528	0.00000	0.00000	0.00000	0.00000	0.0230	0.0000	240.8253
11	0.03779	0.00000	0.00000	0.00000	0.00000	0.0002	0.0000	316.7039

TOTAL MOLAR FLOWRATE : 43101.76100
ENTHALPY : VAPOR -&- LIQUID 2688.1186000 3679.0751000
ENTHALPY DEPARTURE :VAPOR -&- LIQUID 0.00000 0.00000
ENTROPY DEPARTURE :VAPOR -&- LIQUID 0.0000000 0.0000000
VAP/LIQ/2ND PHASE MIX. COMPRESSIBILITY FACTOR : 1.000000

****
STREAM NUMBER 8
****

TEMPERATURE : 177.961 PRESSURE : 3.2023 VAPOR FRACTION : 1.0000

ID	X	Y	FUG	GAMA	K	VP	VZ	M.VOL
49	0.00000	0.00035	0.00000	0.00000	0.00000	6.6956	0.0000	83.8132
46	0.00000	0.00824	0.00000	0.00000	0.00000	263.6228	0.0000	42.4409
2	0.00000	0.92550	0.00000	0.00000	0.00000	80.7463	0.0000	46.1130
3	0.00000	0.05746	0.00000	0.00000	0.00000	5.0260	0.0000	129.5547
4	0.00000	0.00780	0.00000	0.00000	0.00000	0.6248	0.0000	167.8166
5	0.00000	0.00020	0.00000	0.00000	0.00000	0.1468	0.0000	207.8786
6	0.00000	0.00040	0.00000	0.00000	0.00000	0.0815	0.0000	203.3705
7	0.00000	0.00001	0.00000	0.00000	0.00000	0.0092	0.0000	240.0745
8	0.00000	0.00003	0.00000	0.00000	0.00000	0.0230	0.0000	240.8253
11	0.00000	0.00000	0.00000	0.00000	0.00000	0.0002	0.0000	316.7039

TOTAL MOLAR FLOWRATE : 15323.23400
ENTHALPY : VAPOR -&- LIQUID 2454.2766000 0.0000000
ENTHALPY DEPARTURE :VAPOR -&- LIQUID 0.00000 0.00000
ENTROPY DEPARTURE :VAPOR -&- LIQUID 0.0000000 0.0000000
VAP/LIQ/2ND PHASE MIX. COMPRESSIBILITY FACTOR : 1.000000

****
STREAM NUMBER 10
****

TEMPERATURE : 222.263 PRESSURE : 34.0230 VAPOR FRACTION : 0.0000

ID	X	Y	FUG	GAMA	K	VP	VZ	M.VOL
49	0.00114	0.00000	0.00000	0.00000	0.00000	6.6956	0.0000	83.8132
46	0.00068	0.00000	0.00000	0.00000	0.00000	263.6228	0.0000	42.4409
2	0.25041	0.00000	0.00000	0.00000	0.00000	80.7463	0.0000	46.1130
3	0.24978	0.00000	0.00000	0.00000	0.00000	5.0260	0.0000	129.5547
4	0.27267	0.00000	0.00000	0.00000	0.00000	0.6248	0.0000	167.8166
5	0.03021	0.00000	0.00000	0.00000	0.00000	0.1468	0.0000	207.8786
6	0.10853	0.00000	0.00000	0.00000	0.00000	0.0815	0.0000	203.3705

7	0.02350	0.00000	0.00000	0.00000	0.00000	0.0092	0.0000	240.0745
8	0.02528	0.00000	0.00000	0.00000	0.00000	0.0230	0.0000	240.8253
11	0.03779	0.00000	0.00000	0.00000	0.00000	0.0002	0.0000	316.7039

TOTAL MOLAR FLOWRATE : 43101.76100
ENTHALPY : VAPOR -&- LIQUID 0.0000000 3694.6679000
ENTHALPY DEPARTURE :VAPOR -&- LIQUID 0.00000 0.00000
ENTROPY DEPARTURE :VAPOR -&- LIQUID 0.0000000 0.0000000
VAP/LIQ/2ND PHASE MIX. COMPRESSIBILITY FACTOR : 1.000000

*** SUBSET LOOP COMPLETE ***

FINAL RESULTS

CHESS3 ... TEST CASE FOR ROTATIONAL EQUIPMENTS

STREAM NUMBER	1	2	3	4	
EQUIP CONXION	FR 0 TO 1	FR 1 TO 3	FR 0 TO 2	FR 2 TO 3	FR
VAPOR FRACTION	1.0000	1.0000	0.0000	0.0000	
TEMPERATURE, F	-25.7978	-54.6879	-59.9618	-63.5349	
PRESSURE, PSIA	199.9979	415.0000	599.9934	415.0002	
ENTHALPY, K.BTU	181.9508	174.1086	622.4309	618.1101	
	COMPOSITION, LB-MOLES/UNIT TIME				
CO2	0.02052	0.02052	0.08808	0.08808	
NITROGEN	0.14913	0.14913	0.14913	0.14913	
METHANE	28.48314	28.48314	28.81215	28.81215	
ETHANE	3.63050	3.63050	20.12111	20.12111	
PROPANE	0.92711	0.92711	25.00037	25.00037	
I-BUTANE	0.03843	0.03843	2.83448	2.83448	
N-BUTANE	0.08968	0.08968	10.23009	10.23009	
I-PENTANE	0.00831	0.00831	2.22600	2.22600	
N-PENTANE	0.00610	0.00610	2.39818	2.39818	
N-HEPTANE	0.00100	0.00100	3.59221	3.59221	

TOTAL	33.35390	33.35390	95.45181	95.45181	

STREAM NUMBER	5	6	7	8	
EQUIP CONXION	FR 3 TO 4	FR 4 TO 5	FR 5 TO 6	FR 6 TO 0	FR
VAPOR FRACTION	0.1567	0.2623	1.0000	1.0000	
TEMPERATURE, F	-61.9513	-61.9535	-61.9535	-139.3581	
PRESSURE, PSIA	415.0000	300.0042	300.0042	47.0610	
ENTHALPY, K.BTU	792.2185	792.2185	163.3513	149.1412	
	COMPOSITION, LB-MOLES/UNIT TIME				
CO2	0.10860	0.10860	0.01266	0.01266	
NITROGEN	0.29826	0.29826	0.29826	0.29826	
METHANE	57.29530	57.29530	33.48386	33.48386	
ETHANE	23.75160	23.75160	2.07893	2.07893	
PROPANE	25.92747	25.92747	0.28213	0.28213	
I-BUTANE	2.87291	2.87291	0.00735	0.00735	
N-BUTANE	10.31976	10.31976	0.01465	0.01465	
I-PENTANE	2.23431	2.23431	0.00036	0.00036	
N-PENTANE	2.40429	2.40429	0.00096	0.00096	
N-HEPTANE	3.59321	3.59321	0.00001	0.00001	

TOTAL	128.60571	128.80571	33.78210	33.78210	

STREAM NUMBER	9	10	
EQUIP CONXION	FR 5 TO 7	FR 7 TO 0	FR
VAPOR FRACTION	0.0000	0.0000	
TEMPERATURE, F	-61.9535	-59.6143	
PRESSURE, PSIA	300.0042	500.0017	
ENTHALPY, K.BTU	628.8650	631.5303	

COMPOSITION, LB-MOLES/UNIT TIME

CO2	0.10860	0.10860
NITROGEN	0.06497	0.06497
METHANE	23.81145	23.81145
ETHANE	23.75160	23.75160
PROPANE	25.92746	25.92746
I-BUTANE	2.87291	2.87291
N-BUTANE	10.31974	10.31974
I-PENTANE	2.23431	2.23431
N-PENTANE	2.40429	2.40429
N-HEPTANE	3.59321	3.59321

TOTAL	95.02359	95.02359

```
CHESS3 ... TEST CASE FOR ROTATIONAL EQUIPMENTS


==============================
SUMMARY OF ENERGY REQUIREMENTS:
==============================


--------------------------------------------------------

UNIT NUMBER =    1
COMPRESSOR
NUMBER OF STAGES =     1
COMPRESSION RATIO PER STAGE =    2.075
BREAK HORSEPOWER =        10.570
STAGE    DISCHARGE TEMP. ,DEG F   HEAT EXCH.DUTY: K-BTU
  1                       53.7                   30.780
--------------------------------------------------------
--------------------------------------------------------

UNIT NUMBER =    2
HYDRAULIC TURBINE
RECOVERABLE HORSEPOWER =        1.698
--------------------------------------------------------
--------------------------------------------------------

UNIT NUMBER =    6
GAS EXPANDER
RECOVERABLE HORSEPOWER =        5.583
--------------------------------------------------------
--------------------------------------------------------

UNIT NUMBER =    7
PUMP
BREAK HORSEPOWER =        4.189
--------------------------------------------------------
```

AN EXAMPLE OF INPUT DATA : IDLL=4, IDLV=3, IDH=0

```
CHESS3 ... TEST CASE FOR ROTATIONAL EQUIPMENTS
 10, 4, 3, 0, 0, 0,
 49, 46, 2, 3, 4, 5, 6, 7, 8, 11,
 7, 6, 2, 4, 1,
 1, 'COMP', 'U-1', 1, -2, 5*0,
 2, 'HYTR', 'U-2', 3, -4, 5*0,
 3, 'MIXR', 'U-3', 2, 4, -5, 4*0,
 4, 'VALV', 'U-4', 5, -6, 5*0,
 5, 'ADBF', 'U-5', 6, -7, -9, 4*0,
 6, 'GSXP', 'U-6', 7, -8, 5*0,
 7, 'PUMP', 'U-7', 9, -10, 5*0,
 3, 49*0,
 1, 28.239, 225.0, 0.85, 3, 20*0.0,
 2, 28.239, 0.60, 22*0.0,
 4, 20.414, 0.0, 22*0.0,
 5, 2.0, 23*0.0,
 6, 3.2023, 0.60, 22*0.0,
 7, 34.023, 0.75, 22*0.0,
 2, 4, 5, 6, 7, 8, 9, 10, 92*0,
 1, 0.0, 15129.0, 9.3070, 67.646, 12920.0, 1646.8, 420.54,
     17.434, 40.678, 3.7680, 2.7690, 0.454,
 3, 0.0, 43296.0, 39.952, 67.646, 13069.0, 9126.8, 11340.0,
        1285.7, 4640.3, 1009.7, 1087.8, 1629.4,
 2, 4, 5, 6, 7, 9, 94*0,
 1, 1.0, 1.0, 241.05, 13.609, 0.0, 4*0.0,
 3, 1.0, 0.0, 222.07, 40.827, 0.0, 4*0.0,
 8, 2.0, 8*0.0,
 10, 2.0, 8*0.0,
 20, 5, 0, 0.0001,
 50*0,
 50*0,
 50*0,
```

APPENDIX D

PROGRAM LISTINGS OF SELECTED MODULES

FORTRAN IV VER 59 SOURCE LISTING: 08/16/85 15:01:31

```
      PROGRAM    CHESS3
C
C*****************************************************
C*                   CHESS :3                        *
C*.                  N.J.I.T                         *
C*                   MAY, 1985                       *
C*                JOYDEEP BANERJEE                   *
C*****************************************************
      COMMON  /CNTRL/  NCR,NPRT
      COMMON  /CONTL/  NIN,NOUT,NOCOMP,NE,NEN,KUNITS
      COMMON  /EQPA/   EQPAR(25,50),NEMAX,MAXEQP
      COMMON  /EQPB/   NECALL(50),NEXEQN(50),NAME(50)
      COMMON  /MTST/   ISAVEX(100),SAVEQ(50)
      COMMON  /MIX/    FMIX,ZMIX,BMIX,AA1,3B,BB1,ZMX
      COMMON  /STMA/   SEXTSV(13,100),SINTSV(10,100),NSMAX,MAXSEX,MAXSI
      COMMON  /STRMIN/ SINUM(4),SIFLAG(4),SIVPFR(4),SITEMP(4),SIPRES(4)
     *                 SIENTH(4),SIVISC(4),SITHK(4),SIZ(4),SIS(4),
     *                 SIMOLE(4),SICOMP(10,4),SIKV(10,4)
      COMMON  /STMOUT/ SONUM(4),SOFLAG(4),SOVPFR(4),SOTEMP(4),SOPRES(4)
     *                 SOENTH(4),SOVISC(4),SOTHK(4),SOZ(4),SOS(4),
     *                 SOMOLE(4),SOCOMP(10,4),SOKV(10,4)
      COMMON  /SYSAA/  TITLE(20),COMPNT(10),KOMNAM(40)
      COMMON  /SYSA/   KPM(10,50),KSEM(3,100),N3MAX
      COMMON  /SYSB/   KE1(50),NE1MAX,KE2(50),NE2MAX,KE3(10),NE3MAX,
     *                 KE4(10),NE4MAX,KRET,KRET2,KRET3
      COMMON  /SYSC/   LA,LB,LC,LOOP,LOOPS
      COMMON  /SYSD/  KEFLAG(50),KSFLAG(100),KTRACE,DERROR,NPFREQ,
     *                IPUNCH
      COMMON  /CMPRO/  NC, NCM1,IDLL,IDLV,IDH,LDBUG,ISW,NPNRBL, NDIM,
     *                 ZNAME(2,10), L(10), NTCOMP(10), ITR, ITRMAX,
     *                 NST, NSTM1, NK1, NK2, NK11, NK21, NCASE, NFEED,
     *                NFTOP, NFBTM,LF(8),IDCODE,ICODE,CPCODE(10)
      COMMON  /ZDATA/ CPL(10,4),CPV(10,4),ENP(10,10),ANT(6,10),ADEL(10)
     *                W(10),AX,BX,OMEGA(10),AVAL(10),BVAL(10),MODEAF,
     *                AK(10,10), R(10), Q(10), XL(10),VOL(10),TB(10),
     *                C(180),ALPHA(45),VC(10),TC(10),PC(10),EVAP(10),
     *                OA(10), OB(10), AA(10,10), G(10,10), ZRA(10)
      COMMON  /STREAM/   T,P,Z(10),Y(10),X(10),FRACV,ZVAP,
     *                   EK(10),VP(10),FUG(10),GAM(10),VZ(11),SVAP,
     *                   HOFZ,HVAP,HLIQ,DHV,DSV,XSH,DSL,NOBUB,NODEW
C
C     WRITE (6,99999)
C9999 FORMAT(' ',113X,'PROGRAM CHESS 3')
C
C     SYSTEM LIMITS
C       10 COMPONENTS
C       50 STREAMS
C       100 NODES(PIECES OF EQUIPMENT)
C
      NCR=5
      NPRT=6
C     'MODEAF' IS A SWITCH USED BY THE PENG-ROBINSON
C      EQN. TO CALCULATE INTERACTION PARAMETERS.
C      IT IS SET ON BY THE ROUTINE 'AFLASH' FOR
C      ADIABATIC FLASH CALCULATIONS.
C
```

```
      MODEAF=0
C
C     KODE =  0 REQUIRES AN INITIALIZATION OF ALL VARIABLES
C     KODE = -1 IMPLIES A VARIATION OF THE PREVIOUS CASE
C     KODE =  1 PROBLEM DATA HAS ERROR - TERMINATE PROGRAM
C
      KODE=0
   10 CALL DREAD (KODE)
      IF (KODE) 12,11,20
C
C     CALL NETWORK ANALYZER ROUTINE ... DENETS
C
   11 CALL DENETS(&10)
C
C
C-----CODES FOR LIQUID AND VAPOR PHASE MODELS
C
C     LIQUID PHASE
C        0 = IDEAL
C        1 = VIRIAL EQUATION OF STATE
C        2 = 'NRTL' MODEL OF RENON & PRAUSTNIZ
C        3 = UNIQUAC EQUATION OF STATE
C        4 = CHAO-SEADER PROCEDURE
C        5 = SPECIAL LIBRARY #1 (NRTL)
C        6 = PENG-ROBINSON EQUATION OF STATE
C
C     VAPOR PHASE
C        0 = IDEAL
C        1 = VIRIAL EQUATION OF STATE
C        2 = REDLICH KWONG EQUATION OF STATE
C        3 = SOAVE - REDLICH -KWONG EQUATION OF STATE
C        4 = UNDEFINED NOW.
C        5 = SPECIAL LIBRARY #1 (RK)
C        6 = PENG-ROBINSON EQUATION OF STATE
C
      IF (IDLL.LT.0 .OR. IDLL.GT.6) IDLL=0
      IF (IDLV.LT.0 .OR. IDLV.GT.6) IDLV=0
C
   12 IF (KODE.EQ.-1) GO TO 14
C
C     ACCESS DATA RETRIEVAL PROGRAM
C
      WRITE (NPRT,13)
   13 FORMAT ('1')
      IF (IDLV.EQ.5) CALL ZPVT
      IF (IDLL.EQ.5) CALL ZNRTL
      IF (IDLL.EQ.6.AND.IDLV.EQ.6) CALL COMPID
      IF (IDLL.EQ.4.AND.IDLV.EQ.4) CALL COMPID
      IF (IDLL.EQ.4) CALL COMPID
      IF (IDLL.EQ.4.AND.IDLV.EQ.2) CALL COMPID
      IF (IDLL.EQ.0.AND.IDLV.EQ.0) CALL COMPID
      IF (IDLL.EQ.4.AND.IDLV.EQ.3) CALL COMPID
      IF (IDLV.EQ.6) CALL COMPID
      IF (IDLV.EQ.3) CALL COMPID
      IF (IDLL.EQ.5.AND.IDLV.EQ.5) CALL CDATA
C
```

```
C*****  PRINTOUT FOR CHOSEN PHASE MODEL CODES
C
   14 WRITE (NPRT,15) IDLL,IDLV,IDH
   15 FORMAT ('0VAPOR-LIQUID EQUILIBRIUM DATA CODES:'/
     *          5X, 'LIQUID =', I4 /
     *          5X, 'VAPOR =', I5/
     *          5X, 'ENTHALPY =', I2/)
      IF(IDLL.EQ.4)WRITE(6,155)
      IF(IDLL.EQ.0.AND.IDLV.EQ.0)WRITE(6,156)
      IF(IDLV.EQ.3)WRITE(6,157)
      IF(IDLV.EQ.2)WRITE(6,158)
      IF(IDLV.EQ.6)WRITE(6,159)
      IF (IDLL.EQ.6)WRITE (6,160)
      IF (IDH.EQ.0) WRITE(NPRT,161)
      IF (IDH.EQ.1) WRITE(NPRT,162)
      IF (IDH.EQ.2) WRITE(NPRT,163)
155   FORMAT('0','LIQUID PHASE MODEL  :',' CHAO-SEADER EQN.')
156   FORMAT('0','IDEAL GAS AND IDEAL LIQUID STATE MODELS')
157   FORMAT('0','VAPOR PHASE MODEL   : SOAVE-REDLICH-KWONG EQN.')
158   FORMAT('0','VAPOR PHASE MODEL   :',' REDLICH-KWONG EQN.')
159   FORMAT('0','VAPOR PHASE MODEL   :',' PENG-ROBINSON EQN.')
160   FORMAT('0','LIQUID PHASE MOODEL  :','PENG-ROBINSON EQN.')
161   FORMAT('0','ENTHALPY CORRECTION : FOR BOTH PHASES.')
162   FORMAT('0','ENTHALPY CORRECTION : FOR VAPORS ONLY')
163   FORMAT('0','ENTHALPY CORRECTIONS ARE NOT CALCULATED')
C
C*****            ******          *******
C
      IF (KODE.EQ.-1) GO TO 18
C
C     INITIALIZE ALL DEFINED STREAMS & CHECK STREAM FLAGS
C
      CALL INIT
      CALL DCHECK (KODE)
      IF (KODE.EQ.1) GO TO 20
C
C     PRINT OUT THE FLOW SHEET NETWORK & THE ASSOCIATED STREAMS
C
   18 WRITE (NPRT,13)
      CALL DPRINT
C
C
C----- THE FOLLOWING SUPPLIES THE HEADINS FOR
C-----THE TABLES TO BE PRINTED FOR SUMMARIZING
C-----STREAM CONDITIONS AND PROPERTIES AT THE
C-----OUTLET  OF EACH EQUIPMENT.
C-----COULD BE REMOVED WITH IPT<>1.
C
      IPT=1
      IF(IPT.NE.1)GO TO 67
      WRITE(6,13)
      WRITE(6,133)
133     FORMAT('0FOLLOWING TABLES TRACE THE CHANGES IN THE THERMODYNAMI
     * PROPERTIES.')
      WRITE(6,1331)
1331  FORMAT('0THE STREAM CONDITIONS AT THE OUTLET OF EACH ',
```

```
     ; 'EQUIPMENT NODE ARE TABULATED')
      WRITE(6,134)
 134  FORMAT('0UNITS ARE  :GM.MOLE  CALORIES  OK  ATM  CC')
      WRITE(6,136)
 136  FORMAT('0ID = STANDARD COMPONENT IDENTIFICATION # OF CHESS')
      WRITE(6,137)
 137  FORMAT(' X, Y = LIQUID AND VAPOR COMPOSITIONS')
      WRITE(6,138)
 138  FORMAT(' FUG, GAMA= FUGACITY AND ACTIVITY COEFFICIENTS')
      WRITE(6,1381)
 1381 FORMAT(' K = EQUILIBRIUM RATIOS')
      WRITE(6,139)
 139  FORMAT(' VP= VAPOR PRESSURES VIA ANTOINE EQN.')
      WRITE(6,141)
 141  FORMAT(' VZ= COMP. FACTOR FOR COMPONENTS')
      WRITE(6,142)
 142  FORMAT(' M.VOL= MOLAL VOLUMES')
      WRITE(6,1335)
 1335 FORMAT('0')
C****         *******          *******
C
C     EVALUATE THE NETWORK INCLUDING ALL RECYCLES
C     BY CALLING SUBSET
C
   67 CALL SUBSET
C
C     PRINT OUT THE FINAL RESULTS
C
      WRITE (NPRT,100)
  100 FORMAT ( 1H1, 'FINAL RESULTS' )
      CALL TPRINT
      CALL EPRINT
      KODE=-1
      GO TO 10
C
   20 STOP
      END
```

```
      SUBROUTINE ADBF
C
      COMMON  /CNTRL/  NCR,NPRT
      COMMON  /CONTL/  NIN,NOUT,NOCOMP,NE,NEN,KUNITS
      COMMON  /MIX/    FMIX,ZMIX,BMIX,AA1,BB,BB1,ZMX
      COMMON   /SYSB/  KE1(50),NE1MAX,KE2(50),NE2MAX,KE3(10),NE3MAX,
     *                 KE4(10),NE4MAX,KRET,KRET2,KRET3
      COMMON  /SYSD/   KEFLAG(50),KSFLAG(100),KTRACE,DERROR,NPFREQ,
     *                 IPUNCH
      COMMON  /EQPA/   EQPAR(25,50),NEMAX,MAXEQP
      COMMON /CMPRO/ NC,NCM1,IDLL,IDLV,IDH,LDBUG,ISW,NPNRBL,NDIM,
     *               ZNAME(2,10),L(10),NTCOMP(10),ITR,ITRMAX,
     *               NST,NSTM1,NK1,NK2,NK11,NK21,NCASE,NFEED,
     *               NFTOP,NFBTM,LF(8),IDCODE,ICODE,CPCODE(10)
      COMMON /ZDATA/ CPL(10,4),CPV(10,4),ENP(10,10),ANT(6,10),ADEL(10),
     *               W(10),AX,BX,OMEGA(10),AVAL(10),BVAL(10),MODEAF,
     *               AK(10,10),R(10),Q(10),XL(10),VOL(10),TB(10),
     *               C(180),ALPHA(45),VC(10),TC(10),PC(10),EVAP(10),
     *               OA(10),OB(10),AA(10,10),G(10,10),ZRA(10)
      COMMON  /STRMIN/ SINUM(4),SIFLAG(4),SIVPFR(4),SITEMP(4),SIPRES(4)
     *                 SIENTH(4),SIVISC(4),SITHK(4),SIZ(4),SIS(4),
     *                 SIMOLE(4),SICOMP(10,4),SIKV(10,4)
      COMMON  /STMOUT/ SONUM(4),SOFLAG(4),SOVPFR(4),SOTEMP(4),SOPRES(4)
     *                 SOENTH(4),SOVISC(4),SOTHK(4),SOZ(4),SOS(4),
     *                 SOMOLE(4),SOCOMP(10,4),SOKV(10,4)
      COMMON  /STREAM/ T, P, Z(10), Y(10), X(10), FRACV, ZVAP,
     *                 EK(10), VP(10),FUG(10),GAM(10),VZ(11),SVAP,
     *                 HOFZ, HVAP,HLIQ,DHV,DSV,XSH,DSL,NOBUB, NODEW
      REAL    TR(10)
      LOGICAL             NONCBF(10)
C
C          EQPAR(1,NE) = EQUIPMENT NUMBER
C          EQPAR(2,NE) = MODE OF FLASH CALCULATION
C
C
C-----'NONCBF(I)' ARE FLAGS ,SET TRUE IF NON-CONDENSIBLES
C-----EXIST IN A STREAM. FOLLOWING COMPONENTS ARE CLASSIFIED:
C-----       H2,O2,N2,NH3,SO2,H2S,CO,CO2,C2H2.
C
C
C------ NPNRBL   IS THE SWITCH USED BY THE PENG-
C------ ROBINSON MODULES TO DECIDE WHETHER THE VAPOR
C------- OR THE LIQUID PHASE IS BEING HANDLED
C
      NPNRBL=0
C
C
      DO 75 I=1,NC
      NONCBF(I)=.FALSE.
      IF (NTCOMP(I).EQ.1)  NONCBF(I)=.TRUE.
      IF (NTCOMP(I).EQ.46) NONCBF(I)=.TRUE.
      IF (NTCOMP(I).EQ.47) NONCBF(I)=.TRUE.
      IF (NTCOMP(I).EQ.48) NONCBF(I)=.TRUE.
      IF (NTCOMP(I).EQ.49) NONCBF(I)=.TRUE.
      IF (NTCOMP(I).EQ.50) NONCBF(I)=.TRUE.
      IF (NTCOMP(I).EQ.51) NONCBF(I)=.TRUE.
```

```
      IF (NTCOMP(I).EQ.63) NONCBF(I)=.TRUE.
      IF (NTCOMP(I).EQ.65) NONCBF(I)=.TRUE.
 75   CONTINUE
C
C
C
      IF (EQPAR(2,NE).LE.0.D .OR. EQPAR(2,NE).GT.6.0) EQPAR(2,NE)=2.0
      MODE=EQPAR(2,NE)+0.1
C
C-----FLAG 'MODEAF' IS USED BY PENG-ROBINSON MODULES.
C
      MODEAF=0
C
C-----FOLLOWING COMPUTES:  .. VAPOR PRESSURES IN ATM ,
C-----          ..SETS PHASE CLASSIFICATION CODE (L(I) VALUES)
C-----    L(I)= -1 FOR NON-VOLATILES
C-----         =  0 FOR NON-CONDENSIBLES
C-----         =  1 FOR NORMAL PHASES(CONDENSIBLES PRESENT)
C-----         =  2 FOR SUPERCRITICAL PHASES
C
C
      DO 99 I=1,NC
      PP=SIPRES(1)
      TT=SITEMP(1)
      PTEST=EXP(ANT(1,I)+ANT(2,I)/(ANT(3,I)+TT)+ANT(5,I)*TT
     *      +ANT(6,I)*TT*TT+ANT(4,I)*ALOG(TT))
      PTEST=PTEST/760.D0
      VP(I)=PTEST
      IF (PP.GE.PC(I).AND.TT.GE.TC(I)) GO TO 91
      IF (PP.LT.PC(I).AND.TT.GT.TC(I)) GO TO 92
      IF (PP.GT.PTEST.AND.PP.LT.PC(I).AND.TT.LT.TC(I)) GO TO 93
      IF (TT.LT.TC(I).AND.PP.LT.PTEST)L(I)=1
      L(I)=1
      GO TO 99
 91   L(I)=2
      GO TO 99
 92   IF (NONCBF(I)) GO TO 925
      GO TO 91
 925  L(I)=0
      GO TO 99
 93   L(I)=-1
C990  WRITE(6,901)TT,PP,PTEST,TC(I),PC(I),L(I)
C901  FORMAT(' ADBF****** T P VP TC PC L ',5F10.5,I3)
 99   CONTINUE
C-----COMPUTES THE SATURATED LIQUID VOLUME AT
C-----THE SYSTEM TEMP. USING THE RACKETT EQN.
C-----MODIFIED BY SPENCER & DANNER.
      DO 399 I=1,NC
      TR(I)=SITEMP(1)/TC(I)
      POWER1=1.D0+(1.D0-TR(I)**(2.0/7.0))
      POWER2=1.6D+0.00693026/(TR(I)-0.655)
      IF (TR(I).LT.0.75) GO TO 391
      VOL(I)=82.06/PC(I)*TC(I)*ZRA(I)**POWER2
      GO TO 399
 391  VOL(I)=82.06/PC(I)*TC(I)*ZRA(I)**POWER1
 399  CONTINUE
```

```
      P=SIPRES(1)
      SOPRES(1)=P
      T=SITEMP(1)
      HOFZ=SIENTH(1)/SIMOLE(1)
      FRACV=SIVPFR(1)
      DO 10 I=1,NOCOMP
   10 Z(I)=SICOMP(I,1)
C
      GO TO (11,12,13,14,15,16), MODE
   11 CALL AFLASH
      GO TO 19
   12 CALL AFNODB
      GO TO 19
   13 CALL TFLASH
      GO TO 19
   14 CALL TFNODB
      GO TO 19
   15 CALL DEWT
      GO TO 19
   16 CALL BUBT
C
   19 SIVPFR(1)=FRACV
      SIENTH(1)=HOFZ*SIMOLE(1)
      SITEMP(1)=T
      SOTEMP(1)=T
C
      IF (NOUT.EQ.2) GO TO 30
      SOVPFR(1)=FRACV
      SOMOLE(1)=SIMOLE(1)
      SOENTH(1)=SIENTH(1)
      DO 20 I=1,NOCOMP
   20 SOCOMP(I,1)=SICOMP(I,1)
      GO TO 50
C
   30 SOVPFR(1)=1.0
      SOVPFR(2)=0.0
      SOPRES(1)=P
      SOTEMP(1)=T
      SOPRES(2)=P
      SOTEMP(2)=T
      SOMOLE(1)=SIMOLE(1)*FRACV
      SOMOLE(2)=SIMOLE(1)*(1.0-FRACV)
      SOENTH(1)=HVAP*SOMOLE(1)
      SOENTH(2)=HLIQ*SOMOLE(2)
      SOZ(1)=ZVAP
      SOZ(2)=ZVAP
      DO 40 I=1,NOCOMP
      SOCOMP(I,1)=Y(I)*SOMOLE(1)
   40 SOCOMP(I,2)=X(I)*SOMOLE(2)
C
   50 RETURN
      END
```

```
      SUBROUTINE FLASH
C     WRITE (6,99999)
C9999 FORMAT(' ',113X,'SUBROUTINE FLASH')
C
C     FLASH ROUTINE... PRESSURE AND TEMPERATURE ARE GIVEN
C
C     DETERMINES THE FRACTION VAPORIZED FOR A ONE LIQUID PHASE SYSTEM
C
C
      COMMON  /CNTRL/  NCR, NPRT
      COMMON  /CMPRO/  NC,NCM1,IDLL,IDLV,IDH,LDBUG,ISW,NPNRBL, NDIM,
     *                 ZNAME(2,10), L(10), NTCOMP(10), ITR, ITRMAX,
     *                 NST, NSTM1, NK1, NK2, NK11, NK21, NCASE, NFEED,
     *                 NFTOP, NFBTM, LF(8),IDCODE,ICODE,CPCODE(10)
      COMMON  /STREAM/ T, P, Z(10), Y(10), X(10), FRACV, ZVAP,
     *                 EK(10), VP(10), FUG(10),GAM(10),VZ(11),SVAP,
     *                 HOFZ, HVAP,HLIQ,DHV,DSV,XSH,DSL,NOBUB,NODEW
      REAL             XX(10), SX(10), XC(10),
     *                 YY(10), SY(10), YC(10)
C
      EQUIVALENCE      (R,FRACV)
C
      DATA             CONV /1.0E-3/, CONV1 /1.0E-4/
      DATA             SMALL /0.00001/
C
C     R IS VAPOR FRACTION
C          IF R IS APPROXIMATELY 1.0, SYSTEM IS ALL VAPOR
C          IF R IS APPROXIMATELY 0.0, SYSTEM IS ALL LIQUID
C
      HVAP=0.0
      HLIQ=0.0
      XSH=0.0
      DHV=0.0
      HOFZ=0.0
C
      KNT=0
      IDX=1
      ISW=0
C
      RMIN=0.0
      RMAX=1.0
C
      UY=0.0
      UX=0.0
      DO 2 I=1,NC
      UY=UY+Y(I)
    2 UX=UX+X(I)
      IF (UY+UX .GT. 0.0) GO TO 13
C
      DO 9 I=1,NC
      IF (L(I)) 6,7,8
C     NON-VOLATILE
    6 RMAX=RMAX-Z(I)
      Y(I)=0.0
      X(I)=Z(I)
      GO TO 9
```

```
C     NON-CONDENSIBLE
    7 RMIN=RMIN+Z(I)
      Y(I)=Z(I)
      X(I)=0.0
      GO TO 9
C     NORMAL AND SUPERCRITICAL
    8 Y(I)=Z(I)/2.0
      X(I)=Y(I)
    9 CONTINUE
      R=(RMIN+RMAX)/2.0
      UY=0.0
      UX=0.0
      DO 12 I=1,NC
      UY=UY+Y(I)
   12 UX=UX+X(I)
C
   13 DO 14 I=1,NC
      Y(I)=Y(I)/UY
   14 X(I)=X(I)/UX
      CALL KCALC
      ISW=1
      GO TO 21
C
   20 CALL KCALC
C
   21 KNT=KNT+1
      IF (LDBUG.EQ.0) GO TO 29
      WRITE (NPRT,25) T, R, KNT
   25 FORMAT (' FLASH  T/R', 2F15.5,I10)
C
   29 K=0
   30 AMAX=RMAX
      AMIN=RMIN
C     IF (R.EQ.1.0) R=0.9999999
      IF (R.EQ.1.0) R=1.0-1.0E-7
      IF (R.EQ.0.0) R=1.0E-7
      F=0.0
      DF=0.0
      DO 80 I=1,NC
      IF (L(I))40,50,60
C     NON-VOLATILE
   40 S=1.0/(1.0-R)
      GO TO 70
C     NON-CONDENSIBLE
   50 S=-1.0/R
      GO TO 70
C     NORMAL AND SUPERCRITICAL
   60 S=(1.0-EK(I))/(1.0+R*(EK(I)-1.0))
   70 F=F+Z(I)*S
   80 DF=DF+Z(I)*S*S
      DR=-F/DF
      K=K+1
C
      IF (LDBUG.EQ.0) GO TO 90
      WRITE (NPRT,85) F,DR,R
   85 FORMAT (5X, 'F-DR-R',3E14.5 )
```

```
      IF (LDBUG.EQ.1) GO TO 90
      DO 86 J=1,NC
   86 WRITE (NPRT,87) J,EK(J),VP(J),FUG(J),GAM(J)
   87 FORMAT (I20,4G20.6)
C
   90 IF (K-20) 99,190,91
   91 WRITE (NPRT,92)
   92 FORMAT ('0FLASH CALCULATION TERMINATED'/
     +          ' CALCULATION CONTINUING' ///)
      GO TO 320
C
   99 IF (ABS(F).LT.CONV1) GO TO 190
C     IF (F) 100,190,110
C 100 AMIN=R
C     GO TO 120
C 110 AMAX=R
C 120 IF ((AMAX-AMIN).LT.CONV1) GO TO 170
      IF (ABS(R-AMIN).LT.CONV1 .OR. ABS(R-AMAX).LT.CONV1) GO TO 190
  130 RNEXT=R+DR
      IF (RNEXT.GE.AMIN) GO TO 150
  140 DR=DR/2.0
      GO TO 130
  150 IF (RNEXT.GT.AMAX) GO TO 140
      R=RNEXT
C
      IF (ABS(DR).GT.CONV1) GO TO 30
C
C 170 DO 180 I=1,NC
C 180 X(I)=(X(I)+SX(I))/2.0
C     GO TO 20
C
  190 IF (LDBUG.GE.2) WRITE (NPRT,200) R
  200 FORMAT (5X, 'R', E14.5)
      DO 240 I=1,NC
      IF (L(I))210,220,230
C     NON-VOLATILE
  210 XX(I)=Z(I)/(1.0-R)
      YY(I)=0.0
      GO TO 240
C     NON-CONDENSIBLE
  220 XX(I)=0.0
      YY(I)=Z(I)/R
      GO TO 240
C     NORMAL AND SUPERCRITICAL
  230 XX(I)=Z(I)/(1.0+R*(EK(I)-1.0))
      YY(I)=EK(I)*XX(I)
  240 CONTINUE
C
      IF (IDLL+IDLV.EQ.0) GO TO 320
C
  250 IF (KNT.EQ.50) GO TO 91
      GO TO (340,260), IDX
C
  260 IF (IDLL.EQ.0) GO TO 290
      IF ((ABS(R).LT.CONV1 .OR. ABS(R-1.0).LT.CONV1) .AND. KNT.GE.10)
     *    GO TO 290
```

```
      DO 280 I=1,NC
      IF (L(I).EQ.0 .OR. Z(I).LT.SMALL) GO TO 280
      IF (ABS(X(I)-XX(I))/X(I) .GT. CONV) GO TO 410
  280 CONTINUE
C
  290 IF (IDLV.NE.1) GO TO 320
      IF ((ABS(R).LT.CONV1 .OR. ABS(R-1.0).LT.CONV1) .AND. KNT.GE.10)
     *    GO TO 320
      DO 310 I=1,NC
      IF (L(I).LT.0 .OR. Z(I).LT.SMALL) GO TO 310
      IF (ABS(Y(I)-YY(I))/Y(I) .GT. CONV) GO TO 410
  310 CONTINUE
C
  320 UX=0.0
      UY=0.0
      DO 322 I=1,NC
      X(I)=XX(I)
      Y(I)=YY(I)
      UX=UX+X(I)
  322 UY=UY+Y(I)
      DO 325 I=1,NC
      X(I)=X(I)/UX
  325 Y(I)=Y(I)/UY
      ISW=0
      IF (ABS(R-1.0).GT.CONV1) GO TO 330
      DO 327 J=1,NC
  327 Y(J)=Z(J)
      CALL VAPH
      GO TO 337
  330 IF (ABS(R).GT.CONV1) GO TO 335
      DO 333 J=1,NC
  333 X(J)=Z(J)
      CALL LIQH
      GO TO 337
  335 CALL VAPH
      CALL LIQH
  337 HOFZ=HVAP*R+HLIQ*(1.0-R)
      IF (LDBUG.EQ.0) GO TO 339
      WRITE (NPRT,338) HOFZ,HVAP,HLIQ
  338 FORMAT (20X,3F20.4)
  339 RETURN
C
  340 IF (IDLL.EQ.0) GO TO 370
      DO 360 I=1,NC
      SX(I)=X(I)
      XC(I)=XX(I)
  360 X(I)=(XX(I)+X(I))/2.0
C
  370 IF (IDLV.NE.1) GO TO 400
      DO 390 I=1,NC
      SY(I)=Y(I)
      YC(I)=YY(I)
  390 Y(I)=(YY(I)+Y(I))/2.0
  400 IDX=2
      GO TO 20
C
```

```
  410 IF (IDLL.EQ.0) GO TO 450
      UX=0.0
      DO 430 I=1,NC
      IF (L(I).EQ.0 .OR. Z(I).LT.SMALL) GO TO 430
      IF (ABS(X(I)-XX(I))/X(I) .LE. CONV) GO TO 425
      CALL WEG (X(I),XX(I),SX(I),XC(I))
      GO TO 429
  425 X(I)=XX(I)
  429 UX=UX+X(I)
  430 CONTINUE
      DO 440 I=1,NC
  440 X(I)=X(I)/UX
C
  450 IF (IDLV.NE.1) GO TO 20
      UY=0.0
      DO 470 I=1,NC
      IF (L(I).LT.0 .OR. Z(I).LT.SMALL) GO TO 470
      IF (ABS(Y(I)-YY(I))/Y(I) .LE. CONV) GO TO 455
      CALL WEG (Y(I),YY(I),SY(I),YC(I))
      GO TO 459
  455 Y(I)=YY(I)
  459 UY=UY+Y(I)
  470 CONTINUE
      DO 480 I=1,NC
  480 Y(I)=Y(I)/UY
      GO TO 20
C
      END
```

```
      SUBROUTINE AFLASH
C     WRITE (6,99999)
C9999 FORMAT(' ',113X,'SUBROUTINE AFLASH')
C
C     ADIABATIC FLASH
C
      COMMON  /CMPRO/  NC,NCM1,IDLL,IDLV,IDH,LDBUG,ISW,NPNRBL, NDIM,
     *                 ZNAME(2,10), L(10), NTCOMP(10), ITR, ITRMAX,
     *                 NST, NSTM1, NK1, NK2, NK11, NK21, NCASE, NFEED,
     *                 NFTOP, NFBTM, LF(8),IDCODE,ICODE,CPCODE(10)
      COMMON  /ZDATA/ CPL(10,4),CPV(10,4),ENP(10,10),ANT(6,10),ADEL(10),
     *                 W(10),AX,BX,OMEGA(10),AVAL(10),BVAL(10),MODEAF,
     *                 AK(10,10), R(10), Q(10), XL(10),VOL(10),TB(10),
     *                 C(180), ALPHA(45),VC(10),TC(10),PC(10),EVAP(10),
     *                 OA(10), OB(10), AA(10,10), G(10,10), ZRA(10)
      COMMON  /STREAM/ T, P, Z(10), Y(10), X(10), FRACV, ZVAP,
     *                 EK(10), VP(10), FUG(10),GAM(10),VZ(11),SVAP,
     *                 HOFZ, HVAP,HLIQ,DHV,DSV,XSH,DSL,NOBUB,NODEW
      COMMON /CONTL/  NIN,NOUT,NOCOMP,NE,NEN,KUNITS
C
      DATA             CONV/1.E-4/
C
      DIMENSION       RETAIN(5)
C
C
C     FRACV = VAPOR FRACTION
C       2    SUPERHEATED VAPOR
C      -1    SUBCOOLED LIQUID
C
      NODB=0
      GO TO 1
C
      ENTRY AFNODB
      NODB=1
C
    1 HSAVE=HOFZ
      TSAVE=T
      ISW=0
      STEP=20.0
C
      MODEAF=1
      NPNRBL=0
      SUM=0.0
      DO 5 J=1,NC
      X(J)=0.0
      Y(J)=0.0
    5 SUM=SUM+Z(J)
      DO 6 J=1,NC
    6 Z(J)=Z(J)/SUM
C
      IF (FRACV.EQ.1.0) GO TO 10
      IF (FRACV.EQ.0.0) GO TO 115
      IF (ABS(FRACV-2.0) .LT. CONV) GO TO 10
      IF (ABS(FRACV-(-1.0)) .LT. CONV) GO TO 115
      IF (NODB.NE.0) GO TO 199
C
```

```
      CALL DEWT
      IF (NODEW.EQ.2) GO TO 10
      IF (NODEW.NE.0) GO TO 100
      TDEW=T
      HDEW=HVAP
      IF (HSAVE.LT.HDEW) GO TO 100
      GO TO 15
C
   10 TDEW=273.16
      DO 11 J=1,NC
   11 Y(J)=Z(J)
      CALL VAPH
      HDEW=HVAP
C
   15 ST=TDEW
      SH=HDEW-HSAVE
      T=TDEW+20.0
C
C-----THE FOLLOWING COUNTERS, JK AND NOSC,ARE PROVIDED TO PREVENT
C-----OSCILLATORRY BEHAVIOUR DUE TO MAXIMA IN 'DHV' VALUES
C-----NEAR THE CRITICAL POINTS
C
C-----IF CONVERGENCE IS NOT ACHIEVED WITHIN 20 ITERATIONS,
C-----10 MORE ITERATIONS ARE PERMITTED WITH A STEP SIZE
C-----OF 5 DEGREES TO BEGIN WITH. IF NO CONVERGENCE
C-----IS ARRIVED AT AFTER 30 ITERATIONS, THE LOOP
C----- IS EXITED AND THE AVERAGE OF THE LAST FIVE
C----- VALUES ARE TAKEN TO BE THE FINAL.
      NOSC=0
C
      JK=0
C
   20 CALL VAPH
      H=HVAP-HSAVE
      IF (ABS(H/HSAVE) .LT. CONV) GO TO 30
      SLOPE=(SH-H)/(ST-T)
      DT=-H/SLOPE
      IF (ABS(DT) .LT. 0.50) GO TO 30
      SH=H
      ST=T
C
      NOSC=NOSC+1
      JK=JK+1
      IF(JK.EQ.6)JK=1
      RETAIN(JK)=T
C
C
      IF (NOSC.GT.20) STEP=5.0
      IF (NOSC.GT.30) GO TO 25
C
C
      IF (ABS(DT) .GT. STEP) DT=SIGN(STEP,DT)
      T=T+DT
      GO TO 20
C
C
```

```
25     RTSUM=0.0
C
       DO 26 I=1,5
26     RTSUM=RTSUM+RETAIN(I)
C
       T=RTSUM/5.0
       CALL VAPH
C
    30 FRACV=1.0
       DO 40 J=1,NC
    40 X(J)=0.0
       HLIQ=0.0
       XSH=0.0
       HVAP=HSAVE
       HOFZ=HSAVE
       GO TO 300
C
   100 CALL BUBT
       IF (NOBUB.EQ.2) GO TO 110
       IF (NOBUB.NE.0) GO TO 200
   110 TBUB=T
       HBUB=HLIQ
       IF (HSAVE.GT.HBUB) GO TO 200
       GO TO 116
C
   115 TBUB=273.16
       DO 111 J=1,NC
   111 X(J)=Z(J)
       CALL LIQH
       HBUB=HLIQ
C
   116 ST=TBUB
       SH=HBUB-HSAVE
       T=TBUB-20.0
   120 CALL LIQH
       H=HLIQ-HSAVE
       IF (ABS(H/HSAVE) .LT. CONV) GO TO 130
       SLOPE =(SH-H)/(ST-T)
       DT=-H/SLOPE
       IF (ABS(DT) .LT. 0.50) GO TO 130
       SH=H
       ST=T
       IF (ABS(DT) .GT. STEP) DT=SIGN(STEP,DT)
       T=T+DT
       GO TO 120
C
   130 FRACV=0.0
       HVAP=0.0
       DHV=0.0
       DO 140 J=1,NC
   140 Y(J)=0.0
       HLIQ=HSAVE
       HOFZ=HSAVE
       GO TO 300
C
   200 IF (NODEW.EQ.0 .AND. NOBUB.EQ.0) GO TO 203
```

```
FORTRAN IV  VER 59   SOURCE LISTING: AFLASH  SUBROUTINE  08/16/85  15:03:37  F
          IF (NOBUB.EQ.0) GO TO 201
          IF (NODEW.EQ.0) GO TO 202
    199   T=273.16
          TBUB=0.0
          TDEW=2000.0
          GO TO 205
    201   T=TBUB+20.0
          GO TO 205
    202   T=TDEW-20.0
          GO TO 205
    203   T=TBUB+(HSAVE-HBUB)*(TDEW-TBUB)/(HDEW-HBUB)
    205   DO 206 J=1,NC
          Y(J)=0.0
    206   X(J)=0.0
          ID=1
    210   CALL FLASH
          GO TO (220,230), ID
    220   SH=HOFZ-HSAVE
          ST=T
          T=T-SIGN(10.0,SH)
          ID=2
          GO TO 238
    230   H=HOFZ-HSAVE
          IF (HSAVE.NE.0.0) GO TO 232
          IF (ABS(H) .LT. 0.1) GO TO 240
          GO TO 234
    232   IF (ABS(H/HSAVE) .LT. CONV) GO TO 240
    234   SLOPE=(SH-H)/(ST-T)
          DT=-H/SLOPE
          IF (ABS(DT) .LT. 0.01) GO TO 240
          SH=H
          ST=T
          IF (ABS(DT) .GT. STEP) DT=SIGN(STEP,DT)
          T=T+DT
    238   T=AMIN1(T,TDEW-0.5)
          T=AMAX1(T,TBUB+0.5)
          GO TO 210
    240   HOFZ=HSAVE
C
    300   RETURN
          END
```

```
      SUBROUTINE PENROB(T,P,Y,VP,FUG,DHV,DSV)
C-----THIS SUBPROGRAMME USES THE 'PENG-ROBINSON' EQN.
C-----OF STATE TO PREDICT; .PURE COMPONENT
C-----FUGACITY RATIO, .MIXTURE FUGACITIES, .THE
C-----ENTHALPY DEPARTURE, .THE ENTROPY DEPARTURE.
C--------THE BINARY INTERACTION PARAMETERS ARE
C-----CALCULATED IN SUBROUTINE'DELTIJ' .
C
C
C
      REAL     Y(10),VP(10),FUG(10),AM(10),TR(10),
     *         PR(10),AP(10),AC(10),A(10),B(10),TERM(10),
     *         AT(10),ACIJ(10,10),ACIJO(10,10),TEMP(10),
     *         YAT(10),YATT(10),SA(10),AL(10),BL(10),
     *         INTR(10,10),AIJ(10,10),DLT(10),SAB(10)
      COMMON  /CMPRO/   NC,NCM1,IDLL,IDLV,IDH,LDBUG,ISW,NPNRBL,
     *                  NDIM,ZNAME(2,10),L(10),NTCOMP(10),
     *                  ITR,ITRMAX,NST,NSTM1,NK1,NK2,NK11,
     *                  NK21,NCASE,NFEED,NFTOP,NFBTM,LF(8),
     *                  IDCODE,ICODE
      COMMON  /STREAM/   T21,P1,Z1(10),Y1(10),X(10),FRACV,ZVAP,
     *                  EK(10),VP1(10),FUG1(10),GAM(10),VZ(11),SVAP,
     *                  HOFZ,HVAP,HLIQ,DHV1,DSV1,XSH,DSL,NOBUB,NODEW
      COMMON /ZDATA/ CPL(10,4),CPV(10,4),ENP(10,10),ANT(6,10),ADEL(10),
     *               W(10),AX,BX,OMEGA(10),AVAL(10),BVAL(10),MODEAF,
     *               AK(10,10),R(10),Q(10),XL(10),VOL(10),TB(10),
     *               C(180),ALPHA(45),VC(10),TC(10),PC(10),EVAP(10),
     *               OA(10),OB(10),AD(10,10),G(10,10),ZRA(10)
      COMMON  /SYSAA/   TITLE(20),COMPNT(20),KOMNAM(20)
      COMMON  /MIX/  FMIX,ZMIX,BMIX,AA1,BB,BB1,ZMX
C
C
C
      AA=0.0
      BB=0.0
      DERV=0.0
      T1=SQRT(1./T)
      DO 10 J=1,NC
C-----A(J),B(J)   :PARAMETERS IN THE P-R EQN.OF STATE
C-----AC(J)       :COMPONENT PROPERTY DEPENDENT FACTOR OF A(J)
C-----AP(J)       :TEMP.DEPENDENT FACTOR OF A(J)
C
      AM(J)=0.37464+(1.54226-0.26992*OMEGA(J))*OMEGA(J)
      TR(J)=T/TC(J)
      PR(J)=P/PC(J)
      AP(J)=(1.+AM(J)*(1.-SQRT(TR(J))))**2
      AC(J)=0.457235*(0.082057*TC(J))**2/PC(J)
      A(J)=AC(J)*AP(J)
      B(J)=0.077796*0.082057*TC(J)/PC(J)
      AT(J)=AM(J)/SQRT(TC(J))
      YAT(J)=Y(J)*AT(J)
      YATT(J)=Y(J)*(1.0+AP(J))*T1-YAT(J)
      ACIJO(J,J)=AC(J)
      ACIJ(J,J)=AC(J)
      INTR(J,J)=0.0
      AL(J)=A(J)*P/(0.082057*T)**2
```

```
      BL(J)=B(J)*P/0.082057/T
      AIJ(J,J)=ACIJ(J,J)*AP(J)
      FUG(J)=1.0
 10   CONTINUE
      IF(NC.EQ.1) GO TO 60
C-----ROUTINE 'DELTIJ' SUPPLIES THE INTERACTION
C-----PARAMETERS.
C
      CALL DELTIJ(INTR,DLT)
      DO 20 I=2,NC
      I1=I-1
      DO 20 J=1,I1
C-----ACIJ(I,J),ACIJO(I,J): A PART OF THE TERM TO BE SUMMED
C                   UP TOWARDS THE MIXTURE A PARAMETER
C-----AIJ(I,J) : PART OF MIXTURE 'A' PARAMETER,
C-----INTR(I,J): THE BINARY INTERACTION PARAMETER
C                   USED IN THE MIXTURE A VALUE & THE
C                   DEPARTURE FUNCTIONS
C-----DLT(I)    :INTERACTION PARAMETERS FOR CERTAIN
C                 1<--->1 INTERACTING COMPOUNDS
C
C
      ACIJO(I,J)=SQRT(AC(I)*AC(J))
      ACIJ(I,J)=ACIJO(I,J)*(1.-INTR(I,J))
      ACIJO(J,I)=ACIJO(I,J)
      INTR(J,I)=INTR(I,J)
      ACIJ(J,I)=ACIJ(I,J)
 20   CONTINUE
      DO 30 I=2,NC
      ACIJ(I,1)=ACIJ(I,1)*(1.D-DLT(I))
      ACIJ(1,I)=ACIJ(I,1)
 30   CONTINUE
      DO 35 I=1,NC
      I1=I-1
      DO 35 J=1,I1
      AIJ(I,J)=ACIJ(I,J)*SQRT(AP(J)*AP(I))
 35   AIJ(J,I)=AIJ(I,J)
      DO 50 I=1,NC
      SA(I)=0.0
      DO 40 J=1,NC
C
C-----COMPUTES THE MIXTURE A & B PARAMETERS
C-----ALSO DETERMINES A FACTOR OF THE D(A(I))/D(T) DERIVATIVE
C-----'DERV'
C
C
      D1=Y(J)*YAT(I)*SQRT(AP(J))+Y(I)*YAT(J)*SQRT(AP(I))
      DERV=DERV+D1*T1*ACIJ(I,J)
 40   SA(I)=SA(I)+Y(J)*AIJ(I,J)
      AA=AA+SA(I)*Y(I)
      BB=BB+Y(I)*B(I)
 50   CONTINUE
 55   ZMIX=NC+1
      BB1=BB
      BB=BB*P/0.082057/T
      AA1=AA
      AA=AA*P/(0.082057*T)**2
C
```

```
C-----COMPUTES THE  COMP.FACTOR OF THE MIXTURE
C-----VIA SUBROUTINE CALLS
C
      CALL PEROBZ(AA,BB,ZMIX1)
      VZ(11)=ZMIX1
      ZMX=ZMIX1
      ZMIX=ZMIX1
      Z=ZMIX1
      GO TO 70
C-----FOLLOWING DEFINES PURE COMPONENT PARAMETERS
C-----FOR ONE -COMPONENT STREAMS
C
60    AA=0.457235*(0.082057*TC(1))**2/PC(1)*AP(1)
      BB=0.077796*0.082057*TC(1)/PC(1)
      GO TO 55
70    DERV=(-1./2.)*DERV
      TERM1=ALOG((Z+2.414*BB)/(Z-0.414*BB))
      TERM1=TERM1/2.828
      IF (BB1.EQ.0.0)BB1=1.0E-8
      TERM1=TERM1/BB1
C-----THE DEPARTURES OF ENTHALPY AND ENTROPY ARE ESTIMATED.
C
      DHV=1.9872*T*(ZMX-1.0)+TERM1*(T*DERV-AA1)
      DHV1=DHV
      DSV=1.9872*ALOG(ZMX-BB)+TERM1*DERV
      DSV1=DSV
789   CONTINUE
C
C-----  NPNRBL  =  LIQ. PHASE SWITCH FOR THIS MODULE
C------          =  0    :   VAPOUR PHASE MIXTURES
C----            =  98   :   LIQUID PHASE MIX. FUGACITY COEFF.
C----            =  99   :   LIQUID PHASE EXCESS ENTHALPY OF MIXING
C
      IF (NPNRBL.EQ.99)  RETURN
      Z=NC+1
      CALL PEROBZ(AA,BB,Z)
      VZ(11)=ZMIX1
      ZMIX2=Z
      IF (NPNRBL.EQ.94) RETURN
      IF (NPNREL.EQ.95) RETURN
      ZBB=Z-BB
      TERM2=-ALOG(ZBB)
      TERM3=AA*ALOG((Z-0.414*BB)/(Z+2.414*BB))
      DO 90 I=1,NC
C
C-----FUG(J)=FUGACITY COEFFICIENT FOR COMPONENTS
C           IN A MIXTURE
C
      BIB=B(I)/BB1
      SAB(I)=SA(I)*2./AA1-BIB
      TERM(I)=(Z-1.)*BIB+TERM3*SAB(I)/BB/2.828
      TERM4=TERM2+TERM(I)
      FUG(I)=1.0
      FUG(I)=FUG(I)/EXP(TERM4)
90    CONTINUE
      IF (NDIM.EQ.0)GO TO 100
      CALL ONEDI(P,T,Y(NDIM),AK,ZDIM,ZNOD)
      DO 95 J=1,NC
95    FUG(J)=FUG(J)/ZNOD
      FUG(NDIM)=1./ZDIM
100   RETURN
      END
```

FORTRAN IV VER 59 SOURCE LISTING: PEROBZ SUBROUTINE 08/16/85 15:03:37

```
      SUBROUTINE PEROBZ(A,B,Z)
C
C-----THIS SUBROUTINE PREDICTS THE COMPRESSIBILITY FACTORS
C-----USING PENG-ROBINSON EQN.(CUBIC FORM)
C--------NEWTON-RAPHSON ALGORITHM IS UTILIZED;TOLERANCE
C-----FIGURE OF !DZ!/Z <=0.001 IS SPECIFIED.
C--------DEBUGGING AID;COMPONENT# UPON INVOCATION
C--------ITERATION LIMIT :100 LOOPS
C
C
      COMMON  /CMPRO/  NC,NCM1,IDLL,IDLV,IDH,LDBUG,ISW,NPNRBL,
     *                 NDIM,ZNAME(2,10),L(10),NTCOMP(10),
     *                 ITR,ITRMAX,NST,NSTM1,NK1,NK2,NK11,
     *                 NK21,NCASE,NFEED,NFTOP,NFBTM,LF(8),
     *                 IDCODE,ICODE
C
C
C
      K=Z
      Z=1.0
      IF(NPNRBL.EQ.99) Z=1.0E-2
      IF (NPNRBL.EQ.98) Z=1.0E-2
      J=0
      AB1=A-3.*B*B-2.*B
      AB2=A*B-B*B-B*B*B
      AB3=1.-B
150   FN=Z**3-Z**2*AB3+Z*AB1-AB2
      DF=3.*Z*Z-2.*Z*AB3+AB1
      DZ=-FN/DF
      J=J+1
      IF (J.GT.100) GO TO 200
      IF (ABS(DZ)/Z.LT.0.001)GO TO 250
      DZ=SIGN(AMIN1(ABS(DZ),0.1*Z,0.1),DZ)
      Z=Z+DZ
      GO TO 150
200   IF(NPNRBL.GT.0)Z=AMAX1(Z,0.1)
250   IF(LDBUG.EQ.2)WRITE(6,300)K,A,B,P,J,Z
300   FORMAT('***PEROBZ*K,A,B,P,J,Z**',I5,3G15.6,I5,G15.6)
      RETURN
      END
```

FORTRAN IV VER 59   SOURCE LISTING: DELTIJ SUBROUTINE 08/16/85 15:03:37

```
      SUBROUTINE DELTIJ(DIJ,DELTA)
C
C-----THIS SUBROUTINE SUPPLIES THE INTERACTION PARAMETERS
C-----FOR 20 COMPOUNDS SPECIFIED BY PENG-ROBINSON.
C-----THE VALUES ARE DERIVED EMPERICALLY THRU'
C-----BINARY VLE DATA.FOR THE REMAINING COMPOUNDS,
C-----THE VALUE IS ASSUMED TO BE ZERO.
C
C
      REAL           DIJ(10,10),DELTA(10)
      COMMON  /CMPRO/  NC,NCM1,IDLL,IDLV,IDH,LDBUG,ISW,NPNRBL,
     *                 NDIM,ZNAME(2,10),L(10),NTCOMP(10),
     *                 ITR,ITRMAX,NST,NSTM1,NK1,NK2,NK11,
     *                 NK21,NCASE,NFEED,NFTOP,NFBTM,LF(8),
     *                 IDCODE,ICODE
      COMMON /ZDATA/CPL(10,4),CPV(10,4),ENP(10,10),ANT(6,10),ADEL(10),
     *             W(10),AX,BX,OMEGA(10),AVAL(10),BVAL(10),MODEAF,
     *             AK(10,10),R(10),Q(10),XL(10),VOL(10),TB(10),
     *             C(180),ALPHA(45),VC(10),TC(10),PC(10),EVAP(10),
     *             OA(10),OB(10),AD(10,10),G(10,10),ZRA(10)
      COMMON  /SYSAA/  TITLE(20),COMPNT(20),KOMNAM(20)
      COMMON  /EQPA/  EQPAR(25,50),NEMAX,MAXEQP
      COMMON  /CONTL/ NIN,NOUT,NOCOMP,NE,NEN,KUNITS
      REAL     AIN(190)/66*0.0,0.036,0.05,0.08,0.095,
     *          0.09,0.095,7*0.1,0.13,0.135,2*0.13,
     *          3*0.125,0.1,0.115,2*0.11,-0.02,0.085,
     *          0.084,0.075,0.05,2*0.06,0.065,2*0.06,
     *          0.055,0.05,0.045,0.18,0.1,0.04,2*0.02,8*0.0,
     *          0.01,0.18,0.09,0.0,0.04,2*0.02,8*0.0,
     *          0.01,0.16,0.075,2*0.0,0.035,2*0.02,8*0.0,
     *          0.01,2*0.1,3*0.0,2*0.5,9*0.48,26*0.0/
      INTEGER     COMPN1(10)/10*0/
      REAL     S(60)/-1.5240,0.5328E-02,-0.3982E-05,-0.9682,
     *              0.3384E-02,-0.2354E-05,-1.038,
     *              0.3601E-02,-0.2739E-05,-9.9931,
     *              0.3166E-02,-0.2333E-05,-0.9931,
     *              0.3166E-02,-0.2333E-05,-0.9246,
     *              0.3045E-02,0.2276E-05,21*0.0,
     *              -2.238,0.67E-02,-0.4686E-05,-0.5572,
     *              0.1879E-02,-0.1274E-05,-0.3896,
     *              0.1565E-02,-0.1142E-05,15*0.0/
C
C
C
      DO 100 I=1,NC
C
C-----THE PURE COMPONENT ID#S ARE MATCHED
C     IN THIS LOOP.THE COMPONENTS
C     NOT ENCOUNTERED REMAIN WITH AN ID#
C     OF ZERO.
C
      COMPN1(I)=0
      IF(NTCOMP(I).EQ.2)COMPN1(I)=1
      IF(NTCOMP(I).EQ.3)COMPN1(I)=2
      IF(NTCOMP(I).EQ.4)COMPN1(I)=3
      IF(NTCOMP(I).EQ.5)COMPN1(I)=4
```

```
      IF(NTCOMP(I).EQ.6)COMPN1(I)=5
      IF(NTCOMP(I).EQ.7)COMPN1(I)=6
      IF(NTCOMP(I).EQ.8)COMPN1(I)=7
      IF(NTCOMP(I).EQ.10)COMPN1(I)=8
      IF(NTCOMP(I).EQ.11)COMPN1(I)=9
      IF(NTCOMP(I).EQ.12)COMPN1(I)=10
      IF(NTCOMP(I).EQ.13)COMPN1(I)=11
      IF(NTCOMP(I).EQ.14)COMPN1(I)=12
      IF(NTCOMP(I).EQ.46)COMPN1(I)=13
      IF(NTCOMP(I).EQ.49)COMPN1(I)=14
      IF(NTCOMP(I).EQ.50)COMPN1(I)=15
      IF(NTCOMP(I).EQ.41)COMPN1(I)=16
      IF(NTCOMP(I).EQ.40)COMPN1(I)=17
      IF(NTCOMP(I).EQ.38)COMPN1(I)=18
      IF(NTCOMP(I).EQ.62)COMPN1(I)=19
  100 CONTINUE
      IF(NC.EQ.1)GO TO 375
      NC1=NC-1
      DO 300 II=1,NC1
      I=COMPN1(II)
      NC2=II+1
      DIJ(II,II)=0.0
      DO 300 JJ=NC2,NC
      J=COMPN1(JJ)
      IF(J.LT.I)GO TO 250
      KIJ=I+(J-1)*(J-2)/2
      GO TO 270
  250 KIJ=J+(I-1)*(I-2)/2
  270 DIJ(JJ,II)=AIN(KIJ)
      DIJ(II,JJ)=DIJ(JJ,II)
  300 CONTINUE
      IF (MODEAF.NE.1)GO TO 315
C-----IN THE CASES OF SPECIFIED ENTHALPY FLASH
C-----CALCULATIONS,CERTAIN 1<-->1 INTERACTION
C-----COEFFICIENTS ARE REDEFINED.
      DO 310 I=2,NC
      IF(COMPN1(I).EQ.0)GO TO 310
      J=COMPN1(I)
      KK=3*(J-1)
      DELTA(I)=S(KK+1)+(S(KK+2)+T*S(KK+3))*T
  310 CONTINUE
      GO TO 400
  315 CONTINUE
      DO 350 MN=1,NC
      IF(NTCOMP(MN).NE.62) GO TO 350
      DO 350 I=2,NC
      DELTA(I)=DIJ(I,1)
      IF(NTCOMP(MN).NE.49)GO TO 320
      DELTA(I)=S(40)+(S(41)+S(42)*T)*T
      GO TO 350
  320 IF(NTCOMP(MN).NE.50)GO TO 350
      DELTA(I)=S(43)+(S(44)+S(45)*T)*T
  350 CONTINUE
      GO TO 400
  375 DELTA(1)=0.0
      DIJ(1,1)=0.0
  400 RETURN
      END
```

```
FORTRAN IV  VER 59   SOURCE LISTING: SRKZ    SUBROUTINE  08/16/85  15:03:37
        SUBROUTINE SRKZ(AS,BS,P,T,Z)
C
C
C-----THIS SUBROUTINE USES THE NEWTON-RAPHSON
C-----ALGORITHM TO SOLVE THE 'SRK' EQN.FOR (IN
C-----THE CUBIC FORM)COMPRESSIBILITY FACTOR, Z .
C-----THE TOLERANCE LIMIT IS:!DZ!/Z<0.001
C--------WHEN IT FAILS TO CONVERGE WITHIN
C-----50 ITERATIONS,THE MAX.OF 0.3 OR LAST
C-----Z VALUE IS CHOSEN.
C
C
        COMMON/CNTRL/NCR,NPRT
        COMMON/CMPRO/NC,NCM1,IDLL,IDLV,IDH,LDBUG,ISW,NPNRBL,NDIM,
       *             ZNAME(2,10),L(10),NTCOMP(10),ITR,ITRMAX,
       *             NST,NSTM1,NK1,NK2,NK11,NK21,NCASE,NFEED,
       *             NFTOP,NFBTM,LF(8),IDCODE,ICODE
C
C
C-----Z WAS INITIALIZED TO J OR NC+1 BEFORE
C-----INVOCATION; SO THAT IF THIS ROUTINE
C-----DOES NOT CONVERGE,THE VALUE OF K WOULD
C-----INDICATE (FOR A MIXTURE& A PURE COMP.,RESPECTIVELY)
C-----THE COMPONENT WHOSE Z FAILED TO CONVERGE.
C
        K=Z
        J=0
        A=AS
        B=BS
        D=(A-B-B*B)
C----- Z IS REINITIALIZED TO 1.
        Z=1.
 10     FN=Z**3-Z**2+D*Z-A*B
        DF=3.*Z*Z-2.*Z+D
        DZ=-FN/DF
        J=J+1
        IF (J.GT.50)GO TO 30
        IF(ABS(DZ)/Z.LT.0.001)GO TO 50
        DZ=SIGN(AMIN1(ABS(DZ),0.1*Z,0.1),DZ)
        Z=Z+DZ
        GO TO 10
 30     Z=AMAX1(Z,0.3)
 50     IF (LDBUG.EQ.2)WRITE(NPRT,60)K,A,B,P,J,Z
 60     FORMAT('***SZCALC***K,A,B,P,J,Z**:',I5,3G15.6,I5,G15.6)
        RETURN
        END
```

```
      SUBROUTINE FUGCY (T,P,Y,VP,F,DH)
C
C
      REAL                 Y(10), VP(10), F(10)
C
      COMMON  /CMPRO/  NC,NCM1,IDLL,IDLV,IDH,LDBUG,ISW,NPNRBL, NCIM,
     *                 ZNAME(2,10), L(10), NTCOMP(10), ITR, ITRMAX,
     *                 NST, NSTM1, NK1, NK2, NK11, NK21, NCASE, NFEED,
     *                 NFTOP, NFBTM, LF(8),IDCODE,ICODE,CPCODE(10)
      COMMON  /ZDATA/ CPL(10,4),CPV(10,4),ENP(10,10),ANT(6,10),ADEL(10),
     *                 W(10),AX,BX,OMEGA(10),AVAL(10),BVAL(10),MODLAF,
     *                 AK(10,10), R(10), Q(10), XL(10),VOL(10),TB(10),
     *                 C(180), ALPHA(45),VC(10),TC(10),PC(10),EVAP(10),
     *                 OA(10), OB(10), AA(10,10), G(10,10), ZRA(10)
C
C
      GO TO (10,20,30,20,20,60), IDLV
C
   10 CALL VIRFG (T,P,Y,VP,F,DH)
      GO TO 100
   20 CALL RKFUG (T,P,Y,VP,F,DH,DSV)
      GO TO 100
30    CALL SRKFUG(T,P,Y,VP,F,DH,DSV)
      GO TO 100
60    NPNRBL=0
      CALL PENROB(T,P,Y,VP,F,DH,DSV)
      DO 62 I=1,NC
62    CONTINUE
      NPNRBL=0
C
  100 RETURN
      END


      SUBROUTINE SRKFUG(T,P,Y,VP,FUG,DHV,DSV)
C
C
C
C-----THIS SUBPROGRAM USES THE 'SOAVE-REDLICH-KWONG'
C-----EQUATION OF STATE TO PREDICT;  .FUGACITY
C-----COEFFICIENTS FOR PURE COMPONENTS &
C-----AND FOR COMPONENTS IN A VAPOR MIXTURE,  .THE
C-----ENTHALPY &   .THE ENTROPY  DEPARTURE FUNCTIONS
C-----FOR A VAPOR MIXTURE.
C---------CORRECTIONS ARE ALSO DONE WHEN DIMERS ARE
C-----EXPECTED TO BE PRESENT IN THE VAPOR PHASE.
C
C
C
      REAL              Y(10),VP(10),FUG(10),F(10)
      REAL              AP(10),AM(10),TR(10),PR(10),A(10),B(10)
C
C
      COMMON   /CMPRO/  NC,NCM1,IDLL,IDLV,IDH,LDBUG,ISW,NPNRBL,
```

```
     *                       NDIM,ZNAME(2,10),L(10),NTCOMP(10),
     *                       ITR,ITRMAX,NST,NSTM1,NK1,NK2,NK11,
     *                       NK21,NCASE,NFEED,NFTOP,NFBTM,LF(6),
     *                       IDCODE,ICODE
      COMMON /ZDATA/  CPL(10,4),CPV(10,4),ENP(10,10),ANT(6,10),ADEL(10),
     *                W(10),AX,BX,OMEGA(10),AVAL(10),BVAL(10),MODEAF,
     *                AK(10,10),R(10),Q(10),XL(10),VOL(10),TB(10),
     *                C(180),ALPHA(45),VC(10),TC(10),PC(10),EVAP(10),
     *                OA(10),OB(10),AD(10,10),G(10,10),ZRA(10)
      COMMON  /STREAM/   TX,PX,Z1(10),Y1(10),X(10),FRACV,ZVAP,
     *                   EK(10),VP1(10),FUG1(10),GAM(10),VZ(11),SVAP,
     *                   HOFZ,HVAP,HLIQ,DHV1,DSV1,XSH,DSL,NOBUB,NODEW
      COMMON  /SYSAA/    TITLE(20),COMPNT(20),KOMNAM(80)
      COMMON  /MIX/    FMIX,ZMIX,BMIX,AA1,BB,BB1,ZMX
C
C
C
C      UNITS USED HERE:
C                         P=ATM
C                         V=CC/GRAM-MOLE
C                         T=DEGREES KELVIN
C
C
C
      AA=0.0
      BB=0.0
      HH=0.0
      CC=0.0
      TT=0.0
      DO 100 J=1,NC
C-----A(J),B(J) :PARAMETERS IN THE SRK-EQN. OF STATE
C------AM(J)    :TEMP.DEPENDENT FACTOR OF A(J)
C                IT IS A FUNCTION OF ACCENTRIC FACTOR ALSO.
C
      AM(J)=0.47979+((0.025*OMEGA(J)-0.1925)*OMEGA(J)+1.574)*OMEGA(J)
      TR(J)=T/TC(J)
      P1=1.0+AM(J)*(1.-SQRT(TR(J)))
      AP(J)=P1**2
      PR(J)=P/PC(J)
      A(J)=0.42747*AP(J)*PR(J)/TR(J)/TR(J)
      B(J)=0.08664*PR(J)/TR(J)
100   CONTINUE
      DO 150 J=1,NC
C-----HERE,THE SUGGESTED MIXING RULES ARE APPLIED
C-----TO DETERMINE THE PARAMETERS FOR A MIXTURE.
C---------ALSO CALCULATED ARE: A PART OF THE ENTHALPY
C-----AND ENTROPY DEP.FUNCTIONS  . THE MIXTURE "F" FACTOR.
C
      BB=BB+B(J)*Y(J)
      F(J)=AP(J)/TR(J)
      HHJ=0.5*AM(J)*SQRT(TR(J)/AP(J))
      DO 150 I=1,NC
      D1=SQRT(A(I)*A(J))*(1.-AK(I,J))
      AA=AA+D1*Y(I)*Y(J)
      HH=HH+(1.0-HHJ-0.5*AM(I)*SQRT(TR(I)/AP(I)))*D1*Y(I)*Y(J)
150   CONTINUE
      AA1=AA
      IF (IDLL.EQ.4) GO TO 31
```

```
      DO 30 J=1,NC
      IF(Y(J).EQ.0.0)GO TO 30
      Z=J
      VZ(J)=1.0
C-----L(J)=   -1 FOR NON-VOLATILES
C              0 FOR NON-CONDENSIBLES
C              1 FOR NORMAL CONDITIONS
C              2 FOR SUPER-CRITICALS
C
      IF (L(J)-1)30,20,10
10    FUG(J)=EXP(VOL(J)*P/82.05/T)
      GO TO 30
20    CALL SRKZ(A(J),B(J),VP(J),T,Z)
      VZ(J)=Z
      FUG(J)=EXP(Z-1.0)/((Z-B(J))*((1.0+B(J)/Z)**(A(J)/B(J))))
     *                  *FUG(J)
30    CONTINUE
31    Z=NC+1
C-----THE 'Z' FACTOR FOR A MIXTURE
C
      CALL SRKZ(AA,BB,P,T,Z)
      ZMIX=Z
      ZMX=ZMIX
      VZ(11)=Z
      FN=(Z-1.0)/BB
      DF=ALOG(Z-BB)
      DZ=AA/BB*ALOG(1.0+BB/Z)
C-----THE MIXTURE ENTHALPY DEPARTURE,DHV
C
C     WRITE(6,1228) HH,AA,BB
1228  FORMAT('***SRKFUG++++',' HH AA BB',F20.6,F20.10,F20.13)
      DHV=1.9872*T*(Z-1.-HH/BB*ALOG(1.0+BB/Z))
      DHV1=DHV
      DO 40 J=1,NC
      IF (IDLL.EQ.4) FUG(J)=1.0
      FUG(J)=FUG(J)/EXP(FN*B(J)-DF-DZ*(2.*SQRT(A(J)/AA)-B(J)/
     *       BB))
40    CONTINUE
41    DO 50 J=1,NC
      TT=TT+Y(J)*TC(J)/PC(J)
      DO 50 I=1,NC
      C1=TC(I)*TC(J)/PC(J)/PC(J)*F(I)*F(J)
      C2=SQRT(C1)
      C3=Y(I)*Y(J)*(1.-AK(I,J))*C2
      CC=CC+C3
50    CONTINUE
      FMIX=CC/TT
C-----MIXTURE ENTROPY DEPARTURE
C
      SS=HH-2*NCOUNT
      SS=SS/BB
      BPRT=BB*P/T/1.9872
      DSV=1.9872*(ALOG(1.0-BPRT/Z)-SS*ALOG(1.0+BPRT/Z)+ALOG(Z))
      DSV1=DSV
      IF (NDIM.EQ.0)GO TO 70
      CALL ONEDI(P,T,Y(NDIM),AK,ZDIM,ZNOD)
      DO 60 J=1,NC
C-----IF DIMERS WERE EXPECTED
60    FUG(J)=FUG(J)/ZNOD
      FUG(NDIM)=1.0/ZDIM
70    RETURN
      END
```

```
      SUBROUTINE KCALC
C     WRITE (6,99999)
C9999 FORMAT(' ',113X,'SUBROUTINE KCALC')
C
C     ROUTINE TO CALCULATE K VALUES
C
C
      COMMON  /SYSAA/  TITLE(20),COMPNT(10),KOMNAM(40)
      COMMON  /SYSC/   LIMIT, LIMIT2, LIMIT3, LOOP, LOOPS
      COMMON  /CMPRO/  NC,NCM1,IDLL,IDLV,IDH,LDBUG,ISW,NPNREL, NDIM,
     *                 ZNAME(2,10), L(10), NTCOMP(10), ITR, ITRMAX,
     *                 NST, NSTM1, NK1, NK2, NK11, NK21, NCASE, NFEED,
     *                 NFTOP, NFBTM, LF(8),IDCODE,ICODE,CPCODE(10)
      COMMON  /ZDATA/ CPL(10,4),CPV(10,4),ENP(10,10),ANT(6,10),ADEL(10),
     *                 W(10),AX,BX,OMEGA(10),AVAL(10),BVAL(10),MODEAF,
     *                 AK(10,10), R(10), Q(10), XL(10),VOL(10),TB(10),
     *                 C(180), ALPHA(45),VC(10),TC(10),PC(10),EVAP(10),
     *                 OA(10), OB(10), AA(10,10), G(10,10), ZRA(10)
      COMMON  /STREAM/ T, P, Z(10), Y(10), X(10), FRACV, ZVAP,
     *                 EK(10), VP(10), FUG(10),GAM(10),VZ(11),SVAP,
     *                 HOFZ, HVAP,HLIQ,DHV,DSV,XSH,DSL,NOBUB,NODEW
      REAL  KOMNAM
      REAL            XSAT(10),PSFUG(10),SFUG(10)
      INTEGER               COMPNT
C
C
      TT=T
C
      DHV=0.0
      NPNRBL=0
C
      IF (ISW.NE.0) GO TO 10
      DO 9 J=1,NC
      FUG(J)=1.0
      GAM(J)=1.0
      VP(J)=EXP(ANT(1,J)+ANT(2,J)/(ANT(3,J)+T)+ANT(5,J)*T+ANT(6,J)*T
     *      *T+ANT(4,J)*ALOG(T))
      VP(J)=VP(J)/760.00
    9 CONTINUE
C
   10 IF (NDIM.EQ.0) GO TO 40
      CALL ONEDI (P,TT,Y(NDIM),AKA,ZDIM,ZNODIM)
      VP(NDIM)=(SQRT(1.0+4.0*AKA*VP(NDIM))-1.0)/2.0/AKA
C
C
   40 IF (IDLV.EQ.0) GO TO 100
      CALL FUGCY (TT,P,Y,VP,FUG,DHV)
C
  100 IF (IDLL.EQ.0) GO TO 140
      CALL ACTVY (TT,X,GAM)
      ISW=0
  140 DO 150 J=1,NC
C
C-----IF IDLV=4  :  CHAO- SEADER DEFINITION IS USED
C
C-----FUG(J)     HAS INVERSE OF VAP. PHASE MIX. FUGACITY
C-----           COEFFICIENTS.
C
  145 EK(J)=VP(J)/P*GAM(J)*FUG(J)
      IF (IDLV.EQ.6) EK(J)=FUG(J)*GAM(J)
      IF (IDLV.EQ.0.AND.IDLL.EQ.0)EK(J)=VP(J)/P
150   IF(IDLL.EQ.4)EK(J)=GAM(J)*FUG(J)
200   CONTINUE
      RETURN
      END
```

```
      SUBROUTINE ACTVY (T,X,G)
C
C
      REAL         G(10),NU(10),XRET(10),PFUG(10),QFUG(10),X(10)
C
      COMMON  /CMPRO/  NC,NCM1,IDLL,IDLV,IDH,LDBUG,ISW,NPNRBL, NDIM,
     *                 ZNAME(2,10), L(10), NTCOMP(10), ITR, ITRMAX,
     *                 NST, NSTM1, NK1, NK2, NK11, NK21, NCASE, NFEED,
     *                 NFTOP, NFBTM, LF(8),IDCODE,ICODE,CPCODE(10)
      COMMON  /ZDATA/ CPL(10,4),CPV(10,4),ENP(10,10),ANT(6,10),ADEL(10),
     *                 W(10),AX,BX,OMEGA(10),AVAL(10),BVAL(10),MODEAF,
     *                 AK(10,10), R(10), Q(10), XL(10),VOL(10),TB(10),
     *                 C(180), ALPHA(45),VC(10),TC(10),PC(10),EVAP(10),
     *                 OA(10), OB(10), AA(10,10), G1(10,10), ZRA(10)
      COMMON  /STREAM/ T, P, Z(10), Y(10), X1(10), FRACV, ZVAP,
     *                 EK(10), VP(10), FUG(10),GAM(10),VZ(11),SVAP,
     *                 HOFZ, HVAP,HLIQ,DHV,DSV,XSH,DSL,NOBUB,NODEW
C
      GO TO (10,20,30,40,20,50), IDLL
   10 CALL WILSN (T,X,G)
      GO TO 100
   20 CALL RENON (T,X,G)
      GO TO 100
   30 CALL UNQAC (T,X,G)
      GO TO 100
40    CALL CHAOSD(T,P,X,Y,NU,G,DHL,DSL)
      GO TO 100
50    NPNRBL=98
C----------THIS SWITCH IS FOR LIQUID PHASE
C-----------COMPUTATIONS IN 'PENROB'
      DO 70 J=1,NC
      VP(J)=EXP(ANT(1,J)+ANT(2,J)/(T+ANT(3,J))+ANT(4,J)*ALOG(T)
     *              +ANT(5,J)*T+ANT(6,J)*T*T)
      VP(J)=VP(J)/760.00
70    CONTINUE
      CALL PENROB(T,P,X,VP,PFUG,XSH,DSL)
      DO 80 I=1,NC
      G(I)=1.0/PFUG(I)
80    CONTINUE
C
      NPNRBL=0
  100 RETURN
      END
```

```
      SUBROUTINE CHAOSD(T,P,X,Y,NU,GAMA,DHL,DSL)
C
C
C
C-----THIS SUBPROGRAM EMPLOYS THE 'CHAO-SEADER'
C-----EMPERICAL CORRELATIONS & THE REGULAR
C-----SOLUTION THEORY TO PREDICT;  .ACTIVITY COEFFICIENT
C-----(GAMA) ,       .PURE COMPONENT(AS PAR 'COMPID')
C-----LIQUID PHASE FUGACITY COEFFICIENT(NU),  .ENTHALPY
C-----DEPARTURE(DHL),  .ENTROPY DEPARTURE(DSL).
C--------THE FUG.COEFFICIENTS FOR VAPOR MIXTURES IS
C-----GENERATED VIA 'RK' EQN. AS SUGGESTED BY
C-----CHAO-SEADER.
C
C
C
      REAL      NU(10),PHI(10),LAMDA(10),DELTA(10),DELZV(10)
      REAL      NU1,TR(10),PR(10),TBR(10),VL(10),Y1(10)
      REAL      CH(10),CH2(10),DE(10,10),CP(10,15)
      REAL      X(10),Y(10),K(10),GAMA(10),FUG(10)
      COMMON/SYSAA/    TITLE(20),COMPNT(20),KOMNAM(80)
      COMMON/CMPRO/    NC,NCM1,IDLL,IDLV,IDH,LDBUG,ISW,NPNRBL,NDIM,
     *                 ZNAME(2,10),L(10),NTCOMP(10),ITR,ITRMAX,
     *                 NST,NSTM1,NK1,NK2,NK11,NK21,NCASE,NFEED,
     *                 NFTOP,NFBTM,LF(8),IDCODE,ICODE
      COMMON /ZDATA/CPL(10,4),CPV(10,4),ENP(10,10),ANT(6,10),ADEL(10),
     *             W(10),AX,BX,OMEGA(10),AVAL(10),BVAL(10),MODEAF,
     *             AK(10,10),R(10),Q(10),XL(10),VOL(10),TB(10),
     *             C(180),ALPHA(45),VC(10),TC(10),PC(10),EVAP(10),
     *             OA(10),OB(10),A(10,10),G(10,10),ZRA(10)
      DATA     CT1,CT2,CT3,CT4,CT5,CT6,CT7,CT8,CT9,CT10/10*0.0/
      DATA     CH1,CM1,CN1,CN2,CN3/5*0.0/
      REAL      CP0(15)/-2.10899,0.0,-0.19396,0.02282,0.08852,
     *                 0.0,-0.00872,-0.00353,0.00203,
     *                 -4.23893,8.65808,-1.2206,-3.15244,
     *                 -0.025,2.05135/
      REAL      CP1(15)/2.74283,-0.0211,0.00011,0.0,0.008585,
     *                 9*0.0,1.50709/
      REAL      CP2(15)/-1.54831,0.0,0.02889,-0.01076,
     *                 0.10486,-0.02529,8*0.0,1.36822/
C
C
C
      DO 100 I=1,NC
      IF (NTCOMP(I).EQ.1)GO TO 101
      IF (NTCOMP(I).EQ.2)GO TO 102
      DO 103 J=1,15
      CP(I,J)=CP0(J)
  103 CONTINUE
      GO TO 100
  101 DO 111 J=1,9
  111 CP(I,J)=CP1(J)
      DO 1111 J=10,14
      CP(I,J)=CP0(J)
 1111 CONTINUE
      CP(I,15)=CP1(15)
```

```
      GO TO 100
102   DO 112 J=1,9
112   CP(I,J)=CP2(J)
      DO 1122 J=10,14
      CP(I,J)=CP0(J)
1122  CONTINUE
      CP(I,15)=CP2(15)
100   CONTINUE
C
C
      SMALL=1.0E-20
C
C
      DO 200 I=1,NC
      IF (X(I).LE.SMALL) GO TO 200
C-----VL(I) GIVES THE PURE SPECIES MOLAL VOLUME
C-----CORRECTED FOR THE EXCESS VOLUME OF MIXING,
C-----AS SUGGESTED IN THE EMPERICAL CORRELATION.
C-----IT IS ASSUMED TO BE A FUNCTION OF TEMP.,
C-----PRESSURE & ACCENTRICITY ONLY.
C--------CP(I,N) ARE THE GRAYSON-STREED COEFFICIENTS
C-----FOR CHAO-SEADER EQUATIONS(LIQ.PHASE FUGACITY,
C-----MOLAL VOLUME,ENTHALPY & ENTROPY).THE VALUES
C-----FOR ALL COMPOUNDS EXEPT METHANE & HYDROGEN
C-----ARE THE SAME.
C--------NU(I) ARE THE PURE SPECIES LIQ.PHASE
C-----FUGACITY COEFFICIENTS.
C--------A PART OF ENTHALPY DEPARTURE IS ALSO
C-----CALCULATED (CH(I)) IN THIS LOOP.
C
C
      TR(I)=T/TC(I)
      PR(I)=P/PC(I)
      CT1=CP(I,6)*TR(I)
      CT2=CP(I,7)*TR(I)*TR(I)
      CT3=2.*(CP(I,8)+CP(I,9)*TR(I))
      CT4=CP(I,5)+CT1+CT2+OMEGA(I)*CP(I,14)+CT3
      VL(I)=CT4*2.30258*82.053*T/PC(I)
      CT5=CP(I,11)-CP(I,12)/TR(I)/TR(I)
      CT5=CT5+3.*CP(I,13)*TR(I)*TR(I)
      CT6=CT5*OMEGA(I)
      CT7=2.*CP(I,7)*TR(I)+CP(I,6)
      CT8=2.*CP(I,3)+3.*CP(I,4)*TR(I)
      CT9=CP(I,2)-CP(I,1)/TR(I)/TR(I)
      CT10=CP(I,9)*PR(I)*PR(I)
      CH1=CT9+TR(I)*CT8
      CH1=CH1+CT7*PR(I)
      CH1=CH1+CT10+CT6
      CH(I)=2.30258*1.987*CH1*T*TR(I)
      CN1=CP(I,15)+CP(I,1)/TR(I)+CP(I,2)*TR(I)
      CN1=CN1+CP(I,3)*TR(I)*TR(I)
      CN1=CN1+CP(I,4)*TR(I)**3
      CN1=CN1-ALOG(PR(I))/2.30258
      CN2=CP(I,5)+CP(I,6)*TR(I)
      CN2=CN2+CP(I,7)*TR(I)**2
      CN2=CN2*PR(I)
```

```
      CN3=CP(I,8)+CP(I,9)*TR(I)
      CN3=CN3*PR(I)**2
      CN1=CN1+CN2+CN3
      IF (TR(I).GE.1.0) TR(I)=1.0
C-----THIS MODIFICATION IS IN ACCORDANCE WITH
C-----GRAYSON & STREED :REF-'CHESS' ORIGINAL VERSION.
C-----THE FACTOR OF OMEGA IN LOG(NU(I)) IS EVALUATED
C-----ONLY UPTO THE CRITICAL TEMP. BEYOND WHICH
C-----IT BECOMES ERRONEOUS TO USE TR(I) > 1 VALUES.
      CM1=CP(I,10)+CP(I,11)*TR(I)
      CM1=CM1+CP(I,12)/TR(I)
      CM1=CM1+CP(I,13)*TR(I)**3
      CM1=CM1+CP(I,14)*(PR(I)-.6)
      NU1=CN1+OMEGA(I)*CM1
      NU(I)=(10.00)**(NU1)
200   CONTINUE
      AX=0.0
      DO 320 I=1,NC
      IF (X(I).LE.SMALL) GO TO 320
C--------DELTA(I) IS THE SOLUBILITY PARAMETER.
C--------AX IS THE LIQ.-PHASE MOLAL VOLUME.
C
C
      DELTA(I)=ADEL(I)*SQRT(82.057/1.987)
      AX=AX+X(I)*VL(I)
320   CONTINUE
      IF(AX.EQ.0.0)AX=0.0001
      DO 400 I=1,NC
      IF (X(I).LE.SMALL) GO TO 400
C-----PHI(I) IS THE VOLUME FRACTION
C-----ASSUMING ADDITIVE MOLAL VOLUMES.
C
      PHI(I)=X(I)*VL(I)/AX
400   CONTINUE
      SUMD=0.0
      DHL=0.0
      DSL=0.0
      DO 500 I=1,NC
      IF (X(I).LE.SMALL) GO TO 500
C-----SUMD IS THE SECOND PART OF THE
C-----ENTHALPY DEP. FUNCTION
C
      SUMD=SUMD+PHI(I)*DELTA(I)
500   CONTINUE
      DO 510 I=1,NC
      IF (X(I).LE.SMALL) GO TO 510
C-----GAMA(I) IS THE ACTIVITY COEFF. IN THE
C-----REGULAR SOLUTION;INCLUDES FLORY-HUGGINS'
C-----CORRECTION.
C--------DHL IS ENTHALPY DEPARTURE.
C
C
      D1=DELTA(I)-SUMD
      D1=D1**2
      IF (VL(I).LE.0.0)VL(I)=VOL(I)
      D2=VL(I)*D1/T/82.053
```

```
      GAMA(I)=EXP(D2+1.-VL(I)/AX+ALOG(VL(I)/AX))
C-----THE NUMERATOR OF THE "K-FACTOR" EXPRESSION
C-----IS LUMPED IN THE FOLLOWING  :
      GAMA(I)=GAMA(I)*NU(I)
C
      CH(I)=-CH(I)
      CH2(I)=VL(I)*D1
      DHL=DHL+X(I)*(CH(I)+CH2(I))
 510  CONTINUE
      DO 650 I=1,NC
      IF (X(I).LE.SMALL) GO TO 650
      DELT1=DELTA(I)
      DO 650 J=1,NC
      IF (X(J).LE.SMALL) GO TO 650
      DELT1=(DELT1-DELTA(J))
      DE(I,J)=DELT1**2
 650  CONTINUE
      DSUM=0.0
      GSUM=0.0
      HSUM=0.0
      DO 750 I=1,NC
      IF(X(I).LE.SMALL) GO TO 750
      DO 750 J=1,NC
      IF(X(J).LE.SMALL) GO TO 750
C-----GSUM IS THE DEPARTURE IN THE GIBB'S
C-----FREE ENERGY.
C---------DSL IS THE ENTROPY DEPARTURE
C-----ESTIMATED BY DEFINITION,T*SS=HH-GG.
C
C
      DSUM=DSUM+DE(I,J)*PHI(I)*PHI(J)
      HSUM=HSUM+X(I)*CH2(I)
 750  CONTINUE
      DO 700 I=1,NC
      IF (X(I).LE.SMALL) GO TO 700
      GSUM=GSUM+.5*DSUM*X(I)*VL(I)
 700  CONTINUE
      DSL1=(HSUM-GSUM)/T
      DSL2=0.0
      DO 850 I=1,NC
      IF (X(I).LE.SMALL) GO TO 850
      PGFAC = GAMA(I)*P*X(I)
      DSL2=DSL2+X(I)*((CH(I)+CH2(I))/T-1.9872*ALOG(NU(I)*PGFAC))
 850  CONTINUE
      DSL=DSL1+DSL2
      RETURN
      END
```

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```
      FUNCTION DELCPS(T,P,Y,CPCV)
C
C
C-----THIS FUNCTION PREDICTS THE HEAT CAPACITY FUNCTIONS FOR A
C-----REAL GAS MIXTURE USING THE SOAVE-REDLICH-KWONG EQUATION.
C
C
      COMMON /SYSAA/  TITLE(20),COMPNT(10),KOMNAM(40)
      COMMON /CONTL/  NIN,NOUT,NOCOMP,NE,NEN,KUNITS
      COMMON /STRMIN/ SINUM(4),SIFLAG(4),SIVPFR(4),SITEMP(4),SIPRES(4),
     *                SIENTH(4),SIVISC(4),SITHK(4),SIZ(4),SIS(4),
     *                SIMOLE(4),SICOMP(10,4),SIKV(10,4)
      COMMON  /CMPRO/  NK, NCM1,IDLL,IDLV,IDH,LDBUG,ISW,NPNRBL, NDIM,
     *                 ZNAME(2,10), L(10), NTCOMP(10), ITR, ITRMAX,
     *                 NST, NSTM1, NK1, NK2, NK11, NK21, NCASE, NFEED,
     *                NFTOP, NFBTM,LF(8),IDCODE,ICODE,CPCODE(10)
      COMMON /ZDATA/ CPL(10,4),CPV(10,4),ENP(10,10),ANT(6,10),ADEL(10),
     *              W(10),AX,BX,OMEGA(10),AVAL(10),BVAL(10),MODEAF,
     *              AK(10,10),R(10),Q(10),XL(10),VOL(10),TB(10),
     *              C(180),ALPHA(45),VC(10),TC(10),PC(10),EVAP(10),
     *              OA(10),OB(10),A(10,10),G(10,10),ZRA(10)
      COMMON /MIX/   FMIX,ZMIX,BMIX,AA1,BB,BB1,ZMX
      REAL            Y(10),THETA(10),B(10),TAU(10,10),FF(10),VP(10)
C     WRITE(6,99999)
C9999 FORMAT(' ','FUNCTION DELCPS')
C
C
      OMM=0.0
      BMIX=0.0
      SUM1=0.0
      SUM2=0.0
      SUM3=0.0
      DO 10 I=1,NOCOMP
      OMM=OMM+Y(I)*OMEGA(I)
      THETA(I)=Y(I)*VC(I)**(2./3.)
      SUM1=SUM1+THETA(I)
      B(I)=0.08664*82.057*TC(I)/PC(I)
      VP(I)=EXP(ANT(1,I)+ANT(2,I)/(ANT(3,I)+T)+ANT(5,I)*T+
     *            ANT(6,I)*T*T+ANT(4,I)*ALOG(T))
      VP(I)=VP(I)/760.00
10    CONTINUE
      DO 20 I=1,NOCOMP
      BMIX=BMIX+B(I)
      THETA(I)=THETA(I)/SUM1
20    SUM2=SUM2+THETA(I)*TC(I)
      DO 30 I=1,NOCOMP
      DO 30 J=1,NOCOMP
      K=NTCOMP(I)
      DEL=ABS((TC(I)-TC(J))/(TC(I)+TC(J)))
      TAU(I,J)=SHI(K,DEL)*(TC(I)+TC(J))/2.0
      IF (I.EQ.J) TAU(I,J)=0.0
30    CONTINUE
      DO 40 I=1,NOCOMP
      DO 40 J=1,NOCOMP
40    SUM3=SUM3+THETA(I)*THETA(J)*TAU(I,J)
      TCM=SUM2+SUM3
```

```
      TRM=T/TCM
      YTPC=0.0
      DO 41 J=1,NOCOMP
   41 YTPC=YTPC+Y(J)*TC(J)/PC(J)
      PCM=TCM/YTPC
      AL1=0.48+((0.025*OMM-0.1925)*OMM+1.576)*OMM
      AL2=1.0+AL1*(1.0-SQRT(TRM))
      ALFM=AL2*AL2
      CALL SRKFUG(T,P,Y,VP,FF,DD,SS)
      AMIX=AA1
      ACMIX=AMIX/ALFM
      AL3=AL1*SQRT(TRM)
      AMEG1=AL3*(AL3-AL1-1.0)
      H=BMIX*P/ZMIX
      T1=(1.0+H)/(1.0-H)
      T2=2.0*ACMIX*AMEG1*H/BMIX/82.057/T
      T3=(H*ACMIX*AMEG1/BMIX/82.057/T)**2/T1
      T4=H*(2.0+H)*ACMIX*ALFM/BMIX/82.057/T
      T4=T4/T1
      CPCV=(T1-T2+T3)/(T1-T4)
      T5=ACMIX*AL1*(AL1+1.0)*ALOG(1.0+H)
      T5=T5*SQRT(TRM)/BMIX/T/2.0/82.057
      DELCPS=(T5+CPCV-1.0)*1.9872
      CPCV=CPCV*1.9872
      RETURN
      END
```

```
      FUNCTION DELCPR(T,P,Y,CPCV)
C
C
C
C-----USES PENG-ROBINSON EQN. TO PREDICT THE SPECIFIC HEAT
C-----FUNCTIONS FOR A REAL GAS MIXTURE.
C
C
      COMMON /CONTL/  NIN,NOUT,NOCOMP,NE,NEN,KUNITS
      COMMON /SYSAA/  TITLE(20),COMPNT(10),KOMNAM(40)
      COMMON /STRMIN/ SINUM(4),SIFLAG(4),SIVPFR(4),SITEMP(4),SIPRES(4),
     *                SIENTH(4),SIVISC(4),SITHK(4),SIZ(4),SIS(4),
     *                SIMOLE(4),SICOMP(10,4),SIKV(10,4)
      COMMON /ZDATA/ CPL(10,4),CPV(10,4),ENP(10,10),ANT(6,10),ADEL(10),
     *              W(10),AX,BX,OMEGA(10),AVAL(10),BVAL(10),MODEAF,
     *             AK(10,10),R(10),Q(10),XL(10),VOL(10),TB(10),
     *             C(180),ALPHA(45),VC(10),TC(10),PC(10),EVAP(10),
     *             OA(10),OB(10),A(10,10),G(10,10),ZRA(10)
      COMMON  /CMPRO/  NK, NCM1,IDLL,IDLV,IDH,LDBUG,ISW,NPNRBL, NDIM,
     *                  ZNAME(2,10), L(10), NTCOMP(10), ITR, ITRMAX,
     *                 NST, NSTM1, NK1, NK2, NK11, NK21, NCASE, NFEED,
     *                NFTOP, NFBTM,LF(8),IDCODE,ICODE,CPCODE(10)
      COMMON /MIX/ FMIX,ZMIX,BMIX,AA1,BB,BB1,ZMX
C
C
      REAL           Y(10),THETA(10),TAU(10,10),VP(10),FFF(10)
C
C
      OMGM=0.0
      SUM1=0.0
      SUM2=0.0
      SUM3=0.0
      DO 10 I=1,NOCOMP
      OMGM=OMGM+Y(I)*OMEGA(I)
      THETA(I)=Y(I)*VC(I)**(2./3.)
      SUM1=SUM1+THETA(I)
      VP(I)=EXP(ANT(1,I)+ANT(2,I)/(ANT(3,I)+T)+ANT(5,I)*T+
     *        ANT(6,I)*T*T+ANT(4,I)*ALOG(T))
      VP(I)=VP(I)/760.00
 10   CONTINUE
      DO 20 I=1,NOCOMP
      THETA(I)=THETA(I)/SUM1
 20   SUM2=SUM2+THETA(I)*TC(I)
      DO 30 I=1,NOCOMP
      DO 30 J=1,NOCOMP
      K=NTCOMP(I)
      DEL=ABS((TC(I)-TC(J))/(TC(I)+TC(J)))
      TAU(I,J)=SHI(K,DEL)*(TC(I)+TC(J))/2.0
      IF (I.EQ.J)TAU(I,J)=0.0
 30   CONTINUE
      DO 40 I=1,NOCOMP
      DO 40 J=1,NOCOMP
 40   SUM3=SUM3+THETA(I)*THETA(J)*TAU(I,J)
      TCM=SUM2+SUM3
      KM=0.37464+(1.54226-0.26992*OMGM)*OMGM
      TRM=SQRT(T/TCM)
```

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```
      ALFM=1.0+KM*(1.0-TRM)
      AMAL=ALFM*ALFM
      CALL PENROB(T,P,Y,VP,FFF,DDD,SSS)
      ACM=AA1/AMAL
      H=BB/ZMX
      H1=1.0+2.414*H
      H2=1.0-0.414*H
      H3=2.414-H
      H4=0.414+H
      T1=ACM*KM*ALFM*(1.0-H)*TRM*(H/BB1)
      T1=T1/0.082057/T/H3/H4
      T1=(1.0+T1)**2
      T2=2.0*ACM*AMAL*(1.0+H)*(1.0-H)**2
      T2=T2/0.082057/T/(H1+H2)**2
      T2=1.0-T2
      TERM1=T1/T2
      T3=ACM*KM*(1.0+KM)/4.0/1.414/0.082057
      T3=T3/BB1/TCM/TRM
      TERM2=T3*ALOG(H1/H2)
      DELCPR=1.9872*(TERM1+TERM2-1.0)
      CPCV=1.9872*TERM1
      RETURN
      END
```

```
      FUNCTION SHI(I,DL)
C
C
C
C-----THIS FUNCTION ESTIMATES THE PARAMETER "SHI" FOR THE
C-----TERM "TAU(I,J)" IN THE 'CHUEH-PRAUSNITZ' METHOD
C-----FOR CALCULATING MIXTURE CRITICAL TEMPERATURES.
C-----IT IS USED IN FUNCTIONS 'DELCPS' & 'DELCPR'.
C-----REF:'PROPERTIES OF GASES AND LIQUIDS',3RD.EDN.BY-R:S:P
C
C
C-----FOLLOWING ARE THE CONSTANTS NEEDED FOR THE METHOD.
C
      REAL A(98)/39*0.0076,6*0.0219,2*0.0076,0.0077,0.0953,0.0479,
     *          14*0.0076,0.0785,4*0.0076,9*0.0219,20*0.0076/
      REAL B(98)/39*0.287,6*1.227,2*0.287,-0.095,2.185,-5.725,14*0.287
     *          ,-2.152,4*0.287,9*1.227,20*0.287/
      REAL C(98)/39*1.343,6*24.277,2*5.443,3.528,179.068,-161.319,
     *          14*5.443,-722.676,4*5.443,9*147.673,20*5.443/
      REAL D(98)/39*5.443,6*147.673,2*5.443,3.528,179.068,
     *          -161.319,14*5.443,-722.676,4*5.443,9*147.673,
     *          20*5.443/
      REAL E(98)/39*3.038,6*259.433,0.0,264.522,0.0,14*3.038,0.0,
     *          4*3.038,9*259.433,20*3.038/
C
C
      SHI=(((-E(I)*DL+D(I))*DL-C(I))*DL+B(I))*DL-A(I)
      RETURN
      END
```

```
      SUBROUTINE COMP
C
C
      COMMON  /CNTRL/  NCR,NPRT
      COMMON  /CONTL/  NIN,NOUT,NOCOMP,NE,NEN,KUNITS
      COMMON  /MIX/  FMIX,ZMIX,BMIX,AA1,3B,BB1,ZMX
      COMMON  /SYSC/   LA,LB,LC,LOOP,LOOPS
      COMMON  /SYSD/   KEFLAG(50),KSFLAG(100),KTRACE,DERROR,NPFREQ,
     *                 IPUNCH
      COMMON  /EQPA/   EQPAR(25,50),NEMAX,MAXEQP
      COMMON  /STRMIN/ SINUM(4),SIFLAG(4),SIVPFR(4),SITEMP(4),SIPRES(4),
     *                 SIENTH(4),SIVISC(4),SITHK(4),SIZ(4),SIS(4),
     *                 SIMOLE(4),SICOMP(10,4),SIKV(10,4)
      COMMON  /STMOUT/ SONUM(4),SOFLAG(4),SOVPFR(4),SOTEMP(4),SOPRES(4),
     *                 SOENTH(4),SOVISC(4),SOTHK(4),SOZ(4),SOS(4),
     *                 SOMOLE(4),SOCOMP(10,4),SOKV(10,4)
      COMMON  /ZDATA/ CPL(10,4),CPV(10,4),ENP(13,13),ANT(6,10),ADEL(10),
     *                W(10),AX,BX,OMEGA(10),AVAL(10),BVAL(10),MODEAF,
     *                AK(10,10), R(10), Q(10), XL(10),VOL(10),TB(10),
     *                C(180),ALPHA(45),VC(10),TC(10),PC(10),EVAP(10),
     *                OA(10), OB(10), AA(10,10), G(10,10), ZRA(10)
      COMMON  /CMPRO/  NC,NCM1,IDLL,IDLV,IDH,LDBUG,ISW,
     *                NPNRBL,NDIM,ZNAME(2,10),L(10),NTCOMP(10),
     *                ITR,ITRMAX,NST,NSTM1,NK1,NK2,NK11,NK21,
     *                NCASE,NFEED,NFTOP,NFBTM,LF(8),IDCODE,
     *                ICODE,CPCODE(10)
C
      DIMENSION        Y(10)
      REAL             SIDUM(4,11), SODUM(4,11), SIC(10), SID(11)
C
      EQUIVALENCE      (SINUM,SIDUM), (SONUM,SODUM)
C
C         EQPAR(1,NE) = EQUIPMENT NUMBER
C         EQPAR(2,NE) = DOWNSTREAM PRESSURE, ATM
C         EQPAR(3,NE) = INTERCOOLER/AFTERCOOLER TEMPERATURE, DEG K
C                       (DEFAULT =120F/322.05K)
C         EQPAR(4,NE) = EFFICIENCY (FRACTION)
C                       DEFAULT=0.80
C         EQPAR(5,NE) = # OF STAGES OF COMPRESSION
C         EQPAR(6,NE) = COMPRESSION RATIO PER STAGE
C         EQPAR(7,NE) = TOTAL BRAKE HP, CAL
C
C         EQPAR(11-15,NE) = HEAT REMOVED PER STAGE, CAL
C         EQPAR(16-20,NE) = COMPRESSOR DISCHARGE TEMPERATURE, DEG K
C
C     WRITE (6,99999)
C9999 FORMAT(' ',113X,'SUBROUTINE COMP')
      IF (KUNITS.EQ.1) GO TO 4
      EQPAR(2,NE)=EQPAR(2,NE)/14.696
      IF (EQPAR(3,NE).EQ.0.0) EQPAR(3,NE)=120.0
      EQPAR(3,NE)=(EQPAR(3,NE)-32.0)/1.8+273.16
      IF (EQPAR(4,NE).EQ.0.0) EQPAR(4,NE)=0.80
      EQPAR(25,NE)=0.0
C
C     LOAD THE OUTPUT STREAM WITH THE INPUT STREAM
C
```

```
FORTRAN IV  VER 59   SOURCE LISTING: COMP    SUBROUTINE  08/16/85  15:01:31  P
      4 DO 5 I=3,11
      5 SODUM(1,I)=SIDUM(1,I)
        DO 10 I=1,NOCOMP
     10 SOCOMP(I,1)=SICOMP(I,1)
        IF (EQPAR(2,NE).LT.0.1 .OR. SIPRES(1).GT.EQPAR(2,NE)) GO TO 200
        ESAVE=EQPAR(2,NE)
C
C       DETERMINE THE MAXIMUM NUMBER OF STAGES OF COMPRESSION SO THAT
C       THE STAGE COMPRESSION RATIO IS < 6.0.  MAXIMUM NUMBER OF STAGES
C       IS FIVE (5).
C
        N=0
        RATIO=EQPAR(2,NE)/SIPRES(1)
     20 N=N+1
        IF (RATIO**(1.0/FLOAT(N)) .GT. 6.0) GO TO 20
        NSTAGE=N
        IF (NSTAGE.GT.5) GO TO 200
        EQPAR(5,NE)=NSTAGE
        EQPAR(6,NE)=RATIO**(1.0/FLOAT(NSTAGE))
        EQPAR(7,NE)=0.0
C
        YKK=0.0
C-----PUT VAPOR MOLE FRACTIONS
        DO 21 KK=1,NC
21      YKK=SICOMP(KK,1)+YKK
C
        DO 212 KK=1,NC
212     Y(KK)=SICOMP(KK,1)/YKK
C
C       SAVE THE FEED STREAM
C
        DO 22 I=3,11
     22 SID(I)=SIDUM(1,I)
        DO 23 I=1,NOCOMP
     23 SIC(I)=SICOMP(I,1)
C
C       EACH STAGE OF COMPRESSION IS ACCOMPLISHED IDENTICALLY
C
        T3=EQPAR(3,NE)
        DO 55 N=1,NSTAGE
C       INLET CP-CV VALUE
        T1=SITEMP(1)
        P1=SIPRES(1)
        CP1=0.0
        DO 32 I=1,NOCOMP
        CP1=CP1+SICOMP(I,1)*(((CPV(I,4)*T1+CPV(I,3))*T1+CPV(I,2))
     *      *T1+CPV(I,1))
     32 CONTINUE
        IF (IDLV.EQ.2.OR.IDLV.EQ.4.OR.IDLV.EQ.1)DCP=DELCP(T1,P1,CPCV)
        IF (IDLV.EQ.3)DCP=DELCPS(T1,P1,Y,CPCV)
        IF (IDLV.EQ.6)DCP=DELCPR(T1,P1,Y,CPCV)
        IF (IDLV.EQ.0)DCP=0.0
        IF (IDLV.EQ.0)CPCV=1.9872
        CP1=CP1/SIMOLE(1)
C       WRITE(6,333) CP1,DCP,CPCV
333     FORMAT('   COMP    ',' INLET CPO,DCP,CP-CV',3F15.8)
```

```
      CP1=CP1+DCP
      CV1=CP1-CPCV
      G1=CP1/CV1
      EXP1=(G1-1.0)/G1
      H1=SIENTH(1)
C     OUTLET CP/CV VALUE ... INITIALLY ASSUME A 100K TEMPERATURE RISE
      P2=P1*EQPAR(6,NE)
      T2=T1+100.0
      NTIME=0
   40 CP2=0.0
      DO 42 I=1,NOCOMP
      CP2=CP2+SICOMP(I,1)*(((CPV(I,4)*T2+CPV(I,3))*T2+CPV(I,2))
     *     *T2+CPV(I,1))
   42 CONTINUE
      IF (IDLV.EQ.1.OR.IDLV.EQ.2.OR.IDLV.EQ.4)DCP=DELCP(T2,P2,CPCV)
      IF (IDLV.EQ.3)DCP=DELCPS(T2,P2,Y,CPCV)
      IF (IDLV.EQ.6)DCP=DELCPR(T2,P2,Y,CPCV)
      IF (IDLV.EQ.0)DCP=0.0
      IF (IDLV.EQ.0)CPCV=1.9872
      CP2=CP2/SIMOLE(1)
C     WRITE (6,335) CP2,DCP,CPCV
  335 FORMAT('  OUTLET CPO DCP CP-CV  ',3F20.10)
      CP2=CP2+DCP
      CV2=CP2-CPCV
      G2=CP2/CV2
      EXP2=(G2-1.0)/G2
C     COMPUTE DISCHARGE TEMPERATURE FROM THE COMPRESSOR STAGE
      EXPAVG=(EXP1+EXP2)/2.0
      FACTOR=EQPAR(6,NE)**EXPAVG
      TCALC=T1*FACTOR
      NTIME=NTIME+1
      IF (NTIME.EQ.20) GO TO 48
      IF (ABS(T2-TCALC) .LT. 1.0) GO TO 48
      T2=TCALC
      GO TO 40
   48 EQPAR(N+15,NE)=T2
C     COMPUTE HP REQUIREMENT FOR STAGE
      SCFMIN=SIMOLE(1)/453.59/60.0*379.0
      TSUCR=T1*1.8
      BHP=TSUCR/520.0*0.0643/EXPAVG*SCFMIN*(FACTOR-1.0)/EQPAR(4,NE)
      EQPAR(7,NE)=EQPAR(7,NE)+BHP*2545.1*252.16
C     CALCULATE ENTHALPY AT COMPRESSOR DISCHARGE
      SIPRES(1)=P2
      SITEMP(1)=T2
      EQPAR(2,NE)=4.0
      SIVPFR(1)=1.0
      CALL ADBF
      H2=SIENTH(1)
C     CALCULATE ENTHALPY AT EXIT OF HEAT EXCHANGER
      P3=P2
      SIPRES(1)=P3
      SITEMP(1)=T3
      EQPAR(2,NE)=4.0
      SIVPFR(1)=1.0
      CALL ADBF
      H3=SIENTH(1)
```

```
            SIENTH(1)=H2
      C     CALCULATE AND STORE THE EXCHANGER HEAT DUTY
            EQPAR(N+10,NE)=ABS(H2-H3)
         55 CONTINUE
      C
      C     RESTORE INPUT STREAM ... OUTPUT STREAM LOADED BY FLASH ROUTINE
      C
      C     WRITE (6,892) H1,H2,H3
      892   FORMAT('===COMP H1 H2 H3===',3F20.10)
            DO 64 I=3,11
         64 SIDUM(1,I)=SID(I)
            DO 65 I=1,NOCOMP
         65 SICOMP(I,1)=SIC(I)
            EQPAR(2,NE)=ESAVE
            RETURN
      C
        200 WRITE (NPRT,210) NE
        210 FORMAT ('0***** COMP PRESSURE OR TEMPERATURE WAS NOT SPECIFIED, NE
           * =', I3, ', INPUT TRANSFERED TO OUTPUT')
            RETURN
            END
```

```
      SUBROUTINE GSXP
C     WRITE (6,99999)
C9999 FORMAT(' ',113X,'SUBROUTINE GSXP')
C
      COMMON  /CNTRL/  NCR,NPRT
      COMMON  /CONTL/  NIN,NOUT,NOCOMP,NE,NEN,KUNITS
      COMMON  /SYSD/   KEFLAG(50),KSFLAG(100),KTRACE,DERROR,NPFREQ,
     *                 IPUNCH
      COMMON  /EQPA/   EQPAR(25,50),NEMAX,MAXEQP
      COMMON  /STRMIN/ SINUM(4),SIFLAG(4),SIVPFR(4),SITEMP(4),SIPRES(4)
     *                 SIENTH(4),SIVISC(4),SITHK(4),SIZ(4),SIS(4),
     *                 SIMOLE(4),SICOMP(10,4),SIKV(10,4)
      COMMON  /STMOUT/ SONUM(4),SOFLAG(4),SOVPFR(4),SOTEMP(4),SOPRES(4)
     *                 SOENTH(4),SOVISC(4),SOTHK(4),SOZ(4),SOS(4),
     *                 SOMOLE(4),SOCOMP(10,4),SOKV(10,4)
      COMMON /CMPRO/ NC,NCM1,IDLL,IDLV,IDH,LDBUG,ISW,NPNRBL,
     *               NDIM,ZNAME(2,10),L(10),NTCOMP(10),ITR,
     *               ITRMAX,NST,NSTM1,NK1,NK2,NK11,NK21,NCASE,
     *               NFEED,NFTOP,NFBTM,LF(8),IDCODE,ICODE,CPCODE(10)
      COMMON  /ZDATA/ CPL(10,4),CPV(10,4),ENP(10,10),ANT(6,10),ADEL(10)
     *                 W(10),AX,BX,OMEGA(10),AVAL(10),BVAL(10),MODEAF,
     *                 AK(10,10), R(10), Q(10), XL(10),VOL(10),TB(10),
     *                 C(180),ALPHA(45),VC(10),TC(10),PC(10),EVAP(10),
     *                 OA(10), OB(10), A(10,10), G(10,10), ZRA(10)
      COMMON  /STREAM/ T, P, Z(10), Y(10), X(10), FRACV, ZVAP,
     *                 EK(10), VP(10),FUG(10),GAM(10),VZ(11),SVAP,
     *                 HOFZ, HVAP,HLIQ,DHV,DSV,XSH,DSL,NOBUB, NODEW
C
      REAL             SIDUM(4,11), SODUM(4,11), SIC(10), SID(11)
      REAL              NU(20)
C
      EQUIVALENCE      (SIDUM,SINUM), (SODUM,SONUM)
C
C         EQPAR(1,NE) = EQUIPMENT NUMBER
C         EQPAR(2,NE) = DOWNSTREAM PRESSURE, ATM
C         EQPAR(3,NE) = EFFICIENCY (FRACTION)
C         EQPAR(4,NE) = THEORETICAL HP, CAL
C         EQPAR(5,NE) = RECOVERABLE HP, CAL
C
C         OUTLET STREAM ESTABLISHED VIA AN ADIABATIC FLASH
C
      IF (KUNITS.EQ.1) GO TO 1
      EQPAR(2,NE)=EQPAR(2,NE)/14.696
      EQPAR(25,NE)=0.0
C
    1 DO 5 I=3,11
    5 SODUM(1,I)=SIDUM(1,I)
      DO 10 I=1,NOCOMP
   10 SOCOMP(I,1)=SICOMP(I,1)
      IF (EQPAR(2,NE).LT.0.0001) GO TO 400
      SOPRES(1)=EQPAR(2,NE)
      IF (SIPRES(1).LE.SOPRES(1)) GO TO 400
      IF (EQPAR(3,NE).EQ.0.0) EQPAR(3,NE)=0.75
C
      S=0.0
      SIN=0.0
```

```
      T=SITEMP(1)
      P=SIPRES(1)
      IF(IDLV.EQ.0)GO TO 150
      GO TO (80,80,50,80,80,70), IDLV
 50   CALL SRKFUG(T,P,Y,VP,FUG,DHV,SIN)
      GO TO 150
 70   CALL PENROB(T,P,Y,VP,FUG,DHV,SIN)
      GO TO 150
 80   D=T**1.25
      AA=0.0
      BB=0.0
      DO 110 J=1,NOCOMP
      Y(J)=SICOMP(J,1)/SIMOLE(1)
      IF (Y(J).EQ.0.0) GO TO 110
      AA=AA+OA(J)/D*Y(J)
      BB=BB+OB(J)/T*Y(J)
  110 CONTINUE
      ZVAP=NOCOMP+1
      CALL  ZCALC (AA,BB,P,ZVAP)
      DF=ALOG(ZVAP-BB*P)
      DZ=(AA*AA/BB)*ALOG(1.0+BB*P/ZVAP)
      SIN=1.9872*(DF-ALOG(P)-0.5*DZ)
 150  CALL VAPH
C
C     FOR 100% EFFICIENT GAS-EXPANDER FIND DISCHARGE TEMPERATURE
      TIN=T
      T=T-50
      HIN=HVAP
      P=SOPRES(1)
      ID=1
      NTIME=0
      IF (IDLV.EQ.0)GO TO 240
 200  GO TO (205,205,201,205,205,203) ,IDLV
 201  CALL SRKFUG(T,P,Y,VP,FUG,DHV,S)
      GO TO 215
 203  CALL PENROB(T,P,Y,VP,FUG,DHV,S)
      GO TO 215
  205 D=T**1.25
      AA=0.0
      BB=0.0
      DO 210 J=1,NOCOMP
      IF (Y(J).EQ.0.0) GO TO 210
      AA=AA+OA(J)/D*Y(J)
      BB=BB+OB(J)/T*Y(J)
  210 CONTINUE
      ZVAP=NOCOMP+1
      CALL ZCALC (AA,BB,P,ZVAP)
      DF=ALOG(ZVAP-BB*P)
      DZ=(AA*AA/BB)*ALOG(1.0+BB*P/ZVAP)
      S=1.9872*(DF-ALOG(P)-0.5*DZ)
 215  IF (ABS(S-SIN).LT.0.01) GO TO 240
 216  GO TO (220,230), ID
  220 ID=2
      SSAVE=S
      TSAVE=T
      T=T-SIGN(10.0,S-SIN)
```

```
      GO TO 200
  230 SLOPE=(SSAVE-S)/(TSAVE-T)
      DT=-(S-SIN)/SLOPE
      SSAVE=S
      TSAVE=T
      IF (ABS(DT).GT.20.0) DT=SIGN(20.0,DT)
      T=T+DT
C     WRITE(6,199) T,DT
199   FORMAT('%% T AND DT%%',2F20.10)
      NTIME=NTIME+1
      IF (NTIME.EQ.20) GO TO 240
      GO TO 200
  240 CALL VAPH
      HLOW=HVAP
C
C     POWER RECOVERY
      THP=(HIN-HLOW)*SIMOLE(1)
      EQPAR(4,NE)=THP
      EQPAR(5,NE)=EQPAR(4,NE)*EQPAR(3,NE)
      QVALUE=EQPAR(5,NE)
C
C     DETERMINE EXPANDER DISCHARGE CONDITIONS
C     WRITE(6,3111)SIENTH(1),QVALUE
3111  FORMAT('**INLET ENTH & QVALUE**',2F25.5)
C
C-----IF LIQUID REGION IS REACHED,WE ASSUME
C-----100% EFFICIENCY TO AVOID A PHASE SPLIT
C
      SOENTH(1)=SIENTH(1)-QVALUE
      IF (SIENTH(1).LT.QVALUE) SOENTH(1)=HLOW*SIMOLE(1)
C
      DO 312 I=3,11
      SID(I)=SIDUM(1,I)
  312 SIDUM(1,I)=SODUM(1,I)
      DO 313 I=1,NOCOMP
      SIC(I)=SICOMP(I,1)
  313 SICOMP(I,1)=SOCOMP(I,1)
      SIVPFR(1)=1.00
C-----ONLY SUPERHEATED VAPORS ARE TREATED
C
      ESAVE=EQPAR(2,NE)
      EQPAR(2,NE)=2.0
C
C-----'ADBF' BYPASSED FOR TEMPS < 50 K
      IF(T.LT.50)GO TO 3135
      CALL ADBF
3135  EQPAR(2,NE)=ESAVE
      DO 314 I=3,11
  314 SIDUM(1,I)=SID(I)
      DO 315 I=1,NOCOMP
  315 SICOMP(I,1)=SIC(I)
      GO TO 450
C
  400 WRITE (NPRT,418) NE
  418 FORMAT ('0***** GAS EXPANDER PRESSURE WAS NOT SPECIFIED, NE =',
     *  I3, ', INPUT TRANSFERRED TO OUTPUT.')
C
  450 RETURN
      END
```

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```
      SUBROUTINE HYTR
C     WRITE (6,99999)
C9999 FORMAT(' ',113X,'SUBROUTINE HYTR')
C
C
      COMMON  /CNTRL/  NCR,NPRT
      COMMON  /CONTL/  NIN,NOUT,NOCOMP,NE,NEN,KUNITS
      COMMON  /SYSD/   KEFLAG(50),KSFLAG(100),KTRACE,DERROR,NPFREQ,
     *                 IPUNCH
      COMMON  /EQPA/   EQPAR(25,50),NEMAX,MAXEQP
      COMMON  /STREAM/ T, P, Z(10), Y(10), X(10), FRACV, ZVAP,
     *                 EK(10), VP(10),FUG(10),GAM(10),VZ(11),SVAP,
     *                 HOFZ, HVAP,HLIQ,DHV,DSV,XSH,DSL,NOBUB, NODEW
      COMMON  /STRMIN/ SINUM(4),SIFLAG(4),SIVPFR(4),SITEMP(4),SIPRES(4)
     *                 SIENTH(4),SIVISC(4),SITHK(4),SIZ(4),SIS(4),
     *                 SIMOLE(4),SICOMP(10,4),SIKV(10,4)
      COMMON  /STMOUT/ SONUM(4),SOFLAG(4),SOVPFR(4),SOTEMP(4),SOPRES(4)
     *                 SOENTH(4),SOVISC(4),SOTHK(4),SOZ(4),SOS(4),
     *                 SOMOLE(4),SOCOMP(10,4),SOKV(10,4)
      COMMON  /ZDATA/ CPL(10,4),CPV(10,4),ENP(10,10),ANT(6,10),ADEL(10)
     *                 W(10),AX,BX,OMEGA(10),AVAL(10),BVAL(10),MODEAF,
     *                 AK(10,10), R(10), Q(10), XL(10),VOL(10),TB(10),
     *                 C(180),ALPHA(45),VC(10),TC(10),PC(10),EVAP(10),
     *                 OA(10), OB(10), AA(10,10), G(10,10), ZRA(10)
      REAL             SIDUM(4,11), SODUM(4,11), SIC(10), SID(11)
C
C
      EQUIVALENCE      (SIDUM,SINUM), (SODUM,SONUM)
C
C         EQPAR(1,NE) = EQUIPMENT NUMBER
C         EQPAR(2,NE) = DOWNSTREAM PRESSURE, ATM
C         EQPAR(3,NE) = EFFICIENCY (FRACTION)
C         EQPAR(4,NE) = THEORETICAL HP, CAL
C         EQPAR(5,NE) = RECOVERABLE HP, CAL
C
C         OUTLET STREAM ESTABLISHED VIA AN ADIABATIC FLASH
C
      IF (KUNITS.EQ.1) GO TO 1
      EQPAR(2,NE)=EQPAR(2,NE)/14.696
      EQPAR(25,NE)=0.0
C
    1 DO 5 I=3,11
    5 SODUM(1,I)=SIDUM(1,I)
      DO 10 I=1,NOCOMP
   10 SOCOMP(I,1)=SICOMP(I,1)
      IF (EQPAR(2,NE).LT.0.0001) GO TO 17
      SOPRES(1)=EQPAR(2,NE)
      IF (SIPRES(1).LE.SOPRES(1)) GO TO 17
C
      DELTAP=SIPRES(1)-SOPRES(1)
      FLOW=0.0
      DO 11 I=1,NOCOMP
   11 FLOW=FLOW+SICOMP(I,1)*VOL(I)
      IF (EQPAR(3,NE).EQ.0.0) EQPAR(3,NE)=0.70
      THP=FLOW*DELTAP*24.218E-3
      EQPAR(4,NE)=THP
```

```
      EQPAR(5,NE)=THP*EQPAR(3,NE)
C
      QVALUE=EQPAR(5,NE)
      SOENTH(1)=SIENTH(1)-QVALUE
      DO 12 I=3,11
      SID(I)=SIDUM(1,I)
   12 SIDUM(1,I)=SODUM(1,I)
      DO 13 I=1,NOCOMP
      SIC(I)=SICOMP(I,1)
   13 SICOMP(I,1)=SOCOMP(I,1)
      SIVPFR(1)=0.0
      ESAVE=EQPAR(2,NE)
      EQPAR(2,NE)=2.0
      CALL ADBF
      EQPAR(2,NE)=ESAVE
      DO 14 I=3,11
   14 SIDUM(1,I)=SID(I)
      DO 15 I=1,NOCOMP
   15 SICOMP(I,1)=SIC(I)
      GO TO 20
C
   17 WRITE (NPRT,18) NE
   18 FORMAT ('0***** HYDRAULIC TURBINE PRESSURE WAS NOT SPECIFIED, NE
     *', I3, ', INPUT TRANSFERRED TO OUTPUT.')
C
   20 RETURN
      END
```

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```
      SUBROUTINE PUMP
C     WRITE (6,99999)
C9999 FORMAT(' ',113X,'SUBROUTINE PUMP')
C
C
      COMMON  /CNTRL/  NCR,NPRT
      COMMON  /CONTL/  NIN,NOUT,NOCOMP,NE,NEN,KUNITS
      COMMON  /EQPA/   EQPAR(25,50),NEMAX,MAXEQP
      COMMON  /STRMIN/ SINUM(4),SIFLAG(4),SIVPFR(4),SITEMP(4),SIPRES(4),
     *                 SIENTH(4),SIDUMI(16),SIMOLE(4),SICOMP(10,4)
      COMMON  /STMOUT/ SONUM(4),SOFLAG(4),SOVPFR(4),SOTEMP(4),SOPRES(4),
     *                 SOENTH(4),SODUMO(16),SOMOLE(4),SOCOMP(10,4)
      COMMON  /ZDATA/ CPL(10,4),CPV(10,4),ENP(10,10),ANT(6,10),ADEL(10),
     *                 W(10),AX,BX,OMEGA(10),AVAL(10),BVAL(10),MODEAF,
     *                 AK(10,10), R(10), Q(10), XL(10),VOL(10),TB(10),
     *                 C(180),ALPHA(45),VC(10),TC(10),PC(10),EVAP(10),
     *                 OA(10), OB(10), AA(10,10), G(10,10), ZRA(10)
      REAL             SIDUM(4,11), SODUM(4,11), SIC(10), SID(11)
C
C
      EQUIVALENCE      (SIDUM,SINUM), (SODUM,SONUM)
      ERR=0.0
C
C          EQPAR(1,NE) = EQUIPMENT NUMBER
C          EQPAR(2,NE) = DOWNSTREAM PRESSURE, ATM
C          EQPAR(3,NE) = EFFICIENCY (FRACTION)
C          EQPAR(4,NE) = THEORETICAL HP, CAL
C          EQPAR(5,NE) = BRAKE HP, CAL
C
C          OUTLET STREAM ESTABLISHED VIA AN ADIABATIC FLASH
C
C    TESTING INPUT STREAM VAPOR FRACTION
      IF (KUNITS.EQ.1) GO TO 1
      EQPAR(2,NE)=EQPAR(2,NE)/14.696
      EQPAR(25,NE)=0.0
C
1     IF (SIVPFR(1).LT.0.01)GO TO 4
      IF (SIVPFR(1).GE.0.99) GO TO 25
      GO TO 181
    4 DO 5 I=3,11
    5 SODUM(1,I)=SIDUM(1,I)
      IF(ERR.EQ.1.0)GO TO 20
      DO 10 I=1,NOCOMP
   10 SOCOMP(I,1)=SICOMP(I,1)
      IF (EQPAR(2,NE).LT.0.0001) GO TO 17
      SOPRES(1)=EQPAR(2,NE)
      IF (SOPRES(1).LE.SIPRES(1)) GO TO 17
C
      DELTAP=SOPRES(1)-SIPRES(1)
      FLOW=0.0
      DO 11 I=1,NOCOMP
   11 FLOW=FLOW+SICOMP(I,1)*VOL(I)
      IF (EQPAR(3,NE).EQ.0.0) EQPAR(3,NE)=0.80
      THP=FLOW*DELTAP*24.218E-3
      EQPAR(4,NE)=THP
      EQPAR(5,NE)=THP/EQPAR(3,NE)
```

```
C
      QVALUE=EQPAR(5,NE)-THP
      SOENTH(1)=SIENTH(1)+QVALUE
      DO 12 I=3,11
      SID(I)=SIDUM(1,I)
   12 SIDUM(1,I)=SODUM(1,I)
      DO 13 I=1,NOCOMP
      SIC(I)=SICOMP(I,1)
   13 SICOMP(I,1)=SOCOMP(I,1)
      ESAVE=EQPAR(2,NE)
      EQPAR(2,NE)=2.0
      SIVPFR(1)=0.0
      CALL ADBF
      EQPAR(2,NE)=ESAVE
      DO 14 I=3,11
   14 SIDUM(1,I)=SID(I)
      DO 15 I=1,NOCOMP
   15 SICOMP(I,1)=SIC(I)
      GO TO 20
C
   17 WRITE (NPRT,18) NE
   18 FORMAT ('0***** PUMP PRESSURE WAS NOT SPECIFIED, NE =',I3,
     * ', INPUT TRANSFERED TO OUTPUT.')
      GO TO 20
181   WRITE(NPRT,182)
182   FORMAT('0*****ERROR CONDITION*****INPUT STREAM
     *HAS MORE THAN 1% VAPOR FRACTIONS.')
      WRITE(NPRT,183)
183   FORMAT('0*****INPUT TRANSFERRED TO OUTPUT')
      ERR=1.0
      GO TO 4
C
25    WRITE (NPRT,26)
26    FORMAT('0*****ERROR***SHOULD BE A COMPRESSOR')
      ERR=1.0
      WRITE(NPRT,27)
27    FORMAT('0*****INPUT TRANSFERRED TO OUTPUT')
      GO TO 4
   20 RETURN
      END
```

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```
      SUBROUTINE VALV
C     WRITE (6,99999)
C9999 FORMAT(' ',113X,'SUBROUTINE VALV')
C
C
      COMMON  /CNTRL/  NCR,NPRT
      COMMON  /CONTL/  NIN,NOUT,NOCOMP,NE,NEN,KUNITS
      COMMON  /SYSC/   LA,LB,LC,LOOP,LOOPS
      COMMON  /SYSD/   KEFLAG(50),KSFLAG(100),KTRACE,DERROR,NPFREQ,
     *                 IPUNCH
      COMMON  /EQPA/   EQPAR(25,50),NEMAX,MAXEQP
      COMMON  /STRMIN/ SINUM(4),SIFLAG(4),SIVPFR(4),SITEMP(4),SIPRES(4),
     *                 SIENTH(4),SIVISC(4),SITHK(4),SIZ(4),SIS(4),
     *                 SIMOLE(4),SICOMP(10,4),SIKV(10,4)
      COMMON  /STMOUT/ SONUM(4),SOFLAG(4),SOVPFR(4),SOTEMP(4),SOPRES(4),
     *                 SOENTH(4),SOVISC(4),SOTHK(4),SOZ(4),SOS(4),
     *                 SOMOLE(4),SOCOMP(10,4),SOKV(10,4)
      COMMON  /ZDATA/ CPL(10,4),CPV(10,4),ENP(10,10),ANT(6,10),ADEL(10),
     *                 W(10),AX,BX,OMEGA(10),AVAL(10),BVAL(10),MODEAF,
     *                 AK(10,10), R(10), Q(10), XL(10),VOL(10),TB(10),
     *                 C(180),ALPHA(45),VC(10),TC(10),PC(10),EVAP(10),
     *                 OA(10), OB(10), AA(10,10), G(10,10), ZRA(10)
      REAL             SIDUM(4,11),SODUM(4,11),SIC(10),SID(11)
C
      EQUIVALENCE      (SIDUM,SINUM), (SODUM,SONUM)
C
C          EQPAR(1,NE) = EQUIPMENT NUMBER
C          EQPAR(2,NE) = DOWNSTREAM PRESSURE, ATM
C          EQPAR(3,NE) = INEFFICIENCY (FRACTION)
C          EQPAR(4,NE) = ENERGY INCREASE DUE TO EXPANSION, CAL
C
C          DEFAULT FOR EQPAR(3,NE) IS 0% INEFFICIENCY
C
C          OUTLET STREAM ESTABLISHED VIA AN ADIABATIC FLASH
C
      IF (KUNITS.EQ.1) GO TO 1
      EQPAR(2,NE)=EQPAR(2,NE)/14.696
      EQPAR(25,NE)=0.0
      EQPAR(3,NE)=0.0
      EQPAR(4,NE)=0.0
C
    1 DO 5 I=3,11
    5 SODUM(1,I)=SIDUM(1,I)
      DO 10 I=1,NOCOMP
   10 SOCOMP(I,1)=SICOMP(I,1)
      IF (EQPAR(2,NE).GE.SIPRES(1)) GO TO 17
      SOPRES(1)=EQPAR(2,NE)
      DELTAP=SIPRES(1)-SOPRES(1)
      FLOW=0.0
C     WRITE(6,*) SIPRES(1),SOPRES(1)
      DO 11 I=1,NOCOMP
   11 FLOW=FLOW+SICOMP(I,1)*VOL(I)
      IF (EQPAR(3,NE).EQ.0.0) EQPAR(3,NE)=1.0
      THP=FLOW*DELTAP*24.218E-3
      QVALUE=THP*(1.0-EQPAR(3,NE))
      EQPAR(4,NE)=QVALUE
```

```
          SOENTH(1)=SIENTH(1)+QVALUE
          DO 12 I=3,11
          SID(I)=SIDUM(1,I)
       12 SIDUM(1,I)=SODUM(1,I)
          DO 13 I=1,NOCOMP
          SIC(I)=SICOMP(I,1)
       13 SICOMP(I,1)=SOCOMP(I,1)
          ESAVE=EQPAR(2,NE)
C-----MODIFIED ON CHESS II,'83
          EQPAR(2,NE)=2.0
C-----MODIFIED FROM CHESS II,'83
C
C
C         DO 1112 K=1,NC
C         WRITE(6,1111) I,X(I)
 1111     FORMAT('VALV',I10,F10.8)
 1112     CONTINUE
          IF (LOOP.GT.2) EQPAR(2,NE)=2.0
          CALL ADBF
          EQPAR(2,NE)=ESAVE
          DO 14 I=3,11
       14 SIDUM(1,I)=SID(I)
          DO 15 I=1,NOCOMP
       15 SICOMP(I,1)=SIC(I)
          GO TO 20
C
       17 WRITE (NPRT,18) NE
       18 FORMAT ('0***** VALVE PRESSURE NOT SPECIFIED, NE =', I3,
         *  ', INPUT TRANSFERRED TO OUTPUT')
C
       20 RETURN
          END
```

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```
      SUBROUTINE VAPH
C     WRITE (6,99999)
C9999 FORMAT(' ',113X,'SUBROUTINE VAPH')
C
      COMMON  /CMPRO/  NC,NCM1,IDLL,IDLV,IDH,LDBUG,ISW,NPNRBL, NDIM,
     *                 ZNAME(2,10), L(10), NTCOMP(10), ITR, ITRMAX,
     *                 NST, NSTM1, NK1, NK2, NK11, NK21, NCASE, NFEED,
     *                 NFTOP, NFBTM, LF(8),IDCODE,ICODE,CPCODE(10)
      COMMON  /ZDATA/ CPL(10,4),CPV(10,4),ENP(10,10),ANT(6,10),ADEL(10)
     *                 W(10),AX,BX,OMEGA(10),AVAL(10),BVAL(10),MODEAF,
     *                 AK(10,10), R(10), Q(10), XL(10),VOL(10),TB(10),
     *                 C(180), ALPHA(45),VC(10),TC(10),PC(10),EVAP(10),
     *                 OA(10), OB(10), A(10,10), G(10,10), ZRA(10)
      COMMON  /STREAM/ T, P, Z(10), Y(10), X(10), FRACV, ZVAP,
     *                 EK(10), VP(10), FUG(10),GAM(10),VZ(11),SVAP,
     *                 HOFZ, HVAP,HLIQ,DHV,DSV,XSH,DSL,NOBUB,NODEW
C
C
      NPNRBL=0
      DHV=0.0
      DSV=0.0
      HVAP=0.0
C     WRITE (6,876) T
876   FORMAT('*****TEMP - VAPH**',F10.5)
      DO 10 J=1,NC
   10 HVAP=HVAP+Y(J)*((((ENP(J,10)*T+ENP(J,9))*T+ENP(J,8))*T+ENP(J,7))*
     *     T+ENP(J,6))
      IF (IDH.EQ.2) RETURN
      CALL XSHVP(T,P,X,Y,VP,DHV,DSV)
C     WRITE(6,99) HVAP,DHV
99    FORMAT('****VAPH --HVAP & DHV**',2F25.6)
30    HVAP=HVAP+DHV
C
      RETURN
      END
```

FORTRAN IV VER 59 SOURCE LISTING: 08/16/85 15:03:37

```
      SUBROUTINE LIQH
C
      COMMON  /CMPRO/  NC,NCM1,IDLL,IDLV,IDH,LDBUG,ISW,NPNRBL, NDIM,
     *                 ZNAME(2,10), L(10), NTCOMP(10), ITR, ITRMAX,
     *                 NST, NSTM1, NK1, NK2, NK11, NK21, NCASE, NFEED,
     *                 NFTOP, NFBTM, LF(8),IDCODE,ICODE,CPCODE(10)
      COMMON  /ZDATA/ CPL(10,4),CPV(10,4),ENP(10,10),ANT(6,10),ADEL(10)
     *                 W(10),AX,BX,OMEGA(10),AVAL(10),BVAL(10),MODEAF,
     *                 AK(10,10), R(10), Q(10), XL(10),VOL(10),TB(10),
     *                 C(180), ALPHA(45),VC(10),TC(10),PC(10),EVAP(10),
     *                 DA(10), DB(10), AA(10,10), G(10,10), ZRA(10)
      COMMON  /STREAM/ T, P, Z(10), Y(10), X(10), FRACV, ZVAP,
     *                 EK(10), VP(10), FUG(10),GAM(10),VZ(11),SVAP,
     *                 HOFZ, HVAP,HLIQ,DHV,DSV,XSH,DSL,NOBUB,NODEW
C
C     WRITE (6,99999)
C9999 FORMAT(' ',113X,'SUBROUTINE LIQH')
C
      XSH=0.0
      DSL=0.0
      HLIQ=0.0
      IF(P.GT.1.00.OR.T.GT.300.0)GO TO 20
      DO 10 J=1,NC
      HLIQ=HLIQ+X(J)*((((ENP(J,5)*T+ENP(J,4))*T+ENP(J,3))*T+ENP(J,2))*
     *     T+ENP(J,1))
      IF (CPCODE(J).EQ.2.0)HLIQ=HLIQ-CPL(J,2)*273.16*T
     *   +T*CPL(J,3)*273.16**2-273.16*CPL(J,3)*T*T
10    CONTINUE
C     WRITE(6,99)HLIQ
99    FORMAT('**LIQH       **',F20.8)
      GO TO 30
20    DO 25 K=1,NC
25    HLIQ=HLIQ+X(K)*((((ENP(K,10)*T+ENP(K,9))*T+ENP(K,8))*T
     %           +ENP(K,7))*T+ENP(K,6))
      IF (IDLL.GE.1 .AND. IDH.EQ.0) CALL XSHLQ (T,P,X,Y,VP,XSH,DSL)
C     WRITE(6,199)HLIQ,XSH
199   FORMAT('  LIQH   **HLIQ  XSH  **',2F20.6)
      HLIQ=HLIQ+XSH
C
30    CONTINUE
C
      RETURN
      END
```

FORTRAN IV VER 59 SOURCE LISTING: DREAD SUBROUTINE 08/16/85 15:01:31

```
      SUBROUTINE DREAD (KODE)
C     WRITE (6,99999)
C9999 FORMAT(' ',113X,'SUBROUTINE DREAD')
C
C
      COMMON  /CNTRL/  NCR,NPRT
      COMMON  /CONTL/  NIN,NOUT,NOCOMP,NE,NEN,KUNITS
      COMMON  /SYSA/   KPM(10,50),KSEM(3,100),N3MAX
      COMMON  /EQPA/   EQPAR(25,50),NEMAX,MAXEQP
      COMMON  /STMA/   SEXTSV(13,100),SINTSV(10,100),NSMAX,MAXSEX,MAXSI
      REAL  KOMNAM
      COMMON  /SYSAA/  TITLE(20),COMPNT(10),KOMNAM(40)
      COMMON  /SYSB/   KE1(50),NE1MAX,KE2(50),NE2MAX,KE3(10),NE3MAX,
     *                 KE4(10),NE4MAX,KRET,KRET2,KRET3
      COMMON  /SYSC/   LIMIT,LIMIT2,LIMIT3,LOOP,LOOPS
      COMMON  /SYSD/   KEFLAG(50),KSFLAG(100),KTRACE,DERROR,NPFREQ,
     *                 IPUNCH
      COMMON  /EQPB/   NECALL(50),NEXEQN(50),NAME(50)
      COMMON  /CMPRO/  NC, NCM1,IDLL,IDLV,IDH,LDBUG,ISW,NPNRBL, NDIM,
     *                 ZNAME(2,10), L(10), NTCOMP(10), ITR, ITRMAX,
     *                 NST, NSTM1, NK1, NK2, NK11, NK21, NCASE, NFEED,
     *                NFTOP, NFBTM,LF(8),IDCODE,ICODE,CPCODE(10)
      INTEGER          SNAME(100), ENAME(50), NMLIST(20), KPMKPM(10),
     *                 COMPNT
      REAL             SEX(13), SIN(10), EQP(25)
C
C     AVAILABLE '20' EQUIPMENT SUBROUTINE NAMES;
      DATA NMLIST /'DVDR','DIST','MIXR','ADBF','REAC','VALV','HXER'
     * ,'PUMP','ABSR','COMP','HTCL','OVHD','BOTT','HYTR','CTRL','GSXP',
     * 'SPLT','ADD3','ADD2','ADD1'/
C
    1 FORMAT (8I9)
    2 FORMAT (2X,6G13.5)
    3 FORMAT (' ')
C
      IF (KODE.EQ.0) CALL CLEAN
      READ (NCR,5,ERR=5000,END=5000) TITLE
    5 FORMAT (20A4)
C
      WRITE (NPRT,10)
   10 FORMAT ('1 *** ***  CHESS FLOW SHEET SIMULATION   *** ***'/
     *       '                     VERSION  THREE             '/
     *       '                       JUNE 1985                   ')
C
      WRITE (NPRT,22) TITLE
   22 FORMAT ('0',19A4,A3)
C
C
C     BASIC CONTROL PARAMETERS ... READ IN START
C
C         NOCOMP    NUMBER OF COMPONENTS
C
C         IDLL      LIQUID PHASE CLASSIFICATION CODE
C                           0    IDEAL
C                           1    VIRIAL
C                           2    NRTL
```

```
C                            3    UNIQUAC
C                            4    CHAO-SEADER
C                            5 = SPECIAL LIBRARY #1 (NRTL)
C                            6    PENG-ROBINSON
C
C          IDLV      VAPOR PHASE CLASSIFICATION CODE
C                            0 = IDEAL
C                            1 = VIRIAL EQUATION OF STATE
C                            2 = REDLICH KWONG EQUATION OF STATE
C                            3 = SOAVE - REDLICH -KWONG EQUATION OF STATE
C                            4 = CHAO-SEADER EQN.
C                            5 = SPECIAL LIBRARY #1 (RK)
C                            6 = PENG-ROBINSON EQN. OF STATE
C
C          IDH       ENTHALPY CORRECTION
C                            0    CORRECT BOTH PHASES
C                            1    CORRECT VAPOR PHASE ONLY
C                            2    NO CORRECTION
C
C          LDBUG     DEBUG CODE
C                            0    MINIMUM PRINT OUT OF SEPARATION SYSTEM
C                            1    COMPONENT DATA AND FINAL COLUMN PRO-
C                                      FILES PRINTED
C                            2    CODE 1 + INTERMEDIATE COLUMN PROFILES
C                                      PRINTED
C
C
C
C         KUNITS = 0 ---> PSIA, DEG K , M3TU/HR
C         KUNITS = 1 ---> ATM,  DEG K,  KCAL/HR
C
C
C         SEXTSV(2,STREAM)= STREAM FLAG; 0=INTERMEDIATE
C                                        1=FEED, 2=PRODUCT
C
C
C
C          COMPNT    COMPONENT IDENTIFICATION NUMBERS
C
      IF (KODE.EQ.-1) GO TO 30
      READ (NCR,*) NOCOMP,IDLL,IDLV,IDH,LDBUG,NDIM
      NDIM = 0
      WRITE (NPRT,1) NOCOMP,IDLL,IDLV,IDH,LDBUG,NDIM
      WRITE (NPRT,3)
      READ (NCR,*) (COMPNT(I),I=1,NOCOMP)
      WRITE (NPRT,1) (COMPNT(I),I=1,NOCOMP)
      WRITE (NPRT,3)
      NC=NOCOMP
      NCM1=NC-1
      DO 25 I=1, NOCOMP
   25 NTCOMP(I)=COMPNT(I)
C
   30 READ (NCR,*) NOKPM,NOEQP,NOSEX,NOSIN,KUNITS
      WRITE (NPRT,1) NOKPM,NOEQP,NOSEX,NOSIN,KUNITS
C
C     READ PROCESS MATRIX
```

```
C
      IF (KODE.EQ.-1) GO TO 63
      WRITE (NPRT,301)
  301 FORMAT ('0BEGIN NETWORK READ')
      DO 402 K=1,NOKPM
      READ (NCR,*) KPMKPM
      IF (MOD(K,5).EQ.5) WRITE (NPRT,3)
      WRITE (NPRT,400) KPMKPM
  400 FORMAT (I5,2(6X,A4),7I5)
      I=KPMKPM(1)
      DO 401 J=1,10
  401 KPM(J,I)=KPMKPM(J)
  402 CONTINUE
      WRITE (NPRT,302)
  302 FORMAT (' NETWORK COMPLETE')
      MAXSEX=NOCOMP+3
      MAXSIN=10
      MAXEQP=25
C
C     SET UP EQUIPMENT SUBROUTINE CALLING NUMBER FROM EQUIPMENT NAME
C
      KVOID=0
   51 DO 56 K2=1,50
      IF (KPM(1,K2).EQ.0) GO TO 56
      NEX=KPM(1,K2)
      NEMAX=K2
C
C     NEX IS EQUIPMENT NUMBER OF PROCESS MATRIX ROW 1- KPM(1,K2)
C     KPM(3,K2) IS THE EXTERNAL NAME GIVEN TO THIS UNIT.
C
      I=1
   53 IF (KPM(2,K2).EQ.NMLIST(I)) GO TO 55
      IF (I.GT.20) GO TO 54
      I=I+1
      GO TO 53
   54 WRITE (NPRT,108) NEX,KPM(2,K2)
  108 FORMAT('1IN ''DREAD'' EQUIPMENT NUMBER ''',I3,''' HAS BEEN GIVEN T
     *HE ILLEGAL NAME ''',A4,'''.'// ' THIS DATA IS NOT BEING CALCULATED
     *.'//' PROBLEM HAS BEEN VOIDED.')
      KVOID=1
   55 NECALL(NEX)=I
      NAME(NEX)=KPM(2,K2)
      NEXEQN(NEX)=KPM(3,K2)
   56 CONTINUE
C
C IF THE NUMBER OF EQUIPMENT SUBROUTINE NAMES OR AN EQUIPMENT SUBROU-
C TINE NAME ITSELF IS CHANGED, SUBROUTINE 'EQCALL' MUST BE MODIFIED.
C
      DO 62 J=1,NEMAX
      IF (KPM(1,J).EQ.0) GO TO 62
      DO 61 I=2,8
   61 KPM(I,J)=KPM(I+2,J)
   62 CONTINUE
C
C     READ 'EQPAR' (BY USING EQP1-EQP25) AND 'ENAME'.
C
```

```
   63 IF (NOEQP.EQ.0) GO TO 67
      CALL ZEROX (ENAME,50)
      WRITE (NPRT,303)
  303 FORMAT ('0BEGIN EQUIPMENT DATA READ')
      READ (NCR,*) ENAME
      WRITE (NPRT,1) ENAME
C
      DO 412 K=1,NOEQP
      READ (NCR,*) EQP
      WRITE (NPRT,3)
      WRITE (NPRT,2) EQP
      I=EQP(1)+0.1
      EQP(25)=KUNITS
      DO 411 J=1,25
  411 EQPAR(J,I)=EQP(J)
  412 CONTINUE
      WRITE (NPRT,304)
  304 FORMAT (' EQUIPMENT DATA COMPLETE')
      DO 65 I=1,NEMAX
      J=ENAME(I)
      IF (J.EQ.0) GO TO 65
      IF (ABS(EQPAR(1,J)).LT.1.E-20) EQPAR(1,J)=J
C     WRITE (NPRT,66) J,(EQPAR(K,J),K=1,25)
   65 CONTINUE
C  66 FORMAT (' EQPAR(1,',I2,')=',10G10.2/(13X,10G10.2))
C
      CALL ZEROX (KEFLAG,50)
C
C     READ 'SEXTSV' (BY USING SEX1-SEX50) AND 'SNAME'
C
   67 IF (NOSEX.EQ.0) GO TO 71
      CALL ZEROX (SNAME,100)
      WRITE (NPRT,305)
  305 FORMAT ('0BEGIN STREAM EXTENSIVE LIST READ')
      READ (NCR,*) SNAME
      WRITE (NPRT,1) SNAME
C
      DO 422 K=1,NOSEX
      READ (NCR,*) SEX
      WRITE (NPRT,3)
      WRITE (NPRT,2) SEX
      I=SEX(1)+0.1
      IF (KUNITS.EQ.1)GO TO 418
C
      SEX(2)=SEX(2)*252.16/453.59
      SEX(3)=SEX(3)*453.59
      DO 419 J=1,NOCOMP
  419 SEX(3+J)=SEX(3+J)*453.59
C
418   DO 421 J=1,13
  421 SEXTSV(J,I)=SEX(J)
  422 CONTINUE
      WRITE (NPRT,306)
  306 FORMAT (' STREAM EXTENSIVE LIST COMPLETE')
      DO 68 I=1,100
      J=SNAME(I)
```

```
          IF (J.EQ.0) GO TO 68
          IF (ABS(SEXTSV(1,J)).LT.1.E-20) SEXTSV(1,J)=J
C         WRITE (NPRT,69) J,(SEXTSV(K,J),K=1,13)
       68 CONTINUE
C      69 FORMAT(' SEXTSV(1,',I2,')=',2F3.0,11G10.3/30X,10G10.3 )
C
          IF (KODE.EQ.-1) GO TO 71
          DO 70 I=1,100
       70 IF (ABS(SEXTSV(1,I)) .GT. 1.E-20) NSMAX=I
C
C         READ 'SINTSV' (BY USING SIN1-SIN50) AND 'SNAME'
C
       71 IF (NOSIN.EQ.0) GO TO 75
          CALL ZEROX (SNAME,100)
          WRITE (NPRT,307)
      307 FORMAT ('0BEGIN STREAM INTENSIVE LIST READ')
          READ (NCR,*) SNAME
          WRITE (NPRT,1) SNAME
C
          DO 432 K=1,NOSIN
          READ (NCR,*) SIN
          WRITE (NPRT,3)
          WRITE (NPRT,2) SIN
          I=SIN(1)+0.1
          IF(KUNITS.EQ.1)GO TO 430
C
          IF (SIN(4).NE.0.0) SIN(4)=(SIN(4)-32.0)/1.8+273.16
          SIN(5)=SIN(5)/14.696
          SIN(6)=SIN(6)*252.16
C
  430     DO 431 J=1,10
      431 SINTSV(J,I)=SIN(J)
      432 CONTINUE
          WRITE (NPRT,308)
      308 FORMAT (' STREAM INTENSIVE LIST COMPLETE')
          DO 72 I=1,NSMAX
          J=SNAME(I)
          IF (J.EQ.0) GO TO 72
          IF (ABS(SINTSV(1,J)).LT.1.E-20) SINTSV(1,J)=J
C         WRITE (NPRT,73) J,(SINTSV(K,J),K=1,10)
       72 CONTINUE
C      73 FORMAT (' SINTSV(1,',I2,')=',F3.0,F4.0, 8G10.3)
C
          CALL ZEROX (KSFLAG,100)
C
C         READ EQUIPMENT LISTS FOR RECYCLE CALCULATIONS, KE2, KE3 AND KE4
C         THEIR CONTROL CONSTANTS NE2MAX, NE3MAX AND NE4MAX. WILL BE CALC.
C
       75 WRITE (NPRT,309)
      309 FORMAT ('0BEGIN CALCULATION DATA READ')
          READ (NCR,*) LOOPS,NPFREQ,KTRACE,DERROR
          WRITE (NPRT,1) LOOPS,NPFREQ,KTRACE
          WRITE (NPRT,2) DERROR
          WRITE (NPRT,3)
          READ (NCR,*) KE2
          WRITE (NPRT,1) KE2
```

```
      WRITE (NPRT,3)
      READ (NCR,*) KE3
      WRITE (NPRT,1) KE3
      WRITE (NPRT,3)
      READ (NCR,*) KE4
      WRITE (NPRT,1) KE4
      WRITE (NPRT,310)
  310 FORMAT (' CALCULATION DATA COMPLETE')
C
      NE2MAX=0
      NE3MAX=0
      NE4MAX=0
      DO 76 I=1,50
      IF (KE2(I).EQ.0) GO TO 77
   76 NE2MAX=NE2MAX+1
   77 DO 78 I=1,10
      IF (KE3(I).EQ.0) GO TO 79
   78 NE3MAX=NE3MAX+1
   79 DO 80 I=1,10
      IF (KE4(I).EQ.0) GO TO 81
   80 NE4MAX=NE4MAX+1
C
   81 N3MAX=8
      DO 83 K=2,8
      I=10-K
      DO 82 J=1,NEMAX
      IF (KPM(I,J).NE.0) GO TO 85
   82 CONTINUE
   83 N3MAX=N3MAX-1
   85 CONTINUE
C
C     BUILD UP THE STREAM CONNECTION MATRIX KSEM.
C
      DO 187 M1=1,NEMAX
      IF (KPM(1,M1).LE.0) GO TO 187
  188 M2=KPM(1,M1)
      DO 189 M3=2,N3MAX
      IF (KPM(M3,M1)) 191,187,190
  190 M4=(KPM(M3,M1))
      IF (M4.GT.50)GO TO 3000
      KSEM(3,M4)=M2
      GO TO 192
  191 M4=-(KPM(M3,M1))
      IF (M4.GT.50)GO TO 3000
      KSEM(2,M4)=M2
  192 KSEM(1,M4)=M4
  189 CONTINUE
  187 CONTINUE
C
      IF (KVOID.GT.0) GO TO 5000
C     WRITE (NPRT,1000)
C1000 FORMAT ('1')
      GO TO 5001
 3000 WRITE (NPRT,4000) M1
 4000 FORMAT (' KEYPUNCH ERROR, KPM',I3,' PROBLEM VOIDED.')
 5000 KODE=1
C
 5001 RETURN
      END
```

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```
      SUBROUTINE COMPID
C
C                                   ***** COMPID *****
C
C  PURE COMPONENT ID NUMBERS...
C
C     1. HYDROGEN        18. N-TETRADECANE      35. 1-HEXENE
C     2. METHANE         19. N-PENTADECANE      36. CYCLOPENTANE
C     3. ETHANE          20. N-HEXADECANE       37. METHYLCYCLOPENTANE
C     4. PROPANE         21. N-HEPTADECANE      38. CYCLOHEXANE
C     5. I-BUTANE        22. ETHYLENE           39. METHYLCYCLOHEXANE
C     6. N-BUTANE        23. PROPYLENE          40. BENZENE
C     7. I-PENTANE       24. 1-BUTENE           41. TOLUENE
C     8. N-PENTANE       25. CIS-2-BUTENE       42. O-XYLENE
C     9. NEO-PENTANE     26. TRANS-2-BUTENE     43. M-XYLENE
C    10. N-HEXANE        27. I-BUTENE           44. P-XYLENE
C    11. N-HEPTANE       28. 1,3-BUTADIENE      45. ETHYLBENZENE
C    12. N-OCTANE        29. 1-PENTENE          46. NITROGEN
C    13. N-NONANE        30. CIS-2-PENTENE      47. OXYGEN
C    14. N-DECANE        31. TRANS-2-PENTENE    48. CARBON MONOXIDE
C    15. N-UNDECANE      32. 2-METHYL-1-BUTENE  49. CARBON DIOXIDE
C    16. N-DODECANE      33. 3-METHYL-1-BUTENE  50. HYDROGEN SULFIDE
C    17. N-TRIDECANE     34. 2-METHYL-2-BUTENE  51. SULFUR DIOXIDE
C                    -------------------------------------------
C    52. 2-METHYL-C5     56. 1-HEPTENE          60. C2-CYCLO-C6
C    53. 3-METHYL-C5     57. PROPADIENE         61. ISOPRENE
C    54. 2,2-DI-C1-C4    58. 1,2-BUTADIENE      62. WATER
C    55. 2,3-DI-C1-C4    59. C2-CYCLO-C5
C                    -------------------------------------------
C    63. AMMONIA           73. 1-C1-3-C2-BENZENE83. 1-OCTENE
C    64. CARBON            74. 1-C1-4-C2-BENZENE84. CYCLOPENTENE
C    65. ACETYLENE         75. 1,2,3-MESITYLENE 85. TNS-1,3-DI-C1CYC6
C    66. PROPYNE           76. 1,2,4-MESITYLENE 86. CIS-1,4-DI-C1CYC6
C    67. 1-BUTYNE          77. 1,3,5-MESITYLENE 87. TNS-1,4-DI-C1CYC6
C    68. 2-METHYLPROPENE   78. N-BUTYLBENZENE   88. 1,1-DI-C1-CYC6
C    69. CYCLOPENTENE      79. 2-METHYLHEXANE   89. CIS-1,2-DI-C1CY-C6
C    70. N-PROPYLBENZENE   80. 3-METHYLHEXANE   90. CIS-1,3-DI-C1CY-C6
C    71. I-PROPYLBENZENE   81. 2-METHYLHEPTANE  91. N-OCTADECANE
C    72. 1-C1-2-C2-BENZENE82. 2,2,4-TRIMETHYLC592. N-NONADECANE
C                    -------------------------------------------
C    93. N-EICOSANE        95.CIS-1,2-DI-C1-CYC597. CIS-1,3-DI-C1-CYC5
C    94.1,1-DIMETHYL-CYC5 96.TNS-1,2-DI-C1-CYC598. TNS-1,3-DI-C1-CYC5
C
      COMMON /CONTL/ NIN,NOUT,NOCOMP,NE,NEN,KUNITS
      COMMON/SYSAA/ TITLE(20),COMPNT(10),KOMNAM(40)
      COMMON /CNTRL/ NCR,NPRT
      COMMON /CMPRO/ NC,NCM1,IDLL,IDLV,IDH,LDBUG,ISW,NPNRBL,NDIM,
     *               ZNAME(2,10),L(10),NTCOMP(10),ITR,ITRMAX,
     *               NST,NSTM1,NK1,NK2,NK11,NK21,NCASE,NFEED,
     *                NFTOP,NFBTM,LF(8),IDCODE,ICODE,CPCODE(10)
      COMMON /ZDATA/ CPL(10,4),CPV(10,4),ENP(10,10),ANT(6,10),ADEL(10),
     *               W(10),AX,BX,OMEGA(10),AVAL(10),BVAL(10),MODEAF,
     *               AK(10,10),R(10),Q(10),XL(10),VOL(10),TB(10),
     *               C(180),ALPHA(45),VC(10),TC(10),PC(10),EVAP(10),
     *               OA(10),OB(10),AA(10,10),G(10,10),ZRA(10)
      REAL     ZCD(20),BASEA(20),BASEB(20),LNPHI(20),LNACT(20),LNNU(20)
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      REAL      APH(20),BET(20),GAM(20),DTA(20)
      REAL      AVW(20),MW(20),ALD(20)
C
      INTEGER COUNT,COMPNT
      LOGICAL EXFLAG
C
C     STANDARD COMPONENT NAMES
C
      INTEGER SCNAME(392)
      INTEGER SANAME(156)/' HYD','ROGE','N',' ',' MET','HANE',2*' ',' E
     1H','ANE',' ',' ',' PRO','PANE',2*' ',' I-B','UTAN','E',' ',' N-B'
     2'UTAN','E',' ',' I-P','ENTA','NE',' ',' N-P','ENTA','NE',' ',' NE
     3','-PEN','TANE',' ',' N-H','EXAN','E',' ',' N-H','EPTA','NE',' ',
     4' N-O','CTAN','E',' ',' N-N','ONAN','E',' ',' N-D','ECAN','E',' '
     5' N-U','NDEC','ANE',' ',' N-D','ODEC','ANE',' ',' N-T','RIDE','CA
     6E',' ',' N-T','ETRA','DECA','NE',' N-P','ENTA','DECA','NE',' N-H'
     7'EXAD','ECAN','E',' N-H','EPTA','DECA','NE',' ETH','YLEN','E',' '
     8' PRO','PYLE','NE',' ',' 1-B','UTEN','E',' ',' CIS','-2-B','UTEN'
     9'E',' TRA','NS-2','-BUT','ENE',' I-B','UTEN','E',' ',' 1,3','-BUT
     A,'ADIE','NE',' 1-P','ENTE','NE',' ',' CIS','-2-P','ENTE','NE',' T
     B-','2-PE','NTEN','E',' 2-C','1-1-','BUTE','NE',' 3-C','1-1-','BUT
     C','NE',' 2-C','1-2-','BUTE','NE',' 1-H','EXEN','E',' ',' CYC','LC
     DE','NTAN','E',' C1-','CYCL','O-C5',' ',' CYC','LOHE','XANE',' ',
     E' C1-','CYCL','O-C6',' '/
      INTEGER SBNAME(92)      /' BEN','ZENE',' ',' ',' TOL','UENE',2*'
     F,' O-X','YLEN','E',' ',' M-X','YLEN','E',' ',' P-X','YLEN','E','
     G,' ETH','YLBE','NZEN','E',' NIT','ROGE','N',' ',' OXY','GEN',2*'
     H,' CO',3*' ',' CO2',3*' ',' H2S',3*' ',' SO2',3*' ',' 2-M','ETHY'
     I'L-C5',' ',' 3-M','ETHY','L-C5',' ',' 2,2','-DI-','C1-C','4',' 2,
     J','-DI-','C1-C','4',' 1-H','EPTE','NE',' ',' PRO','PADI','ENE','
     K,' 1,2','-BUT','ADIE','NE',' C2-','CYCL','O-C5',' ',' C2-','CYCL'
     L'O-C6',' ',' ISO','PREN','E',' ',' WAT','ER',2*' '/
      INTEGER SDNAME(144)/' AMM','ONIA',2*' ',' CAR','BON',2*' ',' ACE'
     1'TYLE','NE',' ',' PRO','PYNE',2*' ',' 1-B','UTYN','E',' ',' 2-M',
     2ETHY','LPRO','PENE',' CYC','LOPE','NTEN','E',' N-C','3-BE','NZEN'
     3'E',' I-C','3-BE','NZEN','E',' 1-C','1-2-','C2-B','ENZN',' 1-C',
     4'1-3-','C2-B','ENZN',' 1-C','1-4-','C2-B','ENZN',' 1,2',',3ME',
     5'SITY','LENE',' 1,2',',4ME','SITY','LENE',' 1,3',',5ME','SITY',
     6'LENE',' N-B','UTYL','BENZ','ENE',' 2-M','ETHY','LHEX','ANE',
     7' 3-M','ETHY','LHEX','ANE',' 2-M','ETHY','LHEP','TANE',' 2,2',',4
     8T','RI-C','1-C5',' 1-O','CTEN','E',' ',' CYC','LOPE','NTEN','E',
     9' TNS','-1,3','DIC1','CYC6',' CIS','-1,4','DIC1','CYC6',' TNS','-
     A,4','DIC1','CYC6',' 1,1','-DI-','C1-C','YC6',' CIS','-1,2','DIC1'
     B'CYC6',' CIS','-1,3','DIC1','CYC6',' N-O','CTAD','ECAN','E',' N-N
     C,'ONAD','ECAN','E',' N-E','ICOS','ANE',' ',' 1,1','-DI-','C1-C',
     D'YC5',' CIS','-1,2','DIC1','CYC5',' TNS','-1,2','DIC1','CYC5',' C
     ES','-1,3','DIC1','CYC5',' TNS','-1,3','DIC1','CYC5'/
      EQUIVALENCE (SCNAME(1),SANAME(1)),(SCNAME(157),SBNAME(1))
      EQUIVALENCE (SCNAME(249),SDNAME)
C
C-----ACCENTRIC FACTORS  :REFERENCED FROM'REID-SHERWOOD-PRAUSNITZ'
      REAL AOMEG(98)/-.22,.008,.098,.152,.176,.193,.227,.251,.197,.296,
     1.35,.394,.444,.49,.535,.562,.623,.679,.706,.742,.77,.085,.148,.18
     2,.202,.214,.19,.195,.245,.24,.237,.232,.209,.285,.285,.192,.239,
     3.213,.269,.212,.257,.314,.331,.324,.301,.04,.021,.049,.225,.1,
     4.25,.279,.275,.231,.247,.358,.313,.255,.283,.243,.164,.344,.25,0.
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      *.184,.218,.05,.19,.24,.344,.335,.294,.36,.322,2*.39,.398,.392,.33
      6.289,378,.303,.386,.24,.189,.234,.242,.238,.236,.224,.77,.827,
      7.907,273,4*.269/
C
C      CHAO-SEADER MODIFIED HILDEBRAND SOLUBILITY PARAMETER
C              (CAL./ML.)** 1/2
       REAL DEL(98)/3.25,5.45,5.88,6.00,2*6.73,3*7.021,7.266,7.43,7.551,
      1.649,7.721,7.79,7.84,7.89,7.92,7.96,7.99,8.03,5.8,6.2,4*6.76,6.94
      26*7.055,7.4,8.107,7.849,8.196,7.826,9.158,8.915,8.987,8.818,8.769
      38.787,2.58,4.,3.13,6.,5.634,6.,7.018,7.132,6.712,6.967,7.168,6.85
      4,7.95,7.739,7.743,7.277,7.39,
      A 6.64, 1.00, 4.55, 7.52, 7.56, 6.76, 8.24, 8.64, 8.53, 8.88, 8.72
      B 8.67, 9.08, 8.88, 8.78, 8.52, 7.21, 7.29, 7.35, 6.85, 7.60, 8.24
      C 7.81, 7.79, 7.56, 7.69, 7.93, 7.68, 7.44, 7.41, 7.38, 7.56, 7.89
      D 7.64, 7.57, 7.62/
C
C      VOLUME AT 25 DEG.C. , ML./ G-MOLE
       REAL V25(98)/31.,52.,68.,84.,105.5,101.4,117.4,116.1,123.3,131.6,
      1147.5,163.5,179.6,196.,212.2,228.6,244.9,261.3,277.8,294.1,310.4,
      261.,79.,95.3,91.2,93.8,95.4,88.,110.4,107.8,109.,108.7,112.8,106.
      3,125.8,94.7,113.1,108.7,128.3,89.4,106.8,121.2,123.5,124.,123.1,
      4 36.0,28.4,35.2,53.6,43.6,45.2,132.9,130.6,122.7,131.2,141.7,61.6
      5 83.7,128.8,143.1,100.37,18.076,
      A 54.6,  1.0, 42.8, 64.3, 84.1, 95.4, 91.8,140.2,140.3,137.1,139.7
      B140.2,135.0,137.9,139.6,156.8,148.6,146.7,164.6,166.1,157.9, 91.8
      C143.8,144.1,148.0,144.5,141.6,145.6,327.5,344.7,360.5,130.9,127.8
      D131.5,132.6,131.9/
C
C      CHAO-SEADER CHARACTERISTIC MOLAR VOLUMES - ML./ G-MOLE
       REAL VW(98)/.955,5.,7.88,10.35,13.37,13.,15.36,15.27,15.89,17.64,
      10.05,22.49,24.94,27.42,29.9,32.39,34.88,37.39,39.89,42.41,44.92,6
      288,9.69,12.17,11.71,12.,12.17,11.27,14.55,14.26,14.41,14.31,14.77
      314.14,16.9,12.72,15.33,14.87,17.67,12.26,14.83,17.03,17.28,17.34,
      47.23,2.534,2.871,2.584,6.365,5.081,6.516,17.727,17.473,16.297,
      517.519,19.223,7.721,10.936,17.713,19.916,13.297,2.552,
      6 6.908, 0.001, 4.983, 8.074,11.091,12.169,12.327,19.745,19.714,
      719.392,19.660,19.730,19.178,19.517,19.683,22.229,20.077,19.907,
      822.555,22.622,21.697,12.327,19.987,20.029,20.531,20.073,19.723,
      920.218,47.517,50.152,52.579,17.868,17.548,17.986,18.136,18.041/
C
C-----THE FOLLOWING ARE THE CRITICAL CONSTANTS,
C-----UPDATED VALUES FROM REID-SHERWOOD-PRAUSNITZ'S
C----- "PROPERTIES OF GASES AND LIQUIDS" THIRD EDITION
C----- ARE USED.
C       CRITICAL TEMPERATURES, DEG. K.
        REAL ATC(98)/33.27,190.6,305.43,369.8,408.14,425.17,460.4,469.6,
      1433.76,507.4,540.16,568.8,594.6,617.6,638.8,658.3,675.8,694.,70
      27.,717.,733.,282.4,365.,419.6,435.6,428.6,418.,425.,464.7,476.,47
      3.,465.,450.,470.,504.0,511.6,532.7,553.4,572.1,562.1,591.7,630.2,
      417.,616.2,617.1,126.2,154.6,132.9,304.2,373.2,430.8,497.5,504.4,
      5488.7,499.9,537.2,393.,443.7,569.5,609.,484.,647.3,405.6,0.,308.
      63,402.4,463.7,417.9,506.,638.3,631.,651.,637.,640.,664.5,649.1,6
      737.3,660.5,530.3,535.2,559.6,543.9,566.6,506.,2*598.,590.,591.,6
      806.,591.,745.,756.,767.,547.,564.8,3*553.2/
C
C       CRITICAL PRESSURES, ATM.
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```
        REAL APC(98)/12.8,45.4,48.2,41.9,36.,37.5,33.4,33.3,31.6,29.3,27.
       *24.5,22.8,20.8,19.4,18.,17.,16.,15.,14.,13.,49.7,45.6,39.7,41.5,
       20.5,39.5,42.7,40.,36.,36.,34.,34.7,34.,31.3,44.5,37.4,40.2,34.3,
       3.3,40.6,36.8,35.,34.7,35.6,33.5,49.8,34.5,72.8,88.,77.8,29.7,30.
       *30.4,30.9,28.,54.,44.4,33.5,30.,38.,217.6,111.3,0.,60.6,55.5,46.
       539.5,55.6,5.6,31.6,31.7,30.,28.,29.,34.1,31.9,30.9,28.5,27.,27.8
       624.5,25.3,25.9,55.6,6*29.3,11.9,2*11.,5*34./
 C
 C      CRITICAL VOLUMES,  CC./GMOLE
        REAL AVC(98)/65.,99.,148.,203.,263.,255.,306.,304.,303.,370.,432.
       *492.,548.,603.,660.,713.,780.,830.,2*880.,1000.,129.,181.,240.,
       *234.,238.,239.,221.,3*300.,294.,300.,318.,350.,260.,319.,308.,36
       *,259.,316.,369.,376.,379.,374.,89.5,73.4,93.1,94.,98.5,122.,367.
       *367.,359.,358.,440.,162.,219.,375.,450.,276.,56.,73.,0.,113.,164.
       *220.,239.,254.,440.,428.,460.,490.,470.,2*430.,433.,497.,421.,
       *404.,488.,468.,464.,254.,6*416.,3*779.,360.,368.,3*362./
 C
 C      MOLECULAR WEIGHTS
        REAL AMW(98)/2.016,16.042,30.068,44.094,2*58.12,3*72.146,86.172,
       1100.198,114.224,128.25,142.276,156.302,170.328,184.354,198.38,
       2212.406,226.432,240.458,28.052,42.078,4*56.104,54.088,6*70.13,
       384.156,70.13,2*84.156,98.182,78.108,92.134,4*106.16,28.016,32.,28
       401,44.01,34.08,64.06,4*86.2,98.2,40.1,54.1,98.2,112.2,68.1,18.02,
       A 17.03,12.01,26.036,40.062,54.088,56.104,68.114,8*120.186,134.212
       B 2*100.198, 2*114.224,112.208,68.114, 6*112.208,254.48,268.51,
       C 282.54,5*98.182/
 C
 C      DENSITIES AT 15 DEG. C.,  G./ML.
        REAL DENS(98)/.07,.2,.376,.5076,.5633,.5847,.6246,.63089,.5967,.6
       1384,.68801,.70654,.72146,.7339,.7440,.7525,.7600,.7663,.7720,.773
       2,.7780,.3490,.5226,.6014,.6271,.61,.6005,.6274,.64565,.6607,.6534
       3.6558,.6326,.6776,.67779,.75018,.7534,.78314,.77371,.88417,.87146
       4.88440,.86836,.86532,.87141,.808,1.140,.804,1.101,.790,1.434,.657
       5,.669,.654,.6664,.7015,.657,.658,.771,.7922,.6861,1.0,
       A.6173,1.000,.6150,.6300,.6500,.6004,.7505,.8660,.8660,.8852,.8690
       B.8657,.8987,.8802,.8689,.9650,.6830,.6915,.7021,.6963,.7194,.7505
       C.7892,.7873,.7670,.7854,.8006,.7803,.7856,.7892,.7924,.7593,.7774
       D.7562,.7490,.7535/
 C
 C      **** COEFFICIENTS OF ZERO PRESSURE HEAT CONTENT. *****
 C      ****REVISED DATA-REID-SHERWOOD-PRAUSNITZ :3RD.EDN*****
 C-----EQN. IS: CP(0)=APHA+BETTA*T+GAMA*T**2+DELTA*T**3
 C-----UNITS ARE:  CP IN CALS/GRAM.MOLE-OK ,T IN OK
 C
        REAL APHA(98)/6.483,4.598,1.292,-1.009,-0.332,2.266,-2.275,
       *-0.866,-3.963,-1.054,-1.229,-1.456,0.751,-1.89,-2.005,-2.228,
       *-2.499,-2.623,-2.846,-3.109,-3.336,0.909,0.886,-0.715,0.105,
       *4.375,3.843,-0.403,-0.032,-3.414,0.465,2.525,5.193,2.819,-0.417,
       *-12.808,-11.968,-13.027,-14.789,-8.101,-5.817,-3.786,-6.966,
       *-5.993,-10.294,7.44,6.713,7.373,4.728,7.629,5.697,-2.524,-0.57,
       *-3.973,-3.489,-0.789,2.366,2.675,-13.211,-15.26,-0.815,7.701,
       *6.524,0.,6.41,3.513,2.997,3.834,-9.915,-7.473,-9.402,-3.93,-6.926
       *-6.523,-1.658,-1.115,-4.679,-5.491,-9.408,-1.683,-21.435,-1.782,
       *-.979,-9.915,-15.323,-15.323,-16.806,-17.22,-16.33,-15.564,-3.456
       *-3.7,-5.346,-13.827,-13.29,-13.022,-13.022,-13.022/
 C
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      REAL BETTA(98)/2.215E-3,1.245E-2,4.254E-2,7.315E-2,9.189E-2,7.913
     *E-2,1.21E-1,1.164E-1,1.326E-1,1.39E-1,1.615E-1,1.842E-1,1.618E-1,
     *2.295E-1,2.517E-1,2.744E-1,2.974E-1,3.195E-1,3.422E-1,3.652E-1,
     *3.879E-1,3.74E-2,5.602E-2,8.436E-2,7.054E-2,6.123E-2,6.698E-2,
     *8.165E-2,1.034E-1,1.099E-1,9.988E-2,9.547E-2,9.29E-2,8.381
     *E-2,1.268E-1,1.296E-1,1.524E-1,1.46E-1,1.873E-1,1.133E-1,1.224E-1
     *1.424E-1,1.504E-1,1.443E-1,1.689E-1,-0.324E-2,-0.879E-6,-0.307E-2
     *1.754E-2,3.431E-4,1.6E-2,1.477E-1,1.359E-1,1.503E-1,1.469E-1,1.50
     *E-1,4.273E-2,6.51E-2,1.794E-1,2.124E-1,1.095E-1,5.692E-3,4.595E-4
     *0.0,1.81E-2,4.453E-2,6.553E-2,6.698E-2,1.106E-1,1.788E-1,1.873
     *E-1,1.671E-1,1.742E-1,1.714E-1,1.513E-1,1.49E-1,1.606E-1,1.895E-
     *1,2.064E-1,1.633E-1,2.967E-1,1.858E-1,1.729E-1,1.106E-1,2*2.108E-
     *,2.181E-1,2.149E-1,2.143E-1,2.111E-1,4.101E-1,4.329E-1,4.632E-1,
     *1.832E-1,1.813E-1,3*1.813E-1/
C
      REAL GAMA(98)/-3.298E-6,2.56E-6,-1.657E-5,-3.789E-5,-4.409E-5,-2.
     *47E-5,-6.519E-5,-6.163E-5,-7.879E-5,-7.449E-5,-8.72E-5,-1.002E-4,
     *-4.606E-5,-1.263E-4,-1.385E-4,-1.516E-4,-1.615E-4,-1.773E-4,-1.90
     *E-4,-2.039E-4,-2.169E-4,-1.994E-5,-2.771E-5,-4.754E-5,-2.431E-5,-
     *.675E-5,-2.607E-5,-5.589E-5,-5.534E-5,-6.068E-5,-5.201E-5,-4.648E
     *-5,-4.794E-5,-2.667E-5,-6.933E-5,-7.239E-5,-8.699E-5,-6.027E-5,-1
     *06E-4,-7.206E-5,-6.605E-5,-8.224E-5,-8.95E-5,-8.058E-5,-1.149E-4,
     *6.4E-6,4.17E-6,6.662E-6,-1.338E-5,5.809E-6,-1.185E-5,-8.533E-5,-6
     *.854E-5,-8.314E-5,-8.063E-5,-8.388E-5,-2.822E-5,-3.507E-5,-1.05E-
     *4,-1.22E-4,-7.971E-5,2.521E-6,4.078E-6,0.0,-1.196E-5,-2.803E-5,
     *-3.69E-5,-2.607E-5,-6.16E-5,-1.1E-4,-1.215E-4,-9.341E-5,-1.042E-4
     *-1.01E-4,-7.945E-5,-7.793E-5,-8.819E-5,-1.05E-4,-1.502E-4,
     *-8.92E-5,-2.808E-4,-1.024E-4,-9.641E-5,-6.16E-5,-1.2E-4,-1.198E-4
     *-1.268E-4,-1.199E-4,-1.227E-4,-1.178E-4,-2.291E-4,-2.424E-4,
     *-2.667E-4,-1.075E-4,-1.071E-4,-1.07E-4,-1.07E-4,-1.07E-4/
C
      REAL DELTA(98)/1.826E-9,-2.703E-9,2.08E-9,7.678E-9,6.915E-9,-0.67
     *E-9,1.367E-8,1.267E-8,1.823E-8,1.551E-8,1.829E-8,2.115E-8,-7.121E
     *9,2.701E-8,2.954E-8,3.246E-8,3.555E-8,3.817E-8,4.108E-8,4.418E-8,
     *4.71E-8,4.192E-9,5.266E-9,1.066E-8,-0.147E-9,-2.147E-9,2.173E-9,
     *1.513E-8,1.118E-8,1.303E-8,1.052E-8,7.915E-9,9.579E-9,-1.387E-9,
     *1.446E-8,1.549E-8,1.914E-8,3.156E-9,2.237E-8,1.703E-8,1.173E-
     *8,1.798E-8,2.205E-8,1.629E-8,3.107E-8,-2.79E-9,-2.544E-9,-3.037E-
     *9,4.097E-9,-2.81E-9,3.172E-9,1.931E-8,1.202E-8,1.636E-8,1.629E-
     *8,1.817E-8,6.645E-9,7.378E-9,2.398E-8,2.634E-8,2.389E-8,-0.859E-9
     *-2.83E-9,0.0,3.373E-9,7.701E-9,8.24E-9,2.173E-9,1.298E-8,2.582E-8
     *3.084E-8,2.228E-8,2.388E-8,2.2798E-8,1.579E-8,1.523E-8,1.839E-8,
     *2.047E-8,4.386E-8,1.871E-8,1.103E-7,2.191E-8,2.072E-8,1.298E-8,
     *2*2.552E-8,2.758E-8,2.461E-8,2.624E-8,2.436E-8,4.964E-8,5.267E-8,
     *6.039E-8,2.413E-8,2.422E-8,3*2.429E-8/
C
C
C-----NORMAL BOILING POINTS,DEG. K
       REAL ATB(98)/20.4,111.7,184.5,231.1,261.3,272.7,301.,309.2,282.6,
     1341.9,371.6,398.8,424.,447.3,469.1,489.5,508.6,426.7,543.8,560.,
     2575.2,169.4,225.4,266.9,276.9,274.,266.3,268.7,303.1,310.1,309.5,
     3304.3,293.3,311.7,336.6,322.4,345.,353.9,374.1,353.3,383.8,417.6,
     4412.3,411.5,409.3,77.4,90.2,81.7,194.7,212.8,263.,333.4,336.4,33
     59,331.2,366.8,238.7,284.,376.6,404.9,307.2,373.2,239.7,0.,189.2,
     6250.,281.2,266.3,317.4,432.4,425.6,438.3,434.5,435.2,449.2,442.5,
     *437.9,456.4,363.2,365.,390.8,372.4,394.4,317.4,397.6,397.5,392.5,
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      8392.7,402.9,393.3,589.5,603.1,617.,361.,372.7,3*365./
C
C
C
C-----THE FOLLOWING ARE THE RACKETT PARAMETERS .
C-----THESE HAVE . DATA REGRESSED BY SPENCER &
C-----DANNER,"IMPROVED EQUATION FOR PREDICTING
C-----SAT. LIQUID DENSITY" JOURNAL OF CHEMICAL
C-----AND ENGINEERING DATA :17,#2,1972 ,
C-----               . CRITICAL COMPRESSIBILITY FACTORS
C-----WHERE DATA IS NOT AVAILABLE FROM SPENCER & DANNER
C
C
       REAL ZRAMSD(98)/.3199,.2876,.2789,.2763,.275,.2728,.2716,
      *0.2685,.2723,.2635,.2611,.2576,.2547,.2503,.24,.2466,
      *0.24,3*0.23,.22,.281,.2785,.2736,.2705,.2721,.2727,
      *0.2713,.2944,2*0.28,.262,.282,.28,.26,.2687,.273,.2729,
      *0.2699,.2696,.257,.2633,.2593,.2589,.2626,.2905,
      *0.2909,.2917,.2737,.2851,.268,.267,.273,.272,.27,.28,
      *0.271,0.267,0.269,0.27,.264,.229,.2465,0.0,.2712,.2703,
      *0.27,.2727,.277,.265,4*0.26,.27,.258,.26,2*0.261,
      *0.256,.26,.266,.26,.277,6*0.25,3*0.336,5*0.27/
C
C
C
C-----THE FOLLOWING PARAMETERS INDICATES WHICH SOURCE IS
C-----USED FOR THE LIQUID SPECIFIC HEAT COEFFICIENTS DATA  :
C-----      1=DATA IS REGRESSED BETWEEN THE FREEZING PT.
C-----        AND THE NORMAL BOILING PTS.OF THE COMPONENT.
C-----        THE 'LYMAN-DANNER'PREDICTION METHOD WAS USED,
C-----        REF :"PROPERTIES OF LIQUIDS AND GASES",3RD.EDN.
C-----        UNITS ARE :CPL-->CALS/GM.MOLE/DK ,T-->DK
C-----      2=DATA OBTAINED FROM "HYDROCARBON PROCESSING",46,8,1967.
C-----        AN ARTICLE BY-W.S.TAMPLIN & D.A.ZUZIC.
C-----        CPL=A+B*T+C*T**2+D*T**3  ,IN CALS/GM.MOLE/DC  ,T IN DC
C-----        CONVERSIONS DUE TO TEMP. UNIT IS INCORPORATED IN CODE.
C-----      3=DATA OBTAINED FROM "PHYSICAL PROPERTIES",A 'CHEMICAL
C-----        ENGINEERING' PUBLICATION,BY-CARL L.YAWS.
C-----        UNITS ARE  :CPL IN CALS/GM/DK,  T IN DK
       REAL CPTYPE(98)/4*3.0,4*2.0,1.0,7*2.0,1.0,3*2.0,1.0,2*3.0,
      *3*2.0,1.0,2.0,1.0,8*2.0,3.0,5*2.0,3.0,2.0,4*3.0,1.0,3.0,2*1.0,
      *3*2.0,1.0,4*2.0,2*3.0,1.0,4*1.0,2.0,1.0,2.0,5*1.0,2*2.0,1.0,2*2.C
      *1.0,2.0,1.0,2*2.0,3*1.0,2.0,5*1.C,2.0,4*1.0/
C-----THE FOLLOWING ARE THE COEFFICIENTS OF LIQ. SPECIFIC HEAT :
C-----        CPL=SPHL1+SPHL2*T+SPHL3*T**2+SPHL4*T**3
C
       REAL SPHL1(98)/3.79,1.23,0.1388,0.3326,31.7993,31.8072,37.4372,
      *38.1234,30.8751,43.899,51.6844,58.4915,65.5491,72.6847,79.9498,
      *87.4197,143.753,102.3601,110.447,117.9904,136.6324,-0.3402,.4706,
      *29.3385,28.7748,29.3427,-21.7,27.9619,33.8672,34.6958,35.8566,
      *35.9545,35.4742,35.0291,41.8789,28.4092,35.7877,-1.284,41.7891,
      *31.2646,35.9711,43.103,41.8289,-0.8429,42.4591,-1.064,-0.4587,.56
      *45,-19.3,-404.1,-0.5737,47.431,42.99,43.1081,42.8839,48.4823,-15.
      *,28.5444,42.1086,47.823,34.4949,0.6741,-1.923,0.0,-60.91,6.612,
      *31.1926,-15.046,27.5764,34.076,39.181,51.309,51.051,57.503,49.733
      *49.142,58.11,55.225,50.8207,-50.411,57.4676,59.92,55.3352,27.5764
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      *42.546,42.456,44.818,47.1783,44.054,42.075,147.725,138.707,
      *135.995,41.9763,37.458,22.3897,37.4579,22.3897/
C
       REAL SPHL2(98)/-329.8E-3,-10.33E-3,8.481E-3,2.332E-3,7.6009E-2,
      *5.848E-2,7.3942E-2,6.6571E-2,-0.3893E-1,9.4999E-2,7.5747E-2,
      *8.2209E-2,8.6196E-2,8.2932E-2,7.5836E-2,7.7744E-2,-0.50557,
      *8.053E-2,3.9907E-2,3.8922E-2,-0.8769,6.218E-3,1.683E-3,5.3019E-2,
      *4.8411E-2,4.3362E-2,0.7085,5.6518E-2,-0.3663E-1,5.8063E-2,6.233E-
      *2,6.0298E-2,6.8157E-2,5.4474E-2,7.2299E-2,7.1177E-2,7.7048E-2,
      *13.39E-3,8.9468E-2,4.7709E-2,5.6715E-2,6.9279E-2,7.0207E-2,8.961
      *E-3,7.4669E-2,59.47E-3,32.34E-3,4.798E-3,254.6E-3,7.5539,10.34E-3
      *,-0.1192,-0.6408E-1,9.159E-2,8.4494E-2,8.003E-2,0.6747,4.4089E-2,
      *8.9313E-2,10.6726E-2,7.4755E-2,2.825E-3,31.1E-3,0.0,1.4164,.1794,
      *6.458E-2,0.6404,6.2631E-2,0.8121E-1,0.2433E-1,-0.6592E-1,.7612E-1
      *-0.1375,7.774E-2,8.022E-2,-0.1388,8.606E-2,9.299E-2,1.0551,10.61E
      *2,-0.1552,8.5024E-2,6.263E-2,-0.7479E-1,-0.7424E-1,-0.1025,10.805
      *E-2,-0.9238E-1,-0.7787E-1,-0.2109,10.1419E-2,-0.2374,-0.1492,
      *-0.711E-1,0.8052E-1,-0.711E-1,0.8052E-1/
C
       REAL SPHL3(98)/12170.9E-6,72.0E-6,-56.54E-6,-13.36E-6,2.044E-4,
      *1.9193E-4,2.7035E-4,2.3866E-4,0.1671E-3,5.0E-4,2.0906E-4,2.7364E-
      *4,3.7681E-4,5.8319E-4,10.1152E-4,7.5763E-4,0.1511E-2,6.799E-4,
      *14.0571E-4,14.7679E-4,0.2376E-2,-50.12E-6,-16.82E-6,1.6466E-4,
      *2.6214E-4,1.3583E-4,-0.3455E-2,2.4286E-4,0.1187E-3,2.2389E-4,1.70
      *5E-4,2.0915E-4,1.7583E-4,2.1072E-4,2.5519E-4,2.3504E-4,2.0035E-4,
      *-35.1E-6,1.2454E-4,0.9019E-4,1.7767E-4,1.052E-4,2.8782E-4,-21.45
      *E-6,2.124E-4,-768.7E-6,-395.1E-6,-143.7E-6,-1095.5E-6,-0.4519E-1,
      *-40.28E-6,0.4496E-3,0.2374E-3,0.4405E-4,1.7032E-4,2.9938E-4,
      *-0.3866E-2,2.0535E-4,2.112E-4,2.1519E-4,2.644E-4,-8.371E-6,
      *-110.9E-6,0.0,-0.8709E-2,-0.8241E-3,2.4403E-4,-0.3261E-2,2.077
      *E-4,-0.1708E-3,0.1287E-4,0.2712E-3,0.3033E-3,0.4886E-3,0.9055E-4,
      *3.2532E-4,0.4914E-3,4.11E-4,2.207E-4,-0.3825E-2,6.0033E-4,0.7278
      *E-3,3.2652E-4,2.077E-4,0.3967E-3,0.3948E-3,0.492E-3,2.1395E-4,
      *.916E-3,.7564E-3,2.257E-4,.3545E-3,-0.1536E-3,.3545E-3,-0.1536E-3
C
       REAL SPHL4(98)/-2434.8E-9,-107.3E-9,126.1E-9,30.16E-9,4*0.0,0.159
      *-6,7*0.0,-0.1112E-5,3*0.0,0.5696E-5,-0.1703E-5,126.3E-9,44.07E-
      *9,3*0.0,0.5696E-5,0.0,0.1704E-6,8*0.0,32.27E-9,5*0.0,18.45E-9,
      *3357.3E-9,1575.7E-9,911.95E-9,1573.3E-9,0.8935E-4,52.85E-9,-0.230
      *E-6,0.1931E-7,3*0.0,0.7108E-5,4*0.0,8.601E-9,137.6E-9,0.0,0.3328E
      *6,0.1467E-6,-0.1268E-6,-0.1446E-6,-0.327E-6,2*0.0,-0.326E-6,2*0.0
      *0.4842E-5,0.0,-0.444E-6,2*0.0,-0.2395E-6,-0.2376E-6,-0.331E-6,
      *,-0.5878E-6,-0.48E-6,0.0,-0.1955E-6,0.371E-6,-0.1955E-6,0.371E-6/
C
C
C
C-----HEAT OF VAPORIZATION VALUES AT THE RESPECTIVE NORMAL
C-----BOILING PT.S.REFERENCE  :"PROPERTIES OF GASES AND LIQUIDS"3RD
C-----EDITION.        UNIT OF HVAP IS :CALS/GM.MOLE
C
       REAL AHVAP(98)/216.,1955.,3515.,4487.,5090.,5352.,5900.,6160.,
      *5438.,6896.,7576.,8225.,8823.,9388.,9920.,10430.,10910.,11380.,
      *11820.,12240.,12640.,3237.,4400.,5238.,5580.,5439.,5286.,5370.,
      *6022.,6240.,6230.,6094.,5760.,6287.,6760.,6524.,6950.,7160.,7440.
      *7352.,7930.,8800.,8690.,8600.,8500.,1333.,1630.,1444.,4100.,
      *4460.,5955.,6640.,6710.,6287.,6520.,7430.,4450.,5800.,0.,4050.,
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      *5290.,5970.,5286.,6450.,9140.,8970.,9290.,9210.,9180.,9570.,
      *9380.,9330.,9380.,7330.,7360.,8080.,7411.,8070.,6450.,8090.,8070
      *7790.,7790.,8040.,7840.,13020.,13390.,13740.,7240.,7576.,
      *3*7375.0/
C
C
C-----ANTOINE VAPOR PRESSURE COEFFICIENTS :THE VALUES OF THE
C-----FIRST THREE ARE AVAILABLE.IF DESIRED,THE USER SUPPLIES
C-----THE NEXT THREE. P IS IN MMHG, T IS IN DEG K.
C-----THE EQUATION USED:
C-----LN(PO)=A1+A2/(A3+T)+A4*LN(T)+A5*T+A6*T**2
C
C
C
       REAL ANTO(1,98)/13.63,15.224,15.664,15.726,15.538,15.6782,15.633
      X15.8333,15.2069,15.8366,15.8737,15.9426,15.9671,16.0114,16.0541,
      *16.1134,16.1355,16.148,16.1724,16.1841,16.151,15.5368,15.7027,
      *15.7564,15.8171,15.8177,15.7528,15.7727,15.7645,15.8251,15.9011,
      *15.826,15.7179,15.9238,15.8089,15.8574,15.8023,15.7527,15.7105,
      *15.9008,16.0137,16.1156,16.139,16.0963,16.0195,14.9542,15.4075,
      *14.3686,22.5898,16.104,16.768,15.7476,15.7701,15.5536,15.6802,
      *15.8894,13.1563,16.1039,15.858,15.8125,15.8548,18.3036,16.9481,0.
      X16.348,15.6227,16.0605,15.7528,15.9356,16.0062,15.9722,16.1253,
      *16.1545,16.1135,16.2121,16.219,16.2893,16.0793,15.8261,15.8133,
      *15.9278,15.685,15.963,15.9356,15.7371,15.7333,15.6984,15.6535,
      *15.7438,15.747,16.1232,16.1533,16.4685,15.6973,15.7729,
      *3*15.7594/
C
C
C
       REAL TZ(2,98)/164.9,897.84,1511.42,1872.45,2032.73,2154.9,2477.07
      *2348.67,2034.15,2697.55,2911.32,3120.29,3291.45,3456.8,3614.07,
      *3774.56,3892.91,4008.52,4121.51,4214.91,4294.55,1347.01,1807.53,
      *2132.42,2210.71,2212.32,2125.75,2142.66,2405.96,2459.05,2495.97,
      *2426.42,2333.61,2521.53,2654.81,2588.48,2731.,2766.63,2926.04,
      *2788.51,3096.52,3395.57,3366.99,3346.65,3279.47,588.72,734.55,53
      *0.22,3103.4,1768.69,2302.35,2614.38,2653.43,2489.5,2595.44,2895.5
      *,1054.72,2397.26,2990.13,3183.25,2467.4,3816.44,2132.5,0.,1637.14
      *1850.7,2271.42,2125.75,2583.07,3433.84,3363.6,3535.33,3521.08,
      *3516.31,3670.22,3622.58,3614.19,3633.4,2845.06,2855.66,3079.63,
      *2896.28,3116.52,2583.07,3093.95,3098.39,3063.44,3043.34,3148.35,
      *3081.95,4361.79,4450.44,4680.46,2807.94,2922.3,3*2861.53/
C
C
C
       REAL E(3,98)/3.19,-7.16,-17.16,-25.16,-33.15,-34.42,-40.05,-39.94
      *-45.37,-48.78,-56.51,-63.63,-71.73,-78.67,-85.45,-91.31,-98.93,-1
      *5.4,-111.8,-118.7,-124.,-18.15,-26.15,-33.15,-36.15,-33.15,-33.15
      *-34.3,-39.63,-42.56,-40.18,-40.36,-36.33,-40.31,-47.3,-41.79,-47.
      *,-50.5,-51.75,-52.36,-53.67,-59.46,-58.04,-57.84,-59.95,-6.6,-6.4
      *,-13.15,-.16,-26.06,-35.97,-46.58,-46.02,-43.81,-44.25,-53.97,
      *-77.07,-30.88,-52.47,-58.15,-39.64,-46.18,-32.98,0.,-19.77,-44.07
      *-40.3,-33.15,-39.7,-66.,-63.37,-65.85,-64.64,-64.23,-66.07,-64.59
      *-63.57,-71.77,-53.6,-53.93,-59.46,-52.41,-60.4,-39.7,-57.76,-57.,
      *-54.57,-55.3,-57.31,-55.08,-129.9,-135.6,-141.1,-51.2,-52.94,
      *-51.46,-51.46,-51.46/
```

```
C
      REAL DANTO(4,98)/98*0./
C
      REAL WANTO(5,98)/98*0./
C
      REAL ANTOX(6,98)/98*0./
C
C-----BINARY INTERACTION PARAMETERS FOR THE 'SRK' EQN.
C-----REF:  'PROPERTIES OF GASES AND LIQUIDS'--REID-SHERWOOD-
C-----          PRAUSNITZ. 3RD.EDN. PP-77.
C-----INTERACTION IS SIGNIFICANT FOR THE FOLLOWING POLAR
C-----COMPONENTS: H2S,CO,CO2,N2.
C-----FOR POLAR-POLAR & NON.POLAR-NON.POLAR PAIRS,
C-----INTERACTION IS NEGLECTED(AK(I,J)=0)
C
      REAL AKNTRO(98)/0.0,0.02,0.06,12*0.08,6*0.0,0.04,0.06,14*0.,
     *                8*0.08,53*0.0/
      REAL AKCMON(98)/0.0,-0.02,46*0.0,-0.04,49*0.0/
      REAL AKCDOX(98)/0.0,0.12,6*0.15,0.0,6*0.15,6*0.0,0.15,0.08,
     *                14*0.0,8*0.15,53*0.0/
      REAL AKHTOS(98)/0.0,0.08,2*0.07,4*0.06,0.0,0.05,2*0.04,
     *                3*0.03,6*0.0,2*0.07,14*0.0,8*0.03,
     *                3*0.0,0.12,49*0.0/
C
C
C
      NAMELIST/NSCOMP/ PC,TC,VC,MW,OMEGA,ADEL,AVW,APH,BET,GAM,DTA
     *             ZRA,VOL,TB,ALD,ANT,AK,CPL,CPV,EVAP,CPCODE
C
C     WRITE (6,*) NOCOMP
C     WRITE (6,*) COMPNT
C
      DO 10  I=1,NOCOMP
      J=NTCOMP(I)
      IF(J .GT.100) GO TO 8
      I1=4*(I-1)+1
C     IF((KOMNAM(I1)+KOMNAM(I1+1)+KOMNAM(I1+2)+KOMNAM(I1+3)) .NE. 0)
C    X  GO TO  7
      IF (KOMNAM(I1).NE.0 .AND. KOMNAM(I1+1).NE.0 .AND.
     *   KOMNAM(I1+2).NE.0 .AND. KOMNAM(I1+3).NE.0) GO TO 7
      DO 6  COUNT=1,4
      IK=I1+COUNT-1
      IS=4*(J-1) + COUNT
    6 KOMNAM(IK) = SCNAME(IS)
C-----FOLLOWING ARE THE COMPONENT PROPERTIES
7     PP=APC(J)
      TT=ATC(J)
      OMEGA(I)=AOMEG(J)
      ADEL(I)=DEL(J)
      ZRA(I)=ZRAMSD(J)
      AVW(I)=VW(J)
      PC(I)=PP
      TC(I)=TT
      VC(I)=AVC(J)
      TX1=ATB(J)
      TB(I)=TX1
```

```
      W(I)=AMW(J)
C-----OA & OB ARE THE 'RK' PARAMETERS
      OA(I)=SQRT(0.42748*TC(I)**2.5/PC(I))
      OB(I)=0.08664*TC(I)/PC(I)
C-----FOLLOWING ARE THE ANTOINE EQN. CONSTANTS
      ANT(1,I)=ANTO(1,J)
      ANT(2,I)=-TZ(2,J)
      ANT(3,I)=E(3,J)
      ANT(4,I)=DANTO(4,J)
      ANT(5,I)=WANTO(5,J)
      ANT(6,I)=ANTOX(6,J)
C-----ALD ARE DENSITIES AT 25 DEG.
      ALD(I)=DENS(J)
C-----APH,..,DTA ARE THE IDEAL GAS HEAT CAPACITY COEFFT.S
      APH(I)=APHA(J)
      BET(I)=BETTA(J)
      GAM(I)=GAMA(J)
      DTA(I)=DELTA(J)
C-----CPV(I,N) ARE THE IDEAL GAS HEAT CAPACITY COEFFT.S
      CPV(I,1)=APHA(J)
      CPV(I,2)=BETTA(J)
      CPV(I,3)=GAMA(J)
      CPV(I,4)=DELTA(J)
C-----CPL(I,N) ARE THE LIQUID SP.HEAT COEFFICIENTS
      IF (CPTYPE(J).NE.3.0) GO TO 701
      CPL(I,1)=SPHL1(J)*AMW(J)
      CPL(I,2)=SPHL2(J)*AMW(J)
      CPL(I,3)=SPHL3(J)*AMW(J)
      CPL(I,4)=SPHL4(J)*AMW(J)
      GO TO 702
701   CPL(I,1)=SPHL1(J)
      CPL(I,2)=SPHL2(J)
      CPL(I,3)=SPHL3(J)
      CPL(I,4)=SPHL4(J)
C-----EVAP IS THE ENTHALPY OF VAP. AT NORMAL B.P
702   EVAP(I)=AHVAP(J)
      TR=ATB(J)
C-----ENP(I,N) ARE THE REFERENCE-STATE ENTHALPY
C-----COEFFIECIENTS OF VAPORS(IDEAL)&LIQUIDS AT REF.TEMP. OF NORMAL
C-----BOILING POINTS.
      ENP(I,10)=CPV(I,4)/4.0
      ENP(I,9)=CPV(I,3)/3.0
      ENP(I,8)=CPV(I,2)/2.0
      ENP(I,7)=CPV(I,1)
      ENP(I,6)=EVAP(I)-(((ENP(I,10)*TR+ENP(I,9))*TR+ENP(I,8))*TR+
     *                ENP(I,7))*TR
      ENP(I,5)=CPL(I,4)/4.0
      ENP(I,4)=CPL(I,3)/3.0
      ENP(I,3)=CPL(I,2)/2.0
      ENP(I,2)=CPL(I,1)
      ENP(I,1)=-(((ENP(I,5)*TR+ENP(I,4))*TR+ENP(I,3))*TR+ENP(I,2))*TR
      IF (CPTYPE(J).NE.2.0) GO TO 703
      ENP(I,1)=ENP(I,1)-CPL(I,2)*273.16*TR+CPL(I,3)*273.16*273.16*TR
      ENP(I,1)=ENP(I,1)-TR*273.16*CPL(I,3)*TR
703   CPCODE(I)=CPTYPE(J)
C-----FOLLOWING ARE THE 'SRK' EQN. INTERACTION PARAMETERS.
```

```
C
      DO 71 M=1,NOCOMP
71    AK(I,M)=0.0
      IF(J.EQ.46)GO TO 72
      IF(J.EQ.48)GO TO 73
      IF(J.EQ.49)GO TO 74
      IF(J.EQ.50)GO TO 75
      GO TO 76
72    DO 721 K=1,NOCOMP
      LL=NTCOMP(K)
721   AK(I,K)=AKNTRO(LL)
      GO TO 76
73    DO 731 K=1,NOCOMP
      LL=NTCOMP(K)
731   AK(I,K)=AKCMON(LL)
      GO TO 76
74    DO 741 K=1,NOCOMP
      LL=NTCOMP(K)
741   AK(I,K)=AKCDOX(LL)
      GO TO 76
75    DO 751 K=1,NOCOMP
      LL=NTCOMP(K)
751   AK(I,K)=AKHTOS(LL)
76    GO TO 9
C-----DEBUGGING AID
    8 TT=TC(I)
      PP=PC(I)
    9 BASEB(I)=.0867*TT/PP
      VC(I)=VC(I)* .45359/28.32
      ZCD(I)=PP*VC(I)/(10.73  *TT)
C     WRITE (6,100) I,J
C 100 FORMAT ('OFTN # 100', 5X,2I10)
C     WRITE (6,101) PP,TT
C 101 FORMAT ('OFTN # 101',5X,2G20.5)
      TT=.4278  *TT*TT/PP* SQRT(TT)
C     WRITE (6,102) TT
C 102 FORMAT ('OFTN # 102',5X,G20.5)
      BASEA(I)= SQRT(TT)
C     WRITE (6,103) BASEA(I)
C 103 FORMAT ('OFTN # 103',5X,G20.5)
C     WRITE (6,104)
C 104 FORMAT (/////)
   10 CONTINUE
      IF(EXFLAG) WRITE (6,NSCOMP)
      RETURN
      END
```

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