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Estimation of Thermodynamic Properties of Petroleum Fractions to Supplement the ASPEN Simulator

by
Steven E. Sund

Thesis submitted to the faculty of the Graduate School of the New Jersey Institute of Technology in partial fulfillment of the requirements for the degree of Masters of Science in Chemical Engineering
1989

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1989

APPROVAL SHEET

Title of Thesis: Estimation of Thermodynamic Properties of Petroleum Fractions to Supplement the ASPEN Simulator

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ABSTRACT

Title of Thesis: Estimation of Thermodynamic Properties of Petroleum Fractions to Supplement the ASPEN Simulator

Steven E. Sund, Master of Science, 1989

Thesis directed by: Professor of Chemical Engineering
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The objective of this study was to develop a method of estimating hydrocarbon pseudocomponent data in a format that is consistent with the ASPEN simulator. Although algorithms exist to estimate the pseudocomponent properties, no comprehensive program exists for the public version of ASPEN. A computer program was developed which will take a minimum of input data and can generate the necessary pure component properties for an ASPEN simulation. The program is meant to complement the ASPEN simulator, so the input is similar to ASPEN's input. The output can be incorporated directly into an ASPEN input or can be of the form used by ASPEN's data file management system (DFMS) translator for creation of a user data bank.

The program has the capability to enter all the necessary input needed to generate the pseudocomponent data or will fill in missing values with 'good' estimates. The program is intelligent enough to calculate only the necessary pure component properties which are needed for a particular ASPEN property route. Preferred existing correlations were used whenever available. If no property correlation was found in the literature, the property

constants were estimated using recommended estimation procedures. Parameters for the remaining properties for which no estimation technique could be found were fit using the ASPEN data bank.

An extensive estimation debug and report facility were included to trace the estimation procedure and/or summarize the properties estimated. Error/warning messages were incorporated wherever feasible, as were statistics on the fit of temperature dependent property constants. All parameter fit were performed using Marquardt's method.

Forward

The United States Department of Energy (DOE) in 1976 realized a need for a "rapid, efficient, and consistent means of performing its process evaluation functions"[1]. At the time there was a large push for fossil fuel energy process development in the synthetic fuel area. The DOE wanted a simulator to study synthetic fuel processes such as coal gasification and liquefaction, and oil shale recovery. The need for a steady state process simulator to develop and evaluate proposed processes before pilot plant construction began brought about the ASPEN project. The ASPEN (Advanced **S**imulator for **P**rocess **En**gineering) project was a consortium of university and industry engineers which during the period from 1976 to 1981 developed the final version of ASPEN. The base used to build the ASPEN simulator was the Monsanto FLOWTRAN simulator program. Working versions were introduced and tested by the Chemical profession from 1978 to 1981. The testing community consisted of the petroleum, chemical, construction, paper, metals, and food industries[2,3].

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[1] Joint MIT-ERDA news release on ASPEN project (Nov. 10, 1976

[2] Gallier, P.,L. Evans, H. Britt, J. Boston, P. Gupta, "ASPEN: advanced capabilities for modeling and simulation of industrial processes", ACS Symposium Series, no. 24, 1980,pp 293-308

After the final release of the public version of ASPEN, other commercial versions were produced based on the existing ASPEN code.

The public version ASPEN maintenance was left to the DOE at the Morgantown Energy Technology Center in Morgantown, West Virginia and is now in revision D. This research is meant to be a supplement to the public version of ASPEN as now available on a Vax system.

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[3] Gallier, P., L. Evans, H. Britt, J. Boston, "ASPEN:advanced system for process engineering, Perspect. Comput., vol. 1, 1981, pp 43-49.

Dedication

I would like to dedicate this Thesis to my wife, Janice A. Sund for her patience in my never ending graduate work and to my parents whose suggestion when times were tough was to 'go for it'.

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I. INTRODUCTION

Mathematical modeling and computer simulation have been widely used in the development, design, and improvement of existing processes in the petroleum industry. A standard tool of the petroleum engineer is the flowsheet simulator[1].

Most steady state simulators are component based, that is, they simulate a process with a specified number of components using a given physical property model. It is the engineer's responsibility to be sure that the component properties and model parameters are complete enough to perform the desired simulation, with the desired degree of accuracy.

Crude petroleum is primarily a mixture of carbon and hydrogen with lesser amounts of oxygen, nitrogen, and sulfur. Metals such as nickel and iron as well as minor amounts of inorganic compounds are also found in trace amounts in petroleum crudes[2].

Feed streams, which a petroleum engineer normally encounters, are composed of complex mixtures of organic chemicals of varying compositions and phases. Low boiling mixtures usually consist of discretely identifiable compounds that at normal temperatures and pressures exist a gas. Higher boiling mixtures consist of mixtures which at

normal temperatures and pressures exist largely as a liquid[3]. These liquid streams are called petroleum fractions and can range from light naphtha to heavy crude oil.

A reasonable knowledge of the characteristics of a crude oil is essential in the design of a petroleum based process. Properties of low boiling hydrocarbon liquids have been studied extensively and pure compounds have been identified and produced synthetically in the laboratory[4]. The higher boiling hydrocarbon mixtures consist of hundreds or possibly thousands of compounds[5] with physical properties that approach a continuum, thereby making the separation into discrete compounds impractical.

The study of crude oil has mainly proceeded along the molecular form or series line. The main groups of hydrocarbons studied in the past were paraffin, olefin, napthene, aromatic, diolefin, and cyclic series[6]. The three most abundant types of hydrocarbons in a typical low boiling crude oil are paraffins, napthenes, and aromatics. The paraffins and napthenes are characterized by being stable saturated hydrocarbons. The aromatic series, on the other hand, is chemically active and can react to form valuable products[7]. All three chemical groups are found in high percentages in an 'average' crude. In low boiling fractions of crude, the paraffins predominate and at higher boiling points the aromatics and naphthenes predominate[8].

Simulation of petroleum based streams can be performed on a fraction of particular boiling range called a "cut". The simulation using a petroleum fraction is realized using a single compound to characterize the group of compounds present in the selected fraction or cut. The simulation using cuts is performed by dividing the petroleum stream into a finite number of cuts representing individual pseudocomponents.

Characterization of pure component properties have been correlated successfully using specific gravity, API (American Petroleum Institute)[9] gravity, UOP (Universal Oil Products) or Watson K characterization factor and/or boiling point. With a petroleum cut or fraction the gravity can be measured directly, but the boiling point can not be quantified.

The common procedure used to characterize a petroleum fraction is to obtain a distillation curve in the laboratory. Various distillation techniques are used by the petroleum industry to characterize a petroleum mixture. Some examples from the API are ASTM D86, ASTM D216, and ASTM D1160[10]. All these methods employ one stage distillations and use conversion charts to obtain a True Boiling Point (TBP) curve.

A true boiling point distillation can be performed in a column of 15 to 50 theoretical stages, however the time required for a typical distillation run can be up to 100

hours[11,12]. Recently, gas chromatograph methods (ASTM D2887) have been developed to obtain boiling point distributions which show good agreement with TBP distillations in much shorter times[13,14].

From the data obtained from the distillation, a single compound or set of pseudocompounds based on a boiling range of individual cuts can be selected. The characterization of the physical and thermodynamic properties of these cuts is then accomplished using a combination of one of the gravity types, one of five boiling points, and/or the Watson or UOP K characterization factor.

The five boiling points generally used to characterize the petroleum fraction are volume average, molal average, weight average, cubic average, and mean average boiling points.

The volume average boiling point (VABP), molal average boiling point (MABP), weight average boiling point (WABP), cubic average boiling point (CABP), and mean average boiling point (MeABP) are defined by

$$VABP = \Sigma\ X_{vi}\ T_{bi} \tag{1.1}$$

$$MABP = \Sigma\ X_{i}\ T_{bi} \tag{1.2}$$

$$WABP = \Sigma\ X_{wi}\ T_{bi} \tag{1.3}$$

$$CABP = \left(\Sigma\ X_{vi}\ T_{bi}^{1/3} \right)^{3} \tag{1.4}$$

$$MeABP = (MABP + CABP) / 2 \tag{1.5}$$

where

X_{vi} = volume fraction of component i.

X_{i} = mole fraction of component i.

X_{wi} = weight fraction of component i.

T_{bi} = normal boiling point of component i (°R).

The common order of the boiling points from lowest to highest for a fraction is molal, mean, cubic, volume, and weight average.

Physical and thermodynamic properties of a petroleum fraction are estimated based on the appropriate average boiling point. The volume average boiling point is used for characterization of the viscosity and specific heat, while the weight average boiling point is used to characterize true critical properties of known compounds. The molal average boiling point is used to characterize pseudocritical temperatures and acentric factors, while the mean average

boiling point is used to calculate pseudocritical pressure, molecular weight, and heat of combustion[15].

Empirically determined charts have been prepared to convert from one boiling point to another[16,17]. For narrow cuts all the average boiling points approach each other and the volume average boiling point is used for all the others[18].

The different average boiling points are primarily used to characterize wide boiling cuts or to characterize a full petroleum cut into one pseudocomponent.

The relationship between the API (American Petroleum Institute) gravity and the specific gravity is defined as

$$API = 141.5 / S_g - 131.5 \qquad (1.6)$$

where API is the API gravity and S_g is the specific gravity at 60 °F relative to water at 60 °F. The UOP (Universal Oil Products) or Watson characterization 'K' factor is defined as

$$UOPK = T_b^{1/3} / S_g \qquad (1.7)$$

where T_b is the mean average boiling point of the cut in degrees Rankine. The UOPK is a rough indication of paraffinicity of a hydrocarbon, with high UOPK values indicating high degrees of saturation[19]. It has been found

that petroleum fractions that contain an abundance of paraffinic hydrocarbons have a UOPK of 11.8 to 13.1. Those that contain an abundance of napthenes have a UOPK of 11.0 to 12.7, and those that contain an abundance of aromatics have a UOPK of 9.7 to 12.3. The API, however, has suggested that the UOPK does not accurately characterize fractions containing substantial amounts of olefinic, diolefinic, or aromatic hydrocarbons[20].

The process engineer must decide the preferred boiling point range for the cuts and determine how many cuts to use to characterize the petroleum fraction. In depth characterization of petroleum fractions by expanding the number of pseudocomponents has to be weighed against the increased computer time necessary for the simulation.

The objective of this research is to automate the estimation process for a given set of pseudocomponents to allow the engineer to investigate multiple simulations.

II. THERMODYNAMIC MODELS OF ASPEN

A. Introduction

The physical properties required for an ASPEN run can be divided up into two types, thermodynamic and transport. ASPEN has the capability to perform a simulation of a set of unit operations and then size and cost the final steady state solution. The properties necessary for the simulation part of an ASPEN run are primarily thermodynamic, while those required for the sizing and costing part are primarily transport. ASPEN groups thermodynamic and transport properties into option sets known as SYSOPs. Each SYSOP has a recommended set of thermodynamic and transport models, and requires certain unary and binary parameters to execute the models. The user also has the capability to modify a built in option set or construct one of his own for a particular simulation. Pure component properties are retrieved from one or more data banks and interaction parameters are estimated or user supplied.

ASPEN has the capability to use conventional or non-conventional physical properties. A conventional set of properties exist for conventional compounds found in the petroleum or chemical industry. These conventional compounds take part in all phase and chemical equilibrium

calculations. Non-conventional componential properties, on the other hand, have restrictions as to what phases and reactions can occur. The non-conventional property option is primarily for coal and coal derived materials.

As ASPEN is a steady state process simulator with the added capability to size and cost the process, the existing ASPEN data banks are comprised of primarily thermodynamic properties of conventional compounds. This study will follow this practice by examining conventional thermodynamic properties necessary to run on one of ASPEN's built in SYSOPs[21,22].

B. Conventional Physical Properties

ASPEN's thermodynamic physical properties, for a given unit operation, consist of a subset of the ASPEN major properties. Major properties, as defined in ASPEN, are fugacity coefficient, enthalpy, entropy, free energy, molar volume, viscosity, thermal conductivity, diffusion coefficient, and surface tension. Fugacity coefficient, enthalpy, entropy, free energy, and molar volume are the major properties designated for conventional thermodynamic physical properties. All the conventional thermodynamic physical properties can be calculated for vapor, liquid, or solid phases[23].

C. Conventional Option Sets

There are twelve conventional option sets or SYSOPs. SYSOP0 is the basis of all the other SYSOPs and is always loaded for an ASPEN simulation. Option set SYSOP0 defines how all the five ASPEN major properties are to be calculated. When using SYSOP0 the fugacity coefficients of the vapor, liquid, and solid phases are treated as ideal. The calculation of the molar enthalpy of the vapor is done using ideal gas, Watson[24] for liquid, and ideal mixture for solid. The molar free energy is calculated using ideal gas for vapor, liquid, and solid. The molar entropy of the vapor is calculated using ideal gas, Watson for the liquid, and ideal mixture for the solid. Molar volume is calculated using ideal gas for the vapor phase, Rackett[25] for the liquid phase, and ideal solid for the solid phase.

The other eleven SYSOPs are designed to supplement or replace SYSOP0's calculation of the fugacity coefficient, molar enthalpy, molar free energy, molar entropy, and molar volume for the liquid and vapor phases.

SYSOP1, SYSOP2, SYSOP3, SYSOP4, SYSOP5, and SYSOP14 use the addition of an equation of state (EOS) model to replace the ideal assumptions of SYSOP0. SYSOP1 adds the Redlich-Kwong[26] (RK) equation of state, extended Scatchard-Hildebrand, and Chao-Seider[27] models. SYSOP2 adds

the Redlich-Kwong equation of state, extended Scatchard-Hildebrand, and Grayson-Streed[28] models. SYSOP3 adds the Soave modification to the Redlich-Kwong (SRK) equation of state[29]. SYSOP4 adds the Peng-Robinson (PR) equation of state[30]. SYSOP5 adds the Conformational Solution theory modification of the Benedict-Webb-Rubin (BWR) equation of state[31]. SYSOP14 adds the ASPEN or Mathias modification of the Redlich-Kwong-Soave (ASRK) equation of state[32].

Four other option sets are extensions to the properties of SYSOP0 using an activity coefficient model for the liquid fugacity and the Gibbs free energy of the mixture. SYSOP8 uses the Wilson equation[33], SYSOP9 the Van Laar equation[34], SYSOP10 the NRTL equation[35], and SYSOP12 the UNIQUAC equation[36] to model the Gibbs free energy. In the above four models, the Redlich-Kwong EOS model is used to calculate the vapor mixture properties. The Cavett equation[37] is used to model the mixture enthalpy and the Rackett equation[38] is used to model the molar volume of the mixture.

The last option set, SYSOP12, adds the 1967 ASME water correlations[39].

For a more complete summary and further information on the transport models available in ASPEN's SYSOPs the reader is referred to the ASPEN users manual[40].

D. Universal and model specific parameters

For each of the twelve SYSOPs there is a set of parameters needed for the application of the model to the calculation of the thermodynamic properties. All parameters used for the option sets must be consistent with the internal SI (Systeme Internationale d'Unites) unit structure of ASPEN.

Each of the SYSOPs requires a minimum subset of the available parameters to describe the thermodynamic models completely. These parameters can be broken down into two types, universal and model specific. Universal parameters usually are experimentally determined and are constants that characterize a property of the compound, such as molecular weight and boiling point. Model specific parameters are those which are valid only for a particular model and are derived from component data.

The model specific parameters can be subdivided further into unary, and binary. Unary constants are those which are a function of pure component properties only, such as extended Antoine vapor pressure constants or Rackett Z's. Binary constants are those that describe the interaction between two components and can be used to describe the mixture properties. An example of binary constants are the Peng-Robinson interaction parameters (k_{ij}) which are normally obtained by fitting experimental data.

The advantage of using only universal and unary parameters for a thermodynamic model is that a limited number of measured values can describe a large class of phenomenon. Binary parameters are indicated primarily when experimentally determined data is available[41].

As the fundamental information desired is that which can be determined from pure component data, the following discussion will only involve the universal and unary parameters specific to an option set.

Table 2.1 summarizes the pure component universal and unary parameters available for an ASPEN simulation using one of the built in option sets.

Table 2.1

ASPEN pure component universal & unary parameters

Parameter name	Number Elements	Parameter Units*	Description
MW	1	Kg/Kmole	Molecular Wt.
TFP	1	°K	Normal freezing point
TB	1	°K	Normal Boiling point
TC	1	°K	Critical temperature
PC	1	Pascals	Critical Pressure
VC	1	M^3/Kmole	Critical volume
ZC	1		Critical compressibility factor
OMEGA	1		Acentric Factor
RKTZRA	1	M^3/Kmole	Rackett parameter
VB	1	M^3/Kmole	Liquid molar volume at normal boiling point
CPIG	11	J/Kmole°K	Ideal gas heat capacity
DELTA	1	$(J/M^3)^{\frac{1}{2}}$	Solubility parameter at T_{ref}
MUP	1	Coulomb*M	Dipole moment
PLXANT	9	Pascals	Extended Antoine vapor pressure
MULAND	5	N-Sec/M^2	Modified Andrade model for liquid Viscosity
DHFORM	1	J/Kmole	Standard enthalpy of formation at T_{ref}
DGFORM	1	J/Kmole	Standard free energy of formation at T_{ref}
DHVLB	1	J/Kmole	Enthalpy of vaporization at T_b
DHVLWT	5	J/Kmole	Watson equation for Enthalpy of vaporization
PLCAVT	4	Pascals	Cavett pure component liquid vapor pressure
DHLCVT	1	J/Kmole	Cavett enthalpy parameter
VLCVT1	1	M^3/Kmole	Scatchard Hildebrand Characteristic molar volume parameter
RGYR	1	M	Radius of gyration

* units for unary constants are property units.

Table 2.2 is a summary of the universal and unary parameters necessary for the thermodynamic properties of the twelve SYSOPs.

Table 2.2

Universal and unary parameters for Thermodynamic properties

SYSOP name	Property
SYSOP0	TC, PC, VC, ZC, DHFORM, DGFORM PLXANT, CPIG, DHLWT, RKTZRA
SYSOP1	TC, PC, VC, ZC, DELTA, DHFORM, DGFORM PLXANT, CPIG, VLCVT1, RKTZRA
SYSOP2	TC, PC, VC, ZC, DELTA, DHFORM, DGFORM PLXANT, CPIG, DHLWT, RKTZRA
SYSOP3,4,5,14	TC, PC, OMEGA, DHFORM, DGFORM PLXANT, CPIG
SYSOP8,9,10,11	TC, PC, VC, ZC, DHFORM, DGFORM PLXANT, CPIG, RKTZRA, DHLCVT
SYSOP12	DHFORM, DGFORM, CPIG

Universal parameters are; molecular weight, critical properties, boiling points, Pitzer[42] acentric factor, solubility parameter, enthalpy, and entropy of formation of ideal gas at standard conditions. The remainder are unary model specific parameters.

Some of the ASPEN parameters, as defined in Table 2.1, must represent a range of conditions. The following descriptions of the unary parameters; RKTZRA, CPIG, PLXANT, MULAND, DHVLWT, PLCAVT, DHLCVT, and VLCVT1 need clarification when used by its corresponding ASPEN property model.

The extended Antoine vapor pressure equation for pure component liquid vapor pressure[43] has nine available parameters (PLXANT) and is of the form

$$\ell n(P^{OL}) = C_1 + C_2 / (T + C_3) + C_4 \times T + C_5 \times \ell n(T) + C_6 \times T^{C7} \qquad (2.1)$$

where P^{OL} is liquid vapor pressure in Pascals and T is temperature in degrees Kelvin. Equation (2.1) is used for the range of temperatures of C_8 to C_9. Outside this range the vapor pressure is extrapolated as $\ell n(P^{OL})$ vs. 1/T. Parameters C_1 to C_7 are values fit to experimental data and C_8 and C_9 are lower and upper limits of the correlation. The upper limit default value is 1000 °K.

The Cavett equation for pure component liquid vapor pressure[44] (P^{0L}) has four available parameters (PLCAVT). The Cavett equation has two forms.

For $T_r \geq 0.4$

$$\ell n(P^{0L}/P_c) = (1 - 1/T_r)\ [A_1 + A_2/T_r + A_3/T_r^2 + A_4/T_r^3 + AM\ (A_5 + A_6/T_r + A_7/T_r^2 + A_8/T_r^3]) + \beta(A_{13} + A_{14} \times T_r)\ (T_r - 0.7)\ (T_r - 1)] \qquad (2.2)$$

For $T_r < 0.4$

$$\ell n(P^{0L}/P_c) = A_9 + AM \times A_{10} + (1/T_r - 2.5)\ [A_{11} + AM \times A_{12} + \beta(A_{13} + A_{14} \times T_r)\ (T_r - 0.7)\ (T_r - 1)] \qquad (2.3)$$

where

P_c = is the critical pressure in Pascals.

$T_r = T/T_c$ = is the reduced temperature.

A_1 to A_{14} are universal constants defined in Table 2.3.

$AM = (\alpha - 1)$.

The first two Cavett parameters, α and β, are the two characteristic parameters which are determined from vapor pressure data. A zero value is an acceptable default value for β. The last two Cavett parameters, T_{max} to T_{min}, are the range of temperatures in which the equation is valid. Outside this range the vapor pressure is extrapolated as $\ell n(P^{0L})$ vs. $1/T$.

Table 2.3

Cavett pure component vapor pressure constants

Constant	Value
A_1	8.6956145
A_2	-4.3610863
A_3	2.3312886
A_4	-0.37445964
A_5	0.41089072
A_6	-0.065391702
A_7	0.33193994
A_8	-0.080981301
A_9	-9.7687809
A_{10}	-1.5850550
A_{11}	-6.9238773
A_{12}	-1.1705661
A_{13}	4.7820604
A_{14}	-4.6670294

The ideal gas heat capacity equation[45] has eleven parameters (CPIG). The ideal gas heat capacity equation is of the form:

$$C_p^{0IG} = C_1 + C_2 \times T + C_3 \times T^2 + C_4 \times T^3 + C_5 \times T^4 + C_6 \times T^5 \qquad (2.4)$$

where T is temperature in degrees Kelvin. Equation (2.4) is used for the range of temperature of C_7 to C_8.

For temperatures less than C_7 the ideal gas heat capacity equation is of the form:

$$C_p^{0IG} = C_9 + C_{10} \times T^{C11} \qquad (2.5)$$

where C_1 to C_6 and C_9 to C_{11} are parameters fit to experimental data. For temperatures greater than C_8, the ideal gas heat capacity equation is linearly extrapolated using the slope at C_8. The upper temperature limit default value is 1000 °K. and the values for C_9, C_{10}, and C_{11} cannot be zero.

The extended Watson equation for heat of vaporization[46] has five parameters (DHVLWT). The five Watson parameters are; Δh_1^{vap}, T_1, a, b, and T_{min}. The Watson heat of vaporization equation is of the form:

$$\Delta h^{vap} = \Delta h_1^{vap} \times \left((1 - T/T_c) / (1 - T_1/T_c)^{a+b(1-T/Tc)} \right) \qquad (2.6)$$

where Δh_1^{vap} is the vaporization enthalpy at a reference temperature T_1. T_c is the critical temperature and a and b are empirically determined constants. The original Watson equation values of a = 0.38 and b = 0.0 are the default

values. The lower temperature T_{min} default value is zero and the upper bound of the correlation is T_c.

The Rackett equation for liquid volume[47] uses one parameter (RKTZRA). The form of the equation is

$$V^{0L} = R \times T_c/P_c \times Z_{RA}^{ex} \qquad (2.7)$$

where

$ex = (1 + (1 - T_r)^{2/7})$

T_c = Critical temperature (°K)

P_c = Critical Pressure (Pa)

Z_{RA} = Rackett parameter

R = Gas constant

T_r = Reduced temperature T/T_c

The Rackett 'Z' parameter, Z_{RA}, is an experimentally determined parameter. If no Z_{RA} is supplied then the default of the critical compressibility factor, Z_c, is used.

The Cavett[48] equation for pure saturated liquid enthalpy departure, Δh^{0L}, has an enthalpy parameter, Z_λ, which is experimentally determined (DHLCVT). However, a reasonable estimate is the critical compressibility factor.

The equations used by the Cavett equation are,

for $T_r < 1$

$$\Delta h^{0L}/T_c = \max\left(\Delta h^{0L}_{sub} / T_c \ , \ \Delta h^{0L}_{sup} / T_c\right) \qquad (2.8)$$

or for $T_r \geq 1$

$$\Delta h^{0L}/T_c = \Delta h^{0L}_{sup} / T_c \qquad (2.9)$$

where

T_c is the critical temperature (°K).

T_r is the reduced temperature.

$$\Delta h^{0L}_{sub} / T_c = a_1 + a_2 \ (1-T_r)^{(1-a3(Tr-0.1))}$$

$$\Delta h^{0L}_{sup} / T_c = \max(0.0, b_1 + b_2 \times T_r^2 + b_3 \times T_r^3 + b_4 \times T_r^4 + b_5 \times P_r \times T_r^2)$$

$$a_1 = B_1 + B_2 \ Z_\lambda + B_3 \ Z_\lambda^2 + B_4 \ Z_\lambda^3$$

$$a_2 = B_5 + B_6 \ Z_\lambda + B_7 \ Z_\lambda^2 + B_8 \ Z_\lambda^3$$

$$a_3 = B_9 + B_{10} \ Z_\lambda + B_{11} \ Z_\lambda^2 + B_{12} \ Z_\lambda^3$$

In the above equations Z_λ is the Cavett equation enthalpy parameter and the universal parameters B_1 to B_{12} and b_1 to b_5 are defined in Table 2.4.

Table 2.4

Cavett equation for enthalpy constants

Constant	Value
B_1	-67.022001
B_2	-644.81654
B_3	-1613.1584
B_4	844.13728
B_5	-270.43935
B_6	4944.9795
B_7	-23612.567
B_8	34152.878
B_9	8.9994977
B_{10}	-78.472151
B_{11}	212.61128
B_{12}	-143.59393
b_1	10.273695
b_2	-1.5594238
b_3	0.0193990
b_4	-0.0306083
b_5	-0.1688720

The extended Scatchard-Hildebrand model for liquid mixture activity coefficients uses one estimated parameter, the characteristic volume (VLCVT1). The extended Scatchard-Hildebrand model[49] is given by:

$$\ell n(\gamma_i) = V_i/RT \sum_j \sum_k \phi_j \phi_k (A_{ji} - 0.5A_{jk}) + \Delta n(\gamma_i) \qquad (2.10)$$

where

$A_{ij} = (\delta_i - \delta_j)^2 + 2k_{ij} \delta_i \delta_j$

γ_i = activity coefficient of component i.

V_i = liquid molar volume at 25 °C.

δ_i = solubility parameter at 25 °C.

$\ell n(\gamma_i) = \ell n(V_i/V_m) + 1 - V_i/V_m$

V_m = mole fraction averaged molar volume = $\sum_j X_j V_j$

ϕ_j = volume fraction of j-th component = $X_j V_j/V_m$

k_{ij} = binary interaction parameters for components i & j.

One of the parameters necessary for the calculation is the pure component liquid molar volume at 25 °C (V_i). When this liquid molar is not specified it is estimated by:

$$V_i = V_i^* \times (5.7 + 3.0 \times 298.15 / T_{ci}) \qquad (2.11)$$

where V_i^* is the characteristic volume parameter.

There is, in addition to the thermodynamic properties described above, a unary transport property, known as the modified Andrade model for liquid viscosity[50], which is featured in the ASPEN data bank. The modified Andrade model for liquid viscosity requires five parameters (MULAND). The Andrade pure component equation is defined as:

$$\ell n(\eta^{0L}) = A + B/T + C \times \ell n(T) \qquad (2.12)$$

where η^{0L} is the pure component viscosity and A, B, and C are three experimentally determined parameters. The original Andrade model was given with C set equal to zero[51], but the addition of the C parameter increases the range of applicability of the correlation. The last two parameters define the range of temperatures, T_l to T_h, in which the model is applicable. There are no default values for any of the determined parameters but the T_{min} and T_{max} values have defaults of 0.0 and 1000.0 °K respectively.

E. ASPEN Data banks

The ASPEN data banks store pure component major property model parameters for use by ASPEN for simulation or sizing/costing. ASPEN comes equipped with two system data banks. In addition, the user can create up to four private data banks.

The pure component data banks supplied with ASPEN are the main pure component data bank (ASPENPCD) and the Flowtran based pure component data bank (FLOWTRAN). The main data bank is based on the data bank published by Reid, Prausnitz and Sherwood[52]. The ASPENPCD data bank is an enhancement of this data bank. The enhancements include the addition of an extended range Antoine equation, Rackett parameter, solubility parameter, and Cavett correlation parameters. The FLOWTRAN data bank is a copy of the original Monsanto Flowtran data bank converted to SI units.

The ASPEN user has the option of creating any of four private data banks for components of interest. There are two types of user data banks, packed and unpacked. The unpacked type has space for every possible combination of component and parameter. The packed type contains a link list directory structure, which is based on the component name and identifies the location of the parameters for that component. The ASPENPCD and FLOWTRAN data banks are unpacked types.

The ASPEN user has the option of creating two of the packed and/or two of the unpacked type private data banks. The creation of the private data banks, updating of data banks, or output of parameter data stored in a data bank is accomplished using the ASPEN Data File Management Ssystem (DFMS)[53]. An example of the output obtained from DFMS for the ASPENPCD component water is shown in Table 2.5.

Table 2.5

ASPEN PURE COMPONENT PHYSICAL PROPERTY DATA BANK

COMPONENT: WATER ALIAS: H2O

NAME	SRCODE	REVDATE	NOE	VALUES
MW	1	06/26/86	1	0.180150D+02
TFP	1	06/26/86	1	0.273200D+03
TB	1	06/26/86	1	0.373200D+03
TC	1	06/26/86	1	0.647300D+03
PC	1	06/26/86	1	0.220483D+08
VC	1	06/26/86	1	0.558953D-01
ZC	1	06/26/86	1	0.229000D+00
OMEGA	1	06/26/86	1	0.344000D+00
RKTZRA	1	06/26/86	1	0.243172D+00
VB	1	06/26/86	1	0.196361D-01
CPIG	1	06/26/86	11	0.337381D+05, -0.701756D+01,
				0.272961D-01, -0.166465D-04,
				0.429761D-08, -0.416961D-12,
				0.200000D+03, 0.300000D+04,
				0.332560D+05, 0.189780D-19,
				0.928460D+01
DELTA	1	10/27/86	1	0.479304D+05
MUP	1	06/26/86	1	0.569210D-24
PLXANT	1	06/26/86	9	0.651544D+02, -0.684291D+04,
				0.000000D+00, 0.278351D-02,
				-0.613638D+01, 0.331168D-17,
				0.600000D+01, 0.319267D+03,
				0.647300D+03
MULAND	1	06/26/86	5	-0.122605D+02, 0.151568D+04,
				0.000000D+00, 0.273200D+03,
				0.647300D+03
DHFORM	1	06/26/86	1	-0.241997D+09
DGFORM	1	06/26/86	1	-0.228767D+09
DHVLB	1	06/26/86	1	0.406831D+08
DHVLWT	1	06/26/86	5	0.406831D+08, 0.373200D+03,
				0.310646D+00, 0.000000D+00,
				0.273200D+03
PLCAVT	1	06/26/86	4	0.244413D+01, 0.167808D+01,
				0.258920D+03, 0.647300D+03
DHLCVT	1	06/26/86	1	0.265731D+00
VLCVT1	1	06/26/86	1	0.100000D-01
RGYR	1	06/26/86	1	0.615000D-10

III. MODEL PARAMETER ESTIMATION

A. Introduction

Each of the parameters in the ASPEN pure component data bank is required for a particular thermodynamic or transport model. All the option sets however, do not need every parameter stored in the ASPEN data bank. Table 3.1 is a summary of the thermodynamic and transport parameters that are used for a particular option set. In Table 3.1 an X indicates that the individual property is retrieved by the ASPEN simulator for a particular SYSOP. A - indicates that the property is present in the ASPEN data base but not used for the SYSOP.

Table 3.1

Thermodynamic parameter summary

Property Name	SYSOP number 0	1	2	3	4	5	7	8	10	11	12	14
TC	X	X	X	X	X	X	X	X	X	X	X	X
PC	X	X	X	X	X	X	X	X	X	X	X	X
VC	X	X	X	X	X	X	X	X	X	X	X	X
ZC	X	X	X	X	X	X	X	X	X	X	X	X
OMEGA	X	X	X	X	X	X	X	X	X	X	X	X
PLXANT	X	X	X	X	X	X	X	X	X	X	X	X
CPIG	X	X	X	X	X	X	X	X	X	X	X	X
DHFORM	X	X	X	X	X	X	X	X	X	X	X	X
DGFORM	X	X	X	X	X	X	X	X	X	X	X	X
DHLCVT	-	X	X	-	-	-	-	-	-	-	-	-
TB	X	X	X	X	X	X	X	X	X	X	X	X
VB	X	X	X	X	X	X	X	X	X	X	X	X
DHVLWT	X	X	X	X	X	X	X	X	X	X	X	X
RKTZRA	X	X	X	X	X	X	X	X	X	X	X	X
DHVLB	-	X	X	-	-	-	-	-	-	-	-	-
TFP	-	-	-	-	-	-	-	-	-	-	-	-
DELTA	-	-	-	-	-	-	-	-	-	-	-	-
MUP	X	X	X	X	X	X	X	X	X	X	X	X
MULAND	X	X	X	X	X	X	X	X	X	X	X	X
RGYR	-	-	-	-	-	-	-	-	-	-	-	-
PLCAVT	-	-	-	-	-	-	-	-	-	-	-	-
VLCVT1	-	X	X	-	-	-	-	-	-	-	-	-

Table 3.1 shows that the necessary parameters for any of the built in SYSOPs can be divided up into two types, SYSOP1&2 and others. Option sets one and two are essentially those that came with the original FLOWTRAN simulator. The other option sets, developed by the ASPEN team, have additional parameters which are used to enhance the molar volume and enthalpy major property calculations.

For those major ASPEN properties which are used to calculate the thermodynamic properties, such as enthalpy,

the property is comprised of ideal and departure portions. Most of these models are designed to use a single ASPEN parameter for both portions of the property.

All internal calculations by ASPEN are in SI units, so all parameters used by ASPEN are also in SI units. ASPEN reference conditions are a gas at a temperature of 298.15 degree Kelvin and a pressure of 101325.0 Pascals.

Most of the parameters needed for the models can be explicitly defined, such as the critical properties. Other model parameters are used to represent a range of conditions and are normally found by fitting data to a correlation numerically. Examples of the second type are the ideal gas heat capacity parameters and the Rackett saturated liquid molar volume parameter.

The fitting of a set of data to a correlation and the solving of the resulting system of nonlinear equations can be done by the same method. The method of choice for this general problem of minimization of a function is the Marquardt method[54], which is an explicit Jacobian method. It uses a λ term to combine the quadratic convergence of Newton Raphson[55] near the solution and the robustness of the steepest descent[56] method away from the solution[57]. All model parameter estimation employed Marquardt's method using ASPEN's YSOLVE subroutine (see Appendix B).

The estimation of the model parameters necessary for the characterization of a hydrocarbon pseudocomponent were estimated using API preferred correlations. If no suitable API correlation method was found, other recommended estimation procedures were used. The ASPEN data bank contains sizeable hydrocarbon pure component properties. These were used to obtain the remaining parameters, for which no recommended estimation technique could be found. A summary of the hydrocarbon pure component properties can be found in Tables A.1 to A.3.

B. Molecular weight and critical properties

The molecular weight (MW) and critical properties (TC, PC, VC, and ZC) are attributes which are needed for all the option sets except SYSOP12. These parameters are normally used in the estimation of departure properties and densities using the corresponding states principle[58]. Another use is in the calculation of model parameters such as the default Redlich-Kwong A^* and B^* mixture parameters[59].

The molecular weight and critical properties T_c, P_c, and V_c were estimated using the Riazi Daubert method[60]. This method uses the specific gravity and boiling point of a petroleum fraction to estimate a property by

$$\Phi = A\ T_b^B\ S_g^C \qquad (3.1)$$

where Φ is the physical property of interest, A, B, and C are fit parameters and S_g and T_b are specific gravity and boiling point in °R. The recommended values for A, B, and C for the molecular weight and each of the critical properties is given in Table 3.2. The critical compressibility factor is calculated using the equation

$$Z_c = (P_c \times V_c) / (R \times T_c) \qquad (3.2)$$

where R is the SI gas constant, which has a value of 8314.33 M^3 Pascal/Kmole °K. The Riazi Daubert method, which has been adopted by the American Petroleum Institute (API), is recommended for boiling points in the range of 70 to 295 °F. and API gravities of 6.6 to 95.0[61].

Table 3.2

Riazi Daubert Correlation constants

physical property	Constant A	Constant B	Constant C
MW	4.5673E-5	2.1962	-1.0164
T_c	24.2787	0.58848	0.3596
P_c	3.1228E-5	-2.3125	2.3201
V_c	7.5214E-5	0.2896	-0.7666
λ	8.48585	1.1347	0.0214
$C_p(0)$	4.0394E-7	2.6724	-2.3630
$C_p(600)$	4.9350E-6	2.4219	-1.9436
$C_p(1200)$	8.3520E-6	2.3853	-1.9320
V	7.6211E-5	2.1262	-1.8688

B. Vapor Pressure

Various vapor pressure correlations have been proposed for use with petroleum fractions[62,63,64,65]. One that has seen extensive use in the petroleum industry since 1955 is the Maxwell Bonnell correlation. The Maxwell Bonnell correlation is a method which estimates the vapor pressure of a pure component hydrocarbon or narrow boiling pseudocomponents using the mean average boiling point, specific gravity, and UOP K. This method assumes that the reciprocal temperature of a paraffin hydrocarbon is linearly related to the reciprocal of a base paraffin at equal vapor pressures[66,67,68]. The base paraffin used is normal hexane. The Maxwell Bonnell correlation, as described in API

procedure 5A1.13[69], is used to calculate a vapor pressure at a given temperature by trial and error methods.

The calculation procedure for the vapor pressure P^* (mm Hg), of a fraction that has a volume average boiling point of T_b (°R) and UOP characterization factor of UOPK at a given temperature T (°R), is to first calculate an X value by the equation

$$X = (T_b' / T - 0.0002867 \times T_b') / (748.1 - 0.2145 \times T_b') \quad (3.3)$$

where T_b' is the boiling point (°R) corrected to a UOPK of 12. Next, the calculation of the common logarithm of the pressure ($\log(P^*)$) is determined using,

for $X > 0.0022$ ($P^* < 2$ mmHg)

$$\log(P^*) = (M_1 \times X - M_2) /(M_3 \times X - M_4) \quad (3.4)$$

or for $0.0013 \leq X \leq 0.0022$ (2 mmHg $\leq P^* \leq$ 760 mmHg)

$$\log(P^*) = (M_5 \times X - M_6) /(M_7 \times X - M_8)$$

or for $X < 0.0013$ ($P^* >$ 760 mmHg)

$$\log(P^*) = (M_9 \times X - M_{10}) /(M_{11} \times X - M_{12}) \quad (3.5)$$

Where M_1 to M_{12} values are given in Table 3.3.

Correction of the previous adjusted boiling point is performed by

$$T'_b = T_b - 2.5 \times f \times (UOPK - 12) \times \log(P^*/14.7) \qquad (3.6)$$

where f is a correction factor. The correction factor is defined as $f = 1.0$ for $T_b > 400$ °F and $f = 0.0$ for $T_b < 200$ °F. In the range of T_b of 200 to 400 °F the correction factor is defined by

$$f = (T_b - 659.7)/200 \qquad (3.7)$$

The trial and error continues by iterating the calculation of X and $\log(P^*)$ until the pressure does not change within desired limits.

The above procedure is repeated for fifty temperatures within a range of ± 50 °F of the volume average boiling point. These values of temperature and vapor pressure are converted to SI units and fit to the extended Antoine and Cavett correlations.

The extended Antoine vapor pressure equation parameters (PLXANT) which are fit are C_1, C_2, and C_3 for a the following shortened version of equation (2.1).

$$\ell n(P^{0L}) = C_1 + C_2 / (T + C_3) \qquad (3.8)$$

The Cavett vapor pressure parameters (PLCAVT) α and β are fit to equations (2.2) and (2.3). The recommended[70] value for α is $\omega/0.14123357$ and the recommended range for β is $\pm$ 0.2.

Table 3.3

Maxwell Bonell Correlation constants

Constant	Value
M_1	3000.538
M_2	6.76156
M_3	43.0
M_4	0.987672
M_5	2663.129
M_6	5.994296
M_7	95.76
M_8	0.972546
M_9	2770.085
M_{10}	6.412631
M_{11}	36.0
M_{12}	0.989679

C. Acentric Factor

The acentric factor (OMEGA) is primarily used as a measure of complexity of a molecule[71]. It has been used to describe the amount of branching found in a hydrocarbon.

The acentric factor has been defined to be a function of the vapor pressure[72,73] as:

$$\omega = -\mathrm{Log}(P_r) - 1.000 \qquad (3.9)$$

where P_r is the reduced vapor pressure (P/P_c) at a reduced temperature, T_r, of 0.7.

It has been suggested[74] that the method of Kesler Lee[75,76] is the recommended method for the calculation of acentric factor for hydrocarbons.

The method uses two equations to estimate the acentric factor. For reduced temperatures greater than 0.8

$$\omega = -7.904 + 0.1352 \times \mathrm{UOPK} - 0.007465 \times \mathrm{UOPK}^2 + 8.359 \times T_r + (1.408 - 0.01063 \times \mathrm{UOPK}) / T_r \qquad (3.10)$$

For reduced temperature less than or equal to 0.8

$$\omega = (\ell n(P_r) - 5.92714 + 6.09648/T_r + 1.28862 \times \ell n(T_r) - 0.169347 \times T_r^6) / (15.2518 - 15.6875/T_r - 13.4721 \times \ell n(T_r) + 0.43577 \times T_r^6) \quad (3.11)$$

where

UOPK = UOP characterization factor

T_r = reduced temperature

P_r = reduced vapor pressure at the boiling point

The suggested limits on the Kesler Lee correlation are that the value of ω should be in the range of 0.2 to 1.4.

D. Rackett Saturated Liquid Molar Volume

Correlations to calculate the saturated liquid molar volume have been proposed by various researchers[77,78,79,80,81,82,83]. The primary equation used by ASPEN is the Rackett saturated liquid molar volume model[84].

The Rackett parameter (Z_{RA}) is estimated by fitting data generated by the Gunn Yamada[85,86] correlation to equation (2.7). Fifty data points were generated using Gunn Yamada in the preferred range of reduced temperature of 0.2 to 0.99.

The Gunn Yamada correlation to estimate a molar volume from a known molar volume can be described as:

$$V/V^R = \{ V_r^{(0)}(T_r) \times [1.0 - \omega\Gamma(T_r)] \} / \{ V_r^{(0)}(T_r^R) \times [1.0 - \omega\Gamma(T_r^R)] \} \quad (3.12)$$

where ω is the acentric factor and V^R is a known value for the liquid specific volume at a reference temperature T^R. $\Gamma(T_r)$ is calculate by:

$$\Gamma(T_r) = 0.29607 - 0.09045 \times T_r - 0.04842 \times T_r^2 \quad (3.13)$$

for the reference reduced temperature T_r^R and the desired reduced temperature T_r.
$V_r^{(0)}(T_r)$ is calculated by:

$$V_r^{(0)}(T_r) = 1.0 + 1.3(1 - T_r)^{\frac{1}{3}} \times \mathrm{Log}(1-T_r) - 0.50879(1 - T_r) - 0.91534(1-T_r)^2 \quad (3.14)$$

at the reference reduced temperature and the desired reduced temperature.

E. Solubility Parameter

The solubility parameter (DELTA) is a semiempirical parameter that is used to describe the effects of molecular

interaction potential energy, thermal energy, and volume[87]. Various methods have been proposed to estimate the solubility parameter[88,89].

The method selected to estimate the solubility parameter (δ) is that suggested by API report 1-77[90] using the equation

$$\delta = (E_{25}^{V} \rho)^{\frac{1}{2}} \qquad (3.15)$$

where

E_{25}^{V} = vaporization energy at 25 °C.

ρ = density at 25 °C.

The method calculates the heat of vaporization (h_{25}^{V}) at ASPEN's reference temperature(T_{ref}) of 25 °C. using the Watson equation (2.6). Next the energy of vaporization is calculated using

$$E_{25}^{V} = h_{25}^{V} - R \times T_{ref} / MW \qquad (3.16)$$

where R is the gas constant and MW is the average molecular weight of the fraction. The liquid molar volume at 20 °C. is calculated using Riazi[91] and corrected to T_{ref} using the Gunn Yamada correlation[92]. The solubility parameter is then calculated using the corrected density.

F. Ideal Gas Heat Capacity

Ideal gas heat capacities are normally used in the calculation of enthalpy and entropy. Reliable ideal properties are needed to interrelate enthalpy and entropy due to the fact these properties are correlated in terms of their deviations from ideality[93]. Most correlations of ideal gas heat capacity use a general polynomial form of the heat capacity equation[94,95].

The method used to calculate the ideal gas heat capacity parameters (CPIG) was based on the correlation developed by Riazi[96]. The Riazi correlation uses three equations of form $C_p(T) = A\ T_b^B\ S_g^C$, which estimate the ideal heat capacity at temperatures of 0 °F, 600 °F, and 1200 °F. The three estimated values, converted to SI units, are then used to solve the following subset of equation (2.4).

$$C_p^{0IG} = C_1 + C_2 \times T + C_3 \times T^2 \qquad (3.17)$$

The temperature range for equation (3.17) is 273.15 to 922.04 °K. For temperatures less than 273.15 °K, the estimated values at 0 and 600 °F were used to solve equation (2.5) of the ideal gas heat capacity equation with C_{11} set equal to one.

The resulting shortened equation is:

$$C_p^{0IG} = C_9 + C_{10} \times T \qquad (3.18)$$

G. Enthalpy of Vaporization

When a molecule obtains enough kinetic energy to overcome the restraining forces of the surface liquid and the pressure of the vapor, the molecule vaporizes[97].

The enthalpy of vaporization, or latent heat of vaporization, is the difference between the enthalpy of a saturated vapor and a saturated liquid at a given temperature. Various estimation techniques for the enthalpy of vaporization have been derived from the Clausius-Clapeyron equation[98]. The Clausius-Clapeyron equation describes the shape of the vapor pressure curve as a function of temperature and properties of the molecule. The form of the equation is:

$$dP/dT = \Delta h_v \; / \; (T \; \Delta V) \qquad (3.19)$$

where Δh_v is the enthalpy of vaporization and ΔV is the volume change of the substance from liquid to vapor. For petroleum pseudocomponents, however, the critical properties are only predictions and another approach is desired. The

method of choice is the Riazi Daubert method which uses experimentally measured enthalpies of vaporization at the boiling point to obtain a correlation.

Two values in the ASPEN data bank are related to the enthalpy of vaporization, the enthalpy of vaporization at the boiling point (DHVLB) and the Watson enthalpy of vaporization parameters (DHVLWT). The enthalpy of vaporization at the boiling point is calculated directly from the Riazi Daubert correlation using the parameters given in Table 3.2. The five Watson enthalpy of vaporization parameters are estimated based on the shortened form of equation (2.6).

$$\Delta h^{vap} = \Delta h^{vap}_{1} \times \left((1 - T/T_c) / (1 - T_1/T_c)^a \right. \qquad (3.20)$$

where Δh^{vap}_{1} is the vaporization enthalpy at a the boiling point (T_1), and the exponent 'a' is given the recommended[99] value of 0.38. The value for T_{min} is also set equal to the default value of 0.0.

H. Cavett Enthalpy Parameter

The Flowtran simulator used the Cavett method for calculation of pure saturated liquid enthalpy departure and saturated liquid mixture enthalpy departure[100]. The parameter (DHLCVT) is the Cavett equation enthalpy

parameter, Z_λ, as defined in equation (2.8) and (2.9). This parameter can be reasonably estimated using the critical compressibility factor, Z_c, if no experimental data is available[101]. Experimental data on petroleum pseudocomponents are normally unavailable and the use of the critical compressibility as a default value is recommended.

I. Enthalpy and Gibbs free energy of Formation

The enthalpy of formation at 25 °C (DHFORM) and the Gibbs free energy of formation at 25 °C (DGFORM) are parameters used primarily in SYSOP0, the base option set, upon which all other option sets are built. The pure component and mixture enthalpies, entropies, and free energies for SYSOP0 are calculated[102] using the appropriate polynomial form of C_p^{0IG} and

$$h^{0IG} = \Delta h_f^{0IG} + \int C_p^{0IG}\, dT \tag{3.21}$$

$$s^{0IG} = (\Delta h_f^{0IG} - \Delta g_f^{0IG}) / T_{ref} + \int (C_p^{0IG} / T)\, dT \tag{3.22}$$

$$g^{0IG} = h^{0IG} - T \times s^{0IG} \tag{3.23}$$

where the limits on the integrations are T_{ref} to T and

h^{0IG} = Ideal gas molar enthalpy

Δh_f^{0IG} = Ideal gas standard enthalpy of formation at T_{ref} (DHFORM)

s^{0IG} = Ideal gas molar entropy

Δg_f^{0IG} = Ideal gas standard free energy of formation at T_{ref} (DGFORM)

g^{0IG} = Ideal gas free energy

T_{ref} = reference temperature of 298.15 degree Kelvin

The study of enthalpy or Gibbs free energy of formation has consisted of additive group contribution[103,104,105,106,107] methods or correlations which are a function of reduced temperature or molecular weight[108,109]. These methods are of limited use for hydrocarbon pseudocomponents due to lack of structure information. To obtain reasonable values for the enthalpy and Gibbs free energies of formation a new method had to be developed. The ASPEN data bank contains a wide selection of energies of formation for hydrocarbons. Therefore, the method chosen was to fit the ASPEN data bank values for paraffins, napthenes, and aromatics as suggested by Riazi[110]. The Riazi form, equation (3.1), could not be used due to the presence of positive and negative values for the energies of formation. Therefore, the data was correlated as a function of volume average boiling point, V_b, to a polynomial of the form:

$$\theta = A + B \times V_b + C \times V_b^2 + D \times V_b^3 \qquad (3.24)$$

where θ is the property desired (DHFORM,DGFORM) and A,B, and C are correlated constants. A summary of the best fit parameters for equation (3.24) are shown in Table 3.4. A complete summary of the ASPEN data bank values used for the regression analysis can be found in Tables A.4 to A.6.

Summaries of the regression estimations are found in Tables A.7 to A.12 and Figures A.1 to A.2.

Table 3.4

Enthalpy and Gibbs free energy of formation constants

Type of Petroleum	Constant A	Constant B	Constant C	Constant D
		DHFORM		
Paraffins	5.6803E8	-4.6027E6	9840.17	-8.2377
Napthenes	1.6169E9	-1.0641E7	21793.96	-15.8926
Aromatics	-1.1603E10	8.8977E9	-2.2301E5	183.32
		DGFORM		
Paraffins	-3.0250E7	1.6932E6	-3258.3	2.619
Napthenes	-3.9762E9	-7.781E4	7933.6	-4.7579
Aromatics	-3.9760E9	3.101E7	-77805.4	64.835

J. Characteristic molar volume

The characteristic molar volume parameter (VLCVT1) is an optional parameter which is used in the extended Scatchard-Hildebrand model for liquid mixture activity coefficients. The characteristic volume parameter (V_i^*) is used in the Scatchard-Hildebrand model, as described earlier, only if the molar volume at 25 °C is not specified. When this liquid molar is not specified, equation (2.11) is used to find V_i^* by

$$V_i^* = V_i \; / \; (5.7 + 3.0 \times 298.15 \; / \; T_{ci}) \qquad (3.25)$$

where V_i is an estimated liquid molar volume at 25 °C.

The calculation of the estimated liquid molar volume is achieved by evaluating the liquid molar volume at 20 °C using the Riazi Daubert equation with the values for V found in Table 3.1. This estimated value is corrected to 25 °C by Gunn Yamada to obtain an estimated molar volume. Then the characteristic volume parameter is obtained using equation (3.25).

K. Normal boiling Point

As ASPEN was primarily designed for the simulation of pure components and not petroleum pseudocomponents, the calculation of the normal boiling point (TB) of petroleum fraction is confused by the existence of five boiling points. The five boiling points normally used in the correlation of petroleum pseudocomponent properties are volume average, molal average, weight average, cubic average, and mean average. Each boiling point has an appropriate application to physical properties, as mentioned earlier.

The selection of any of the boiling points becomes arbitrary for narrow enough boiling fractions and therefore the suggested boiling point[111] is the volume average boiling point.

L. Liquid Molar volume at the normal boiling point

The liquid molar volume at the normal boiling point (VB) of a component is used in every ASPEN option set except SYSOP12 for transport properties. Many correlations have been proposed to estimate the liquid molar volume or density[112,113].

The estimation of liquid molar volume at the normal boiling point is achieved by evaluating the liquid molar volume at 20 °C and one atmosphere using the Riazi Daubert equation with the values for V found in Table 3.1. The estimate is then corrected to the 25 °C by Gunn Yamada, using the normal boiling point and acentric factor calculated earlier, to obtain an estimated molar volume at the normal boiling point.

M. Radius of Gyration

The mean radius of gyration (RGYR) is defined as the distance from the axis of rotation, at which the total mass of a body is concentrated without changing its moment of inertia[114]. This parameter is only used in the Hayden-O'Connell[115] Virial equation of state (EOS). This model is a vapor phase EOS model based on the pure component and cross component second Virial coefficients estimated by the Hayden and O'Connell method. This EOS model is only available as a modification of a built in option set or in the construction of a user defined option set.

Although the radius of gyration has been used as a corresponding states correlation parameter[116], the primary use is found in the characterization of the dimension, shape, and branching of a molecule. It has been shown[117,118] that,

$$RGYR \propto g\,[(l^2/6) \times n]^{\frac{1}{2}} \tag{3.26}$$

or by collecting the constants,

$$RGYR \propto C \times n^{p1} \times l^{p2} \tag{3.27}$$

where g and C are constants, p1 and p2 are powers of n, the number of bonds in the molecule and l, the length of the molecule. The number of bonds times the length is proportional to the molecular weight and the UOP characterization factor which gives the form:

$$RGYR = A\ UOPK^B\ MW^C \tag{3.28}$$

Equation (3.28) was the form used for the fitting of the ASPEN data bank values found in Tables A.4 to A.6 for paraffins, napthenes, and aromatics. The best fit constants A, B, and C are defined in Table 3.5 and a summary of the fit can be found in Tables A.13 to A.15.

Table 3.5

Radius of Gyration Correlation constants

Type of Petroleum	Constant A	Constant B	Constant C
Paraffins	4.4908E-12	0.30375	0.80725
Napthenes	5.7662E-12	0.26866	0.76607
Aromatics	3.5630E-13	2.2211	0.38474

N. Dipole Moment

The Dipole moment (MUP) of a molecule is defined by Nelken[119] as "the vector in the direction of negative to positive charge of magnitude Qr, where Q is the charge and r is the charge separation distance". Most estimation procedures are group contribution type, which are not suited to the estimation of petroleum fractions.

The default value for a symmetric molecule, suggested by ASPEN and DIPPR[120] (Design Institute for Physical Property Data), is used for the Dipole moment.

O. Normal Freezing/Melting Point

The normal freezing or melting point (TFP) is the temperature at which a solid melts or a liquid freezes under a pressure of 1 atmosphere. Most estimation techniques are

fair to poor at best[121], due to the lack of an adequate theory for predicting the melting point temperature or enthalpy of melting[122].

Due to this lack of an adequate estimation procedure, a regression analysis was performed using the hydrocarbon normal freezing/melting temperature information from the ASPEN data bank. Although the fit was not totally adequate, petroleum engineers have little use for this parameter and the fit is at least a reasonable estimate to the normal freezing/melting point. The Riazi[123] form was used to fit the freezing/melting point data found in Tables A.4 to A.6 for paraffins, napthenes, and aromatics by:

$$TFP = A\ V_b^B\ S_g^C \qquad (3.29)$$

where V_b is the volume average boiling point and S_g is the specific gravity. The values for A, B, and C are defined in Table 3.6 and a summary of the fit can be found in Tables A.16 to A.18.

Table 3.6

Freezing/Melting point Correlation constants

Type of Petroleum	Constant A	Constant B	Constant C
Paraffins	3.6305E-2	1.4185	-8.5142E-2
Napthenes	32728.4497	-0.62428	6.6091
Aromatics	542.9949	-6.7363E-2	4.0803

P. Andrade Viscosity

The liquid viscosity is a measure of the forces that work against the flow of the liquid when shearing stress is present[124]. The viscosity for a petroleum fluid is normally used in the sizing and costing of process equipment.

The model which is used for the viscosity of SYSOP0 is the extended Andrade model[125]. This model assumes that viscous forces are due to transfer of momentum[126] and is the model most widely used to show the effect of temperature on liquid viscosity[127]. The extended Andrade model for liquid viscosity expands the temperature range of the original Andrade model with the addition of a 'C' parameter as shown in equation (2.12).

The method used to estimate the extended Andrade model parameters (MULAND) was based on the correlation of

Letsou-Stiel[128]. The Letsou-Stiel method can predict viscosities using universal parameters only. Therefore, the Andrade fit is only as good as the estimation derived from this model and if experimental viscosity data is available it should be used to determine the Andrade parameters.

The Letsou-Stiel correlation to estimate viscosity can be described as:

$$\eta^L \xi = (\eta^L \xi)^{(0)} + \omega (\eta^L \xi)^{(1)} \qquad (3.30)$$

where

$\xi = 2.1735E6 (T_c^{1/6} \times P_c^{2/3}) / MW^{1/2}$

ω = Pitzer acentric factor (OMEGA)

The quantities $(\eta^L \xi)^{(0)}$ and $(\eta^L \xi)^{(1)}$ are universal functions defined as

$$(\eta^L \xi)^{(0)} = a_1 + a_2 \times T_r + a_3 \times T_r^2 \qquad (3.31)$$

$$(\eta^L \xi)^{(1)} = a_4 + a_5 \times T_r + a_6 \times T_r^2 \qquad (3.32)$$

where T_r is the reduced temperature and a_1 to a_6 are constants defined in Table 3.7.

Fifty values of viscosity were generated using equations (3.30) to (3.32) in the recommended range ($0.76 \leq T_r \leq 0.98$) of reduced temperatures. The modified Andrade parameters were then fit to this temperature

viscosity data to obtain the A, B, and C parameters of equation (2.12).

Table 3.7

Letsou Stiel Model constants

Constant	Value
a_1	0.015174
a_2	-0.02135
a_3	0.0075
a_4	0.042552
a_5	-0.07674
a_6	0.0340

IV. ESTPRO PROGRAM

A. Introduction

The need was shown by the ASPEN Cooperative Enhancement Group at the 1985 AIChE meeting in Houston Texas on March 25, 1985 for a consistent hydrocarbon pseudocomponent generator. To meet this need, the ESTPRO program was developed to automate the characterization of petroleum fractions to obtain pseudocomponents for the ASPEN simulator. The program was developed on a VAX 11/785 system and written in Fortran 77. The program utilizes a top down structured programming approach. The documentation is structured similar to that used in ASPEN. Each module documentation contains a name, title, brief description, limitations, and variable summary. The program can be resized for a maximum number of pseudocomponent estimations, limited only by available memory. A complete listing of the ESTPRO program is found in Appendix B.

B. Basis and assumptions

The program was written to handle a wide range of input pseudocomponents. Currently, a maximum of 25 pseudocomponents can be estimated using the ESTPRO program during one simulation run. The estimation procedures

developed are only appropriate for olefin free pseudocomponents.

The estimated ranges of applicability are shown in Table 4.1

Table 4.1

ESTPRO Range of application

Parameter name	Range of application
MW	70 to 295 °F, API 6.6 to 95
TFP	paraffins: 110-310 °K napthenes: 130-265 °K aromatics: 173-352 °K
TB	input value
TC	70 to 295 °F, API 6.6 to 95
PC	70 to 295 °F, API 6.6 to 95
VC	70 to 295 °F, API 6.6 to 95
ZC	70 to 295 °F, API 6.6 to 95
OMEGA	0.4 to 1.4
RKTZRA	$0.2 \leq T_r \leq 0.99$
VB	70 to 295 °F, API 6.6 to 95
CPIG	70 to 295 °F, API 6.6 to 95
DELTA	70 to 295 °F, API 6.6 to 95
MUP	default value used
PLXANT	± 50 °R of boiling point
MULAND	$0.76 \leq T_r \leq 0.98$
DHFORM	paraffins: 301-617 °K napthenes: 322-637 °K aromatics: 353-518 °K
DGFORM	paraffins: 301-617 °K napthenes: 322-637 °K aromatics: 353-518 °K
DHVLB	70 to 295 °F, API 6.6 to 95
DHVLWT	70 to 295 °F, API 6.6 to 95
PLCAVT	± 50 °R of boiling point
DHLCVT	default value used
VLCVT1	70 to 295 °F, API 6.6 to 95
RGYR	paraffins: 3.182-8.318 Å napthenes: 2.850-4.367 Å aromatics: 3.004-4.849 Å

The program requires pseudocomponent cut point temperatures and slopes of TBP or ASTM D86 type curves. All input temperatures are assumed to be volume average boiling points and all the other boiling points necessary for the characterization correlations are calculated internally. A summary of the boiling point correction equations used can be found in Table A.19.

The user must be familiar with the ASPEN property option set structure and must know which SYSOP is needed for a particular simulation. Gravities for a cut must be supplied as specific gravity, API gravity, or indirectly as UOPK characterization factor. If any one of the three (S_g, API, UOPK) are given alone, the other two will be estimated. However, if API and S_g or all three are given, the API is used to estimate the other two. If the molecular weight (MW) is not specified it will be estimated using the Riazi[129] correlation with the constants found in Table 3.2. The percent paraffins, napthenes, and aromatics if not specified will be estimated using the March 1969 crude assay characterization of Tia Juana light[130]. A summary of the paraffin, napthene, and aromatic characterization using Tia Juana light can be found in Appendix A. All regressions to obtain unary parameters use a base of 50 generated points.

C. Main features

The program is designed to be consistent with the syntax found in the ASPEN simulator input translator. The syntax is based on primary, secondary, and tertiary key words as is the practice in the ASPEN input and DFMS translators.

The ESTPRO program is designed to give the user the option to enter all the necessary input data needed to generate the pseudocomponents or to let the program approximate the missing values.

The program will calculate only those properties which are needed for a particular ASPEN property route (see Table 3.1) or all the properties available in ASPEN's main pure component data bank. The default property set assumed, if none is specified, is SYSOP0.

ESTPRO output structure is similar to ASPEN's history and report structure. ESTPRO generates a report file with the results of the estimation and a history file which summarizes the history of the estimation calculation.

The history file summarizes the input, constraints specified, and documents the estimation calculation for each component.

The ESTPRO report file can be specified to be in ASPEN input or in DFMS (Data File Management System) form.

The program has two classes of debug options, estimation and report. The debug options, as is the case with the ASPEN debug options, are integers that can range from 0 to 8 where 0 is for a superficial trace output and 8 is used to obtain a detailed trace output.

The report debug option can be used to give a statistical summary of the regression analysis of unary parameters, as well as other estimation information, which will show up as comment lines in the report file. The estimation debug option is used to give varying amounts of output, which is written to the history file, to summarize the estimation calculation of the pseudocomponent properties. An example of the debug print out available is the output of Marquardt information on the progression of the nonlinear fit iteratively.

Error and warning information are also output to the history file. This error/warning information consists of three levels; WARNING, ERROR, and SEVERE ERROR. The WARNING message is output to the history file whenever informational messages are needed, such as when a correlation is used outside the optimal range. The ERROR message is output when corrective action has been taken in the estimation, with the overall estimation calculation continuing. A SEVERE ERROR message is one in which there is an inconsistency present and the estimation stops. An example of a severe error is

the case where the specified ESTPRO input data file cannot be found.

The units used in the input of characterization data can be specified as any available to the ASPEN simulator. These include °F, °R, °C, and °K for temperature and pounds per square inch absolute or gauge, atmospheres, Pascals, and millimeters of mercury.

D. Input

The input to the ESTPRO program has been designed to be consistent with ASPEN's input language. Primary keywords begin input paragraphs as in the ASPEN input. Secondary keywords and tertiary keywords are also used in the ESTPRO program consistent with the ASPEN simulator.

The primary key words used in the ESTPRO program are TITLE, DESC, T-UNITS, P-UNITS, PROP-DATA, PRINT-OPT, and END-INPUT.

The input to the ESTPRO program begins with a single optional title (TITLE) card and up to 50 description (DESC) cards. The only requirement for the title and description cards is that the TITLE and DESC primary keywords must start in column one of the input. An example input illustrating the input format can be seen in the Appendix C, Figure C.1.

The next set of primary keywords are optional and define the temperature and pressure units desired for input

to the ESTPRO program. The T-UNITS= and P-UNITS= primary keywords are used to select input temperature and pressure units. The valid input forms for the T-UNITS= and P-UNITS= primary keywords are

```
T-UNITS= [ cvalu1 ]
P-UNITS= [ cvalu2 ]
```

where:

cvalu1 is the temperature input unit, which must be a one character value from the set; F,R,C,K.
cvalu2 is the pressure input unit, which must be a character value from the set; PSIA,PSIG,ATM,PA,MMHG.

The default values for temperature and pressure units are °F and psia.

The next major paragraph is used to input the characterization data necessary for all the pseudocomponents. The primary keyword PROP-DATA is used to begin the paragraph. The secondary keyword COMP-LIST is used to specify a name for the pseudocomponent which can have up to 32 characters. Under each COMP-LIST is a tertiary keyword CVAL, a characterization variable, and its corresponding value. Valid characterization variables are API=, SG=, VABP=, UOPK=, STBP=, SASTMD86=, PER-PAR=, PER-NAP, and PER-ARO=.

The input is of the form

```
PROP-DATA
  COMP-LIST component name
   CVAL API=        [ rvalu1 ]
   CVAL SG=         [ rvalu2 ]
   CVAL UOPK=       [ rvalu3 ]
   CVAL VABP=       [ rvalu4 ]
   CVAL STBP=       [ rvalu5 ]
   CVAL SASTMD86=   [ rvalu6 ]
   CVAL PER-PAR=    [ rvalu7 ]
   CVAL PER-NAP=    [ rvalu8 ]
   CVAL PER-ARO=    [ rvalu9 ]
```

where:

All the values for **rvalu1** to **rvalu9** must be real numbers.

component name is the name of the component up to 32 characters

rvalu1 is the API value.

rvalu2 is the specific gravity at 60 °F value.

rvalu3 is the UOP characterization factor value.

rvalu4 is the volume average boiling point temperature.

rvalu5 is the slope of the TBP curve value.

rvalu6 is the slope of the ASTM D86 curve value.

rvalu7, **rvalu8**, and **rvalu9** are the percent paraffins, napthenes, and aromatics present in the pseudocomponent respectively.

There are no default values for CVAL's of API=, SG=, VABP=, or UOPK=. The default values for STBP= and SASTMD86= are zero. The default values for PER-PAR=, PER-NAP, and PER-ARO= are all zero and if so specified, will

be estimated based on the boiling point using the Tia Juana light crude assay.

The final major paragraph is used to enter the file management, option set selection, and debug levels.

The primary keyword PRINT-OPT is used to begin the paragraph. The secondary keyword is used to customize the estimation simulation and consists of a secondary keyword and a corresponding parameter. Valid secondary keyword values available are CAL-DEBUG=, REP-DEBUG=, ASPENOUT=, REP-FILE=, and PROP-OPT=.

The input is of the form

```
PRINT-OPT
  CAL-DEBUG= [ ivalu1 ]
  REP-DEBUG= [ ivalu2 ]
  ASPENOUT=  [ cvalu1 ]
  REP-FILE=  [ cvalu2 ]
  PROP-OPT=  [ cvalu3 ]
```

where:

ivalu1 and **ivalu2** are the estimation calculation and report debug options, which must be integers in the range of 0 to 8. The defaults for CAL-DEBUG= and REP-DEBUG= are zero which reduce the CPU time required for the estimation calculation and produce only trace output.

cvalu1 is the type of output desired, which must be a character string from the set INPUT and DFMS. The INPUT parameter produces an ESTPRO report file which can be incorporated directly into an ASPEN input file. The DFMS parameter produces an ESTPRO report file which can be incorporated into a DFMS input file. The default for ASPENOUT= is INPUT.

cvalu2 is the optional file prefix name which is used as the report output file. The name must be less than or equal to 32 characters. The default value when the REP-FILE= secondary keyword is not specified is the ESTPRO input file prefix name.

cvalu3 is the optional name for the option set desired, and must be a character string from the set; SYSOP0, SYSOP1, SYSOP2, SYSOP3, SYSOP4, SYSOP5, SYSOP8, SYSOP9, SYSOP10, SYSOP11, SYSOP12, SYSOP14, SYSOP-1. Each of the character values specifies a valid ASPEN option set and SYSOP-1 is used for generation of all the properties available in ASPEN's main pure component data bank. The default property set assumed if PROP-OPT= is not used is SYSOP0.

The last major paragraph heading is used to instruct the ESTPRO input translator that this is the end of the input file. The primary keyword used is END-INPUT. There are no secondary or tertiary keywords.

A comment card can be embedded into the input file by putting a ';' in column 1 as is the case in the ASPEN input translator.

A complete input data file as required by the ESTPRO program is shown in Appendix C, Figure C.1 and the resulting history and report files are shown in Figures C.2 and C.3.

E. Program Execution

The ESTPRO program has all logical assignment made internally so assignments are not necessary for an ESTPRO run. The execution procedure and corresponding output when used on a Vax system with a ESTPRO input file named ESTPROEX.INP is:

```
$RUN ESTPRO
  Enter input data file name ESTPROEX
    ****************************************
    * SUCCESSFUL OPEN OF INPUT FILE        *
    * SUCCESSFUL OPEN OF HISTORY FILE      *
    * INPUT READ COMPLETE                  *
    * SUCCESSFUL OPEN OF REPORT FILE       *
    * INITIALIZATION OF VARIABLES COMPLETE *
    * CALCULATE NEEDED VALUES COMPLETE     *
    * BEGIN PROPERTY CALCULATION           *
    ****************************************


FINISHED COMPONENT  1 (BP225) C-TIME =  6.61000
FINISHED COMPONENT  2 (BP275) C-TIME =  13.1500
FINISHED COMPONENT  3 (BP324) C-TIME =  20.3800
FINISHED COMPONENT  4 (BP374) C-TIME =  28.2800
FINISHED COMPONENT  5 (BP424) C-TIME =  36.8400
FINISHED COMPONENT  6 (BP475) C-TIME =  46.0900
FINISHED COMPONENT  7 (BP525) C-TIME =  56.0100
FINISHED COMPONENT  8 (BP575) C-TIME =  66.6200

FORTRAN STOP
```

V. RESULTS AND DISCUSSION

A. Introduction

The verification of the accuracy of the ESTPRO program is tied to the resulting ASPEN simulation obtained using the pseudocomponent parameters generated. Using the algorithms described in the previous chapters, a petroleum system was characterized and simulated using the ESTPRO and ASPEN programs. Comparison runs were made using the SimSci PROCESS™ simulator version 3.02.

The calculation runs of the ESTPRO program and the public version D of ASPEN were carried out using the Corporate Technology Vax 11/785 (VMS version 5.02) located at the Corporate headquarters of Allied-Signal in Morristown, New Jersey. The SimSci PROCESS™ runs were carried out using the New Jersey Institute of Technology Vax 8800 (VMS version 4.7) located at the main campus in Newark, New Jersey.

™ - PROCESS is a trademark of Process Simulation International, an affiliate of Simulation Sciences Inc.

B. Simulation comparisons

The analysis of the ESTPRO program pseudocomponent estimation was begun by the characterization of the Tia

Juana light crude assay[131] using eight pseudocomponents. Table 5.1 summarizes the parameters used to characterize the eight pseudocomponents.

Table 5.1

Characterization parameters

Pseudocomponent name	Boiling point °F	API gravity
BP225	225.7	60.53
BP275	275.4	55.32
BP324	324.9	50.12
BP374	374.9	46.07
BP424	424.9	42.40
BP475	475.0	39.44
BP525	525.1	36.66
BP575	575.1	34.13

Characterization data was input to the ESTPRO program and ASPEN properties were generated for SYSOP0, SYSOP3, and SYSOP4. Property option SYSOP0 was chosen to set an ideal base for the calculations. The other two property options sets were chosen to correspond with two compatible equation of state (EOS) property methods available in the PROCESS™ simulator. Option set SYSOP3 uses the Soave modification of the Redlich Kwong EOS[132] and SYSOP4 uses the Peng Robinson EOS[133] to model the Vapor and Liquid phases.

The ESTPRO input for the SYSOP0 characterization of Tia Juana light is shown in Figure C.1. The ESTPRO pseudocomponent results, which can be found in Figure C.3,

were incorporated into an ASPEN input file as shown in Figure C.4.

The simulation selected for the comparison study consisted of a single stage flash of a heavy petroleum stream to obtain the dew point, bubble point, and 50 percent vapor temperatures and compositions. The process flow diagram can be found in Figure C.5. The composition used as the feed to the flash is summarized in Table 5.2.

Table 5.2

Feed stream conditions

Temperature: 400 °F
Pressure: 14.696 PSIA

Pseudocomponent name	Compositions Lb. Moles/hr.
BP225	22.6
BP275	23.5
BP324	22.4
BP374	20.0
BP424	17.4
BP475	15.8
BP525	14.7
BP575	13.8
Total	150.2

The three flash conditions were simulated using each of the three ASPEN property option sets. The same nine flash simulations were completed using the SimSci PROCESS™ simulator. The generalized methods used were LIBRARY (Ideal default), SRK (Soave Redlich-Kwong), and PR (Peng Robinson).

The PROCESS™ LIBRARY method[134] is the recommended method to obtain an ideal simulation. The SRK and PR methods[135] are the methods recommended for heavy hydrocarbons, light hydrocarbons, and synfuels (synthetic fuels) at low to high pressures.

The output report summary with the results of the ASPEN 50/50 split simulation using SYSOP4 can be found in Figure C.6. The corresponding Peng Robinson PROCESS™ listing for the 50/50 split simulation can be found in Figure C.7.

A summary of the temperature results obtained for all the parallel simulations can be found in Table 5.3.

Table 5.3

Simulation temperature result summary

Flash Case	ASPEN temp. °F	PROCESS™ temp. °F	Difference °F	Relative % Difference
50/50 Split				
LIB-IDEAL	366.792	372.064	5.2710	1.417
SRK	375.587	373.953	1.6335	0.437
PR	375.190	373.918	1.2719	0.340
Bubble Pt.				
LIB-IDEAL	283.721	307.761	24.0398	7.811
SRK	312.856	311.376	1.4797	0.475
PR	313.064	311.666	1.3977	0.448
Dew Pt.				
LIB-IDEAL	452.650	450.262	-2.3885	-0.531
SRK	450.584	448.123	2.46100	0.549
PR	448.991	447.865	1.12630	0.251

LIB-IDEAL = LIBRARY vs. Ideal
RKS = Redlich Kwong Soave EOS
PR = Peng Robinson EOS

Summaries of the composition results can be found in Tables 5.4 to 5.9 and Figures C.8 to C.9.

Table 5.4

50/50 Composition simulation result summary
Ideal/LIBRARY for vapor Stream S02

Value Name/ID	PROCESS™ value	ASPEN value	Difference	Relative % Difference
BP225	19.8596	20.0584	-0.1988	-1.0010
BP275	18.6927	19.4985	-0.8058	-4.3108
BP324	15.0166	15.2097	-0.1931	-1.2859
BP374	10.1569	9.9144	0.2425	2.3875
BP424	5.8989	5.5884	0.3105	5.2637
BP475	3.1604	2.8780	0.2824	8.9356
BP525	1.5739	1.3456	0.2283	14.5054
BP575	0.7402	0.6067	0.1335	18.0357
TOTAL	75.0992	75.1000	-0.0008	-0.0011
AVG MW	133.5917	139.8936	-6.3019	-4.7173

Table 5.5

50/50 Composition simulation result summary
Ideal/LIBRARY for liquid Stream S03

Value Name/ID	PROCESS™ value	ASPEN value	Difference	Relative % Difference
BP225	2.7404	2.5415	0.1989	7.2581
BP275	4.8073	4.0014	0.8059	16.7641
BP324	7.3834	7.1902	0.1932	2.6167
BP374	9.8431	10.0855	-0.2424	-2.4626
BP424	11.5011	11.8115	-0.3104	-2.6989
BP475	12.6396	12.9220	-0.2824	-2.2342
BP525	13.1261	13.3544	-0.2283	-1.7393
BP575	13.0598	13.1932	-0.1334	-1.0215
TOTAL	75.1008	75.1000	0.0008	0.0011
AVG MW	185.1822	186.6313	-1.4491	-0.7825

Table 5.6

50/50 Composition simulation result summary
SRK for vapor Stream S02

Value Name/ID	PROCESS™ value	ASPEN value	Difference	Relative % Difference
BP225	19.5087	19.3893	0.1194	0.6120
BP275	18.4279	18.3100	0.1179	0.6398
BP324	14.9641	14.9166	0.0475	0.3174
BP374	10.3217	10.3771	-0.0554	-0.5367
BP424	6.1307	6.2417	-0.1110	-1.8106
BP475	3.3318	3.4229	-0.0911	-2.7343
BP525	1.6543	1.6894	-0.0351	-2.1217
BP575	0.7609	0.7525	0.0084	1.1040
TOTAL	75.1000	75.1000	0.0000	0.0000
AVG MW	134.2066	141.6315	-7.4249	-5.5324

Table 5.7

50/50 Composition simulation result summary
SRK for liquid Stream S03

Value Name/ID	PROCESS™ value	ASPEN value	Difference	Relative % Difference
BP225	3.0913	3.2106	-0.1193	-3.8592
BP275	5.0721	5.1899	-0.1178	-2.3225
BP324	7.4359	7.4833	-0.0474	-0.6374
BP374	9.6783	9.6228	0.0555	0.5734
BP424	11.2693	11.1582	0.1111	0.9859
BP475	12.4682	12.3770	0.0912	0.7315
BP525	13.0457	13.0105	0.0352	0.2698
BP575	13.0391	13.0474	-0.0083	-0.0637
TOTAL	75.1000	75.1000	0.0000	0.0000
AVG MW	184.5679	184.8933	-0.3254	-0.1763

Table 5.8

50/50 Composition simulation result summary
PR for vapor Stream S02

Value Name/ID	PROCESS™ value	ASPEN value	Difference	Relative % Difference
BP225	19.4716	19.3490	0.1226	0.6296
BP275	18.3864	18.2518	0.1346	0.7321
BP324	14.9332	14.8607	0.0725	0.4855
BP374	10.3155	10.3504	-0.0349	-0.3383
BP424	6.1513	6.2593	-0.1080	-1.7557
BP475	3.3664	3.4746	-0.1082	-3.2141
BP525	1.6887	1.7505	-0.0618	-3.6596
BP575	0.7869	0.8033	-0.0164	-2.0841
TOTAL	75.1000	75.1000	0.0000	0.0000
AVG MW	134.3444	141.8196	-7.4752	-5.5642

Table 5.9

50/50 Composition simulation result summary
PR for liquid Stream S03

Value Name/ID	PROCESS™ value	ASPEN value	Difference	Relative % Difference
BP225	3.1284	3.2509	-0.1225	-3.9157
BP275	5.1136	5.2481	-0.1345	-2.6302
BP324	7.4668	7.5392	-0.0724	-0.9696
BP374	9.6845	9.6495	0.0350	0.3614
BP424	11.2487	11.1406	0.1081	0.9610
BP475	12.4336	12.3253	0.1083	0.8710
BP525	13.0113	12.9494	0.0619	0.4757
BP575	13.0131	12.9966	0.0165	0.1268
TOTAL	75.1000	75.1000	0.0000	0.0000
AVG MW	184.4300	184.7052	-0.2752	-0.1492

The two ASPEN equation of state methods (SYSOP3 and SYSOP4) which have an analogous method available in PROCESS™ were further compared. The 50/50 vapor liquid split flash

temperature relative differences were both less than 0.5 percent. The dew point flash temperature relative differences were both less than 1.1 percent and the bubble point temperature relative differences were both less than 0.5 percent.

A comparison of the two ideal flash temperature relative percent differences were -0.531, 7.81, and 1.42 for the dew point, bubble point, and 50 percent vapor temperatures respectively.

The composition comparison for the 50/50 split flash showed that the composition relative percent difference ranges were 1.02 to 18.04, 0.127 to 3.92, and 0.064 to 3.86 for property sets ideal, Redlich Kwong Soave, and Peng Robinson respectively.

The comparison of the nine runs for ASPEN and PROCESS™ show that the equation of state models give closer agreement than the ideal runs.

The discrepancies in the ideal runs can be explained by the difference in the ideal assumptions made in ASPEN and PROCESS™. Although the ASPEN ideal assumptions are clearly defined in the ASPEN technical reference manual, Simulation Sciences documentation gives limited description of the assumptions made for the LIBRARY option set other than that vapor pressure is a major pure component property necessary for the calculation.

The comparison of the Redlich Kwong Soave and Peng Robinson EOS model runs on both simulators show much closer agreement. This is probably due to the similar implementation of these two equation of state models.

Both Peng Robinson and Redlich Kwong Soave are two parameter equation of state models which use the corresponding states principle. The corresponding states principle presumes that the equilibrium properties of a fluid, for all substances, can be expressed as a function of the same dimensionless groups[136]. The dimensionless groups recommended for an equation of state are usually reduced temperature (T/T_c) and reduced pressure (P/P_c). Further semiemperical extensions to improve the accuracy of the corresponding states principle have used the acentric factor as a third correlation parameter. In addition, there are various mixing rules available to calculate mixture properties[137].

All the equation of state correlating parameters are based on the pure component properties estimated by ESTPRO and PROCESS™. Any difference in the estimation methods can cause a discrepancy in the final simulation results.

The ESTPRO program estimates the petroleum properties needed for an ASPEN simulation by procedures discussed earlier. The Cavett correlations are used to generate the petroleum pure component properties needed for a PROCESS™ simulation.

Tables 5.10 to 5.15 summarize the differences in the pure component properties used by both simulators for the test flash calculations.

The average absolute percent deviation between the two characterization correlations vary from a minimum of 0.668 for the critical temperature to a maximum of 8.80 for the acentric factor. Other values for the average absolute percent deviations are 4.19, 6.44, 3.56, and 4.27 for the molecular weight, critical pressure, critical volume, and critical compressibility respectively.

The acentric factor plays an important role in the calculation of the characteristic constants 'a' and 'b ' for the Soave modification of the Redlich Kwong and the Peng Robinson equations of state models.

The differences found in Tables 5.11 and 5.12 indicate that the PROCESS™ correlation estimate of the acentric factor and critical pressure are higher than those used in the ESTPRO program. These differences play a factor in the differences found in the flash results.

Another source of deviation in the simulation results is caused by the different method used to calculate the liquid molar volume. The PROCESS™ procedure uses the API method and the ASPEN simulator uses the Rackett equation as shown earlier.

Table 5.10

Comparison of pure pseudocomponent properties
for Mole Weight(Kg/K-mole)

Name/ID	PROCESS™ value	ASPEN value	Difference	Relative % Difference
BP225	103.976	115.398	-11.422	-10.985
BP275	119.052	128.204	-9.152	-7.687
BP324	134.959	141.984	-7.025	-5.205
BP374	152.907	157.567	-4.660	-3.048
BP424	172.682	174.749	-2.067	-1.197
BP475	194.969	194.045	0.924	0.474
BP525	219.498	215.354	4.144	1.888
BP575	246.330	238.929	7.401	3.005

Table 5.11

Comparison of pure pseudocomponent properties
for Acentric factor

Name/ID	PROCESS™ value	ASPEN value	Difference	Relative % Difference
BP225	0.353	0.297	0.056	15.824
BP275	0.398	0.339	0.059	14.755
BP324	0.438	0.380	0.058	13.139
BP374	0.477	0.426	0.051	10.614
BP424	0.515	0.474	0.041	7.929
BP475	0.554	0.526	0.028	4.989
BP525	0.592	0.581	0.011	1.897
BP575	0.630	0.638	-0.008	-1.286

Table 5.12

Comparison of pure pseudocomponent properties
for Critical pressure (PSIA)

Name/ID	PROCESS™ value	ASPEN value	Difference	Relative % Difference
BP225	435.131	425.397	9.734	2.237
BP275	406.196	385.657	20.539	5.056
BP324	381.216	354.156	27.060	7.098
BP374	352.802	323.497	29.305	8.306
BP424	324.929	296.810	28.119	8.654
BP475	296.008	271.924	24.084	8.136
BP525	268.930	250.340	18.590	6.913
BP575	243.643	231.241	12.402	5.090

Table 5.13

Comparison of pure pseudocomponent properties
for Critical temperature (°F)

Name/ID	PROCESS™ value	ASPEN value	Difference	Relative % Difference
BP225	545.059	555.230	-10.171	1.866
BP275	600.239	608.427	-8.188	1.364
BP324	655.611	661.509	-5.898	0.900
BP374	709.087	712.489	-3.402	0.480
BP424	761.256	762.464	-1.208	0.159
BP475	811.156	810.553	0.603	0.074
BP525	859.799	857.935	1.864	0.217
BP575	906.908	904.317	2.591	0.286

Table 5.14

Comparison of pure pseudocomponent properties for Critical volume (CC/G-mole)

Name/ID	PROCESS™ value	ASPEN value	Difference	Relative % Difference
BP225	406.408	420.800	-14.392	3.541
BP275	453.020	474.701	-21.681	4.786
BP324	501.710	528.725	-27.015	5.385
BP374	561.062	589.770	-28.708	5.117
BP424	628.703	654.082	-25.379	4.037
BP475	709.468	724.599	-15.131	2.133
BP525	800.833	798.268	2.565	0.320
BP575	904.058	875.633	28.425	3.144

Table 5.15

Comparison of pure pseudocomponent properties for Critical compressibility factor

Name/ID	PROCESS™ value	ASPEN value	Difference	Relative % Difference
BP225	0.263	0.263	-0.001	-0.219
BP275	0.259	0.256	0.003	1.295
BP324	0.256	0.249	0.007	2.619
BP374	0.253	0.243	0.010	3.894
BP424	0.250	0.237	0.013	5.079
BP475	0.247	0.232	0.015	6.145
BP525	0.244	0.226	0.017	7.065
BP575	0.241	0.222	0.019	7.903

VI. CONCLUSIONS

1) The ESTPRO program provides a general method to estimate properties necessary for an ASPEN simulation rapidly and consistently.

2) The use of percent paraffins, napthenes, and aromatics as input variables permit a more realistic estimation of petroleum properties.

3) The flash simulation results compared favorably with the SimSci PROCESS™ simulator. The equation of state simulation temperature relative percent differences were all differed by less than 0.6 percent. The equation of state simulation composition relative percent differences all differed by less than 4 percent.

4) The Marquardt method is a simple and efficient method to perform the regression and nonlinear equation solving necessary to obtain unary parameters for hydrocarbon pseudocomponents. Moreover, the use of one subroutine makes the program more compact and efficient.

5) Properties for enthalpy of formation at 25 °C and Gibbs energy of formation at 25 °C can be estimated acceptably using a polynomial form in T_b for napthenes, paraffins, and aromatics.

6) Properties for radius of gyration may be estimated using a modification of the Riazi form. The molecular

weight and UOPK characterization factor are the correlation parameters of choice.

7) The structured Fortran principles used permits the modification of the estimation method with minimum effort.

The ESTPRO program estimates the properties necessary for an ASPEN simulation to a satisfactory degree as shown by the simulation comparison of chapter 5.

These simulations demonstrate that the ESTPRO program is a viable tool for the engineer who must characterize a hydrocarbon stream and can be a reliable aid to the petroleum or chemical engineer who must design a petroleum process within the ASPEN environment.

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APPENDICES

A. Data bank and regression summaries

B. ESTPRO program listing

C. ESTPRO/PROCESS™ Peng Robinson simulation summary

D. ASTM standards

APPENDIX A

Data bank and regression summaries

Figure A.1
Enthalpy of formation using ASPEN data bank

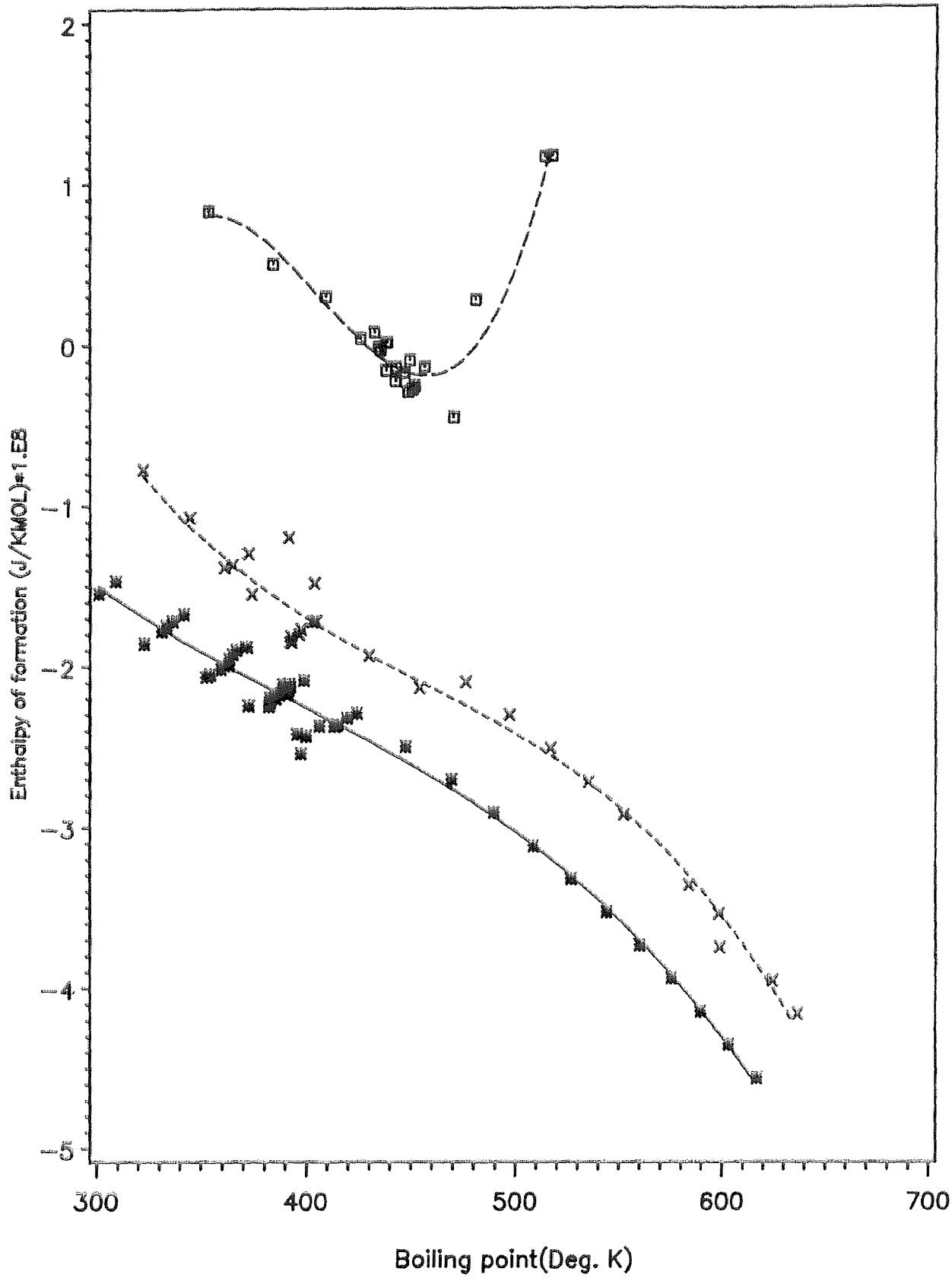

Figure A.2
Gibbs free energy of formation using ASPEN data bank

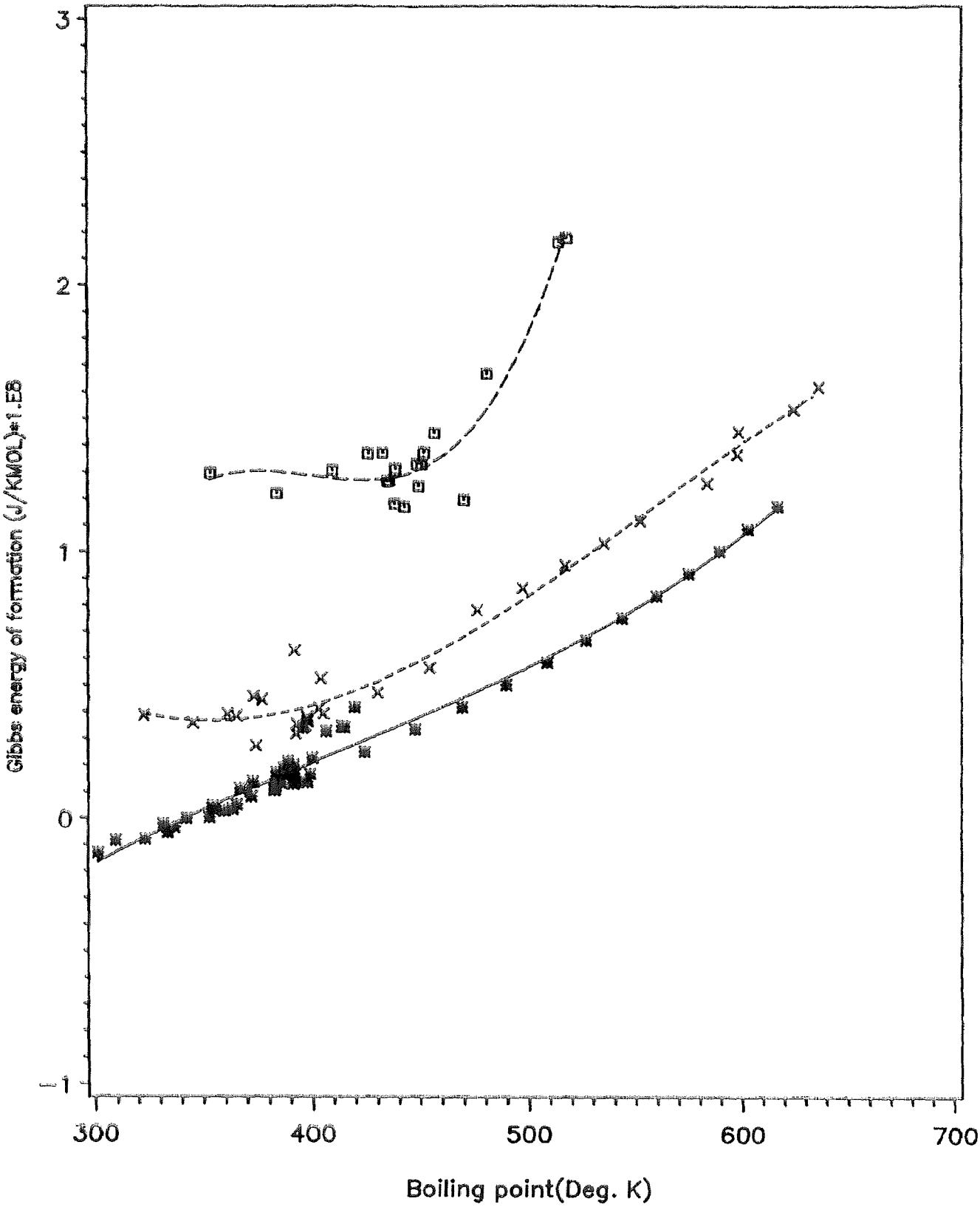

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Figure A.3
Tia Juana Crude Assay % paraffins, napthenes,& aromatics

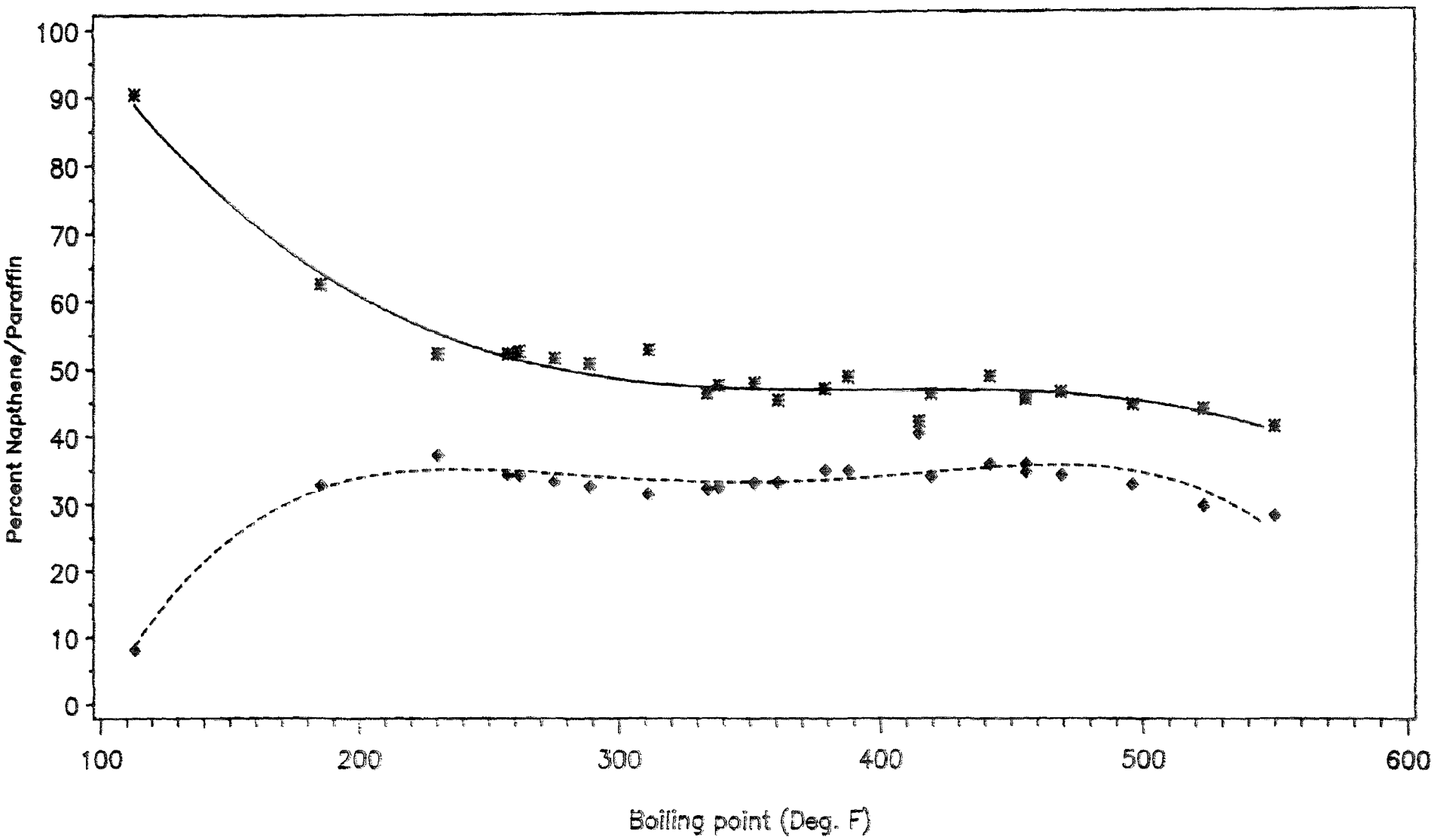

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Figure A.4
Correction of mean average boiling point based on TBP curve

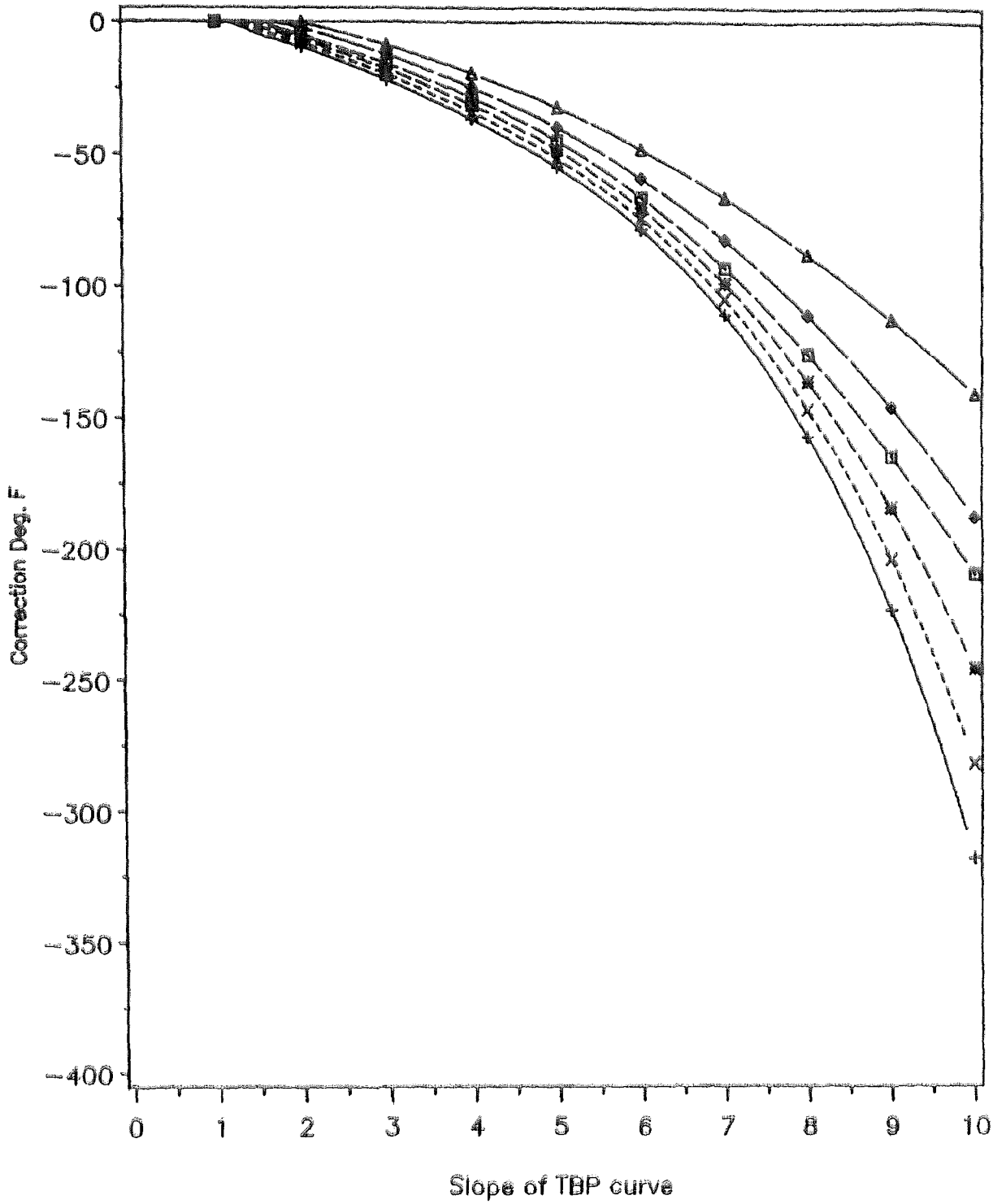
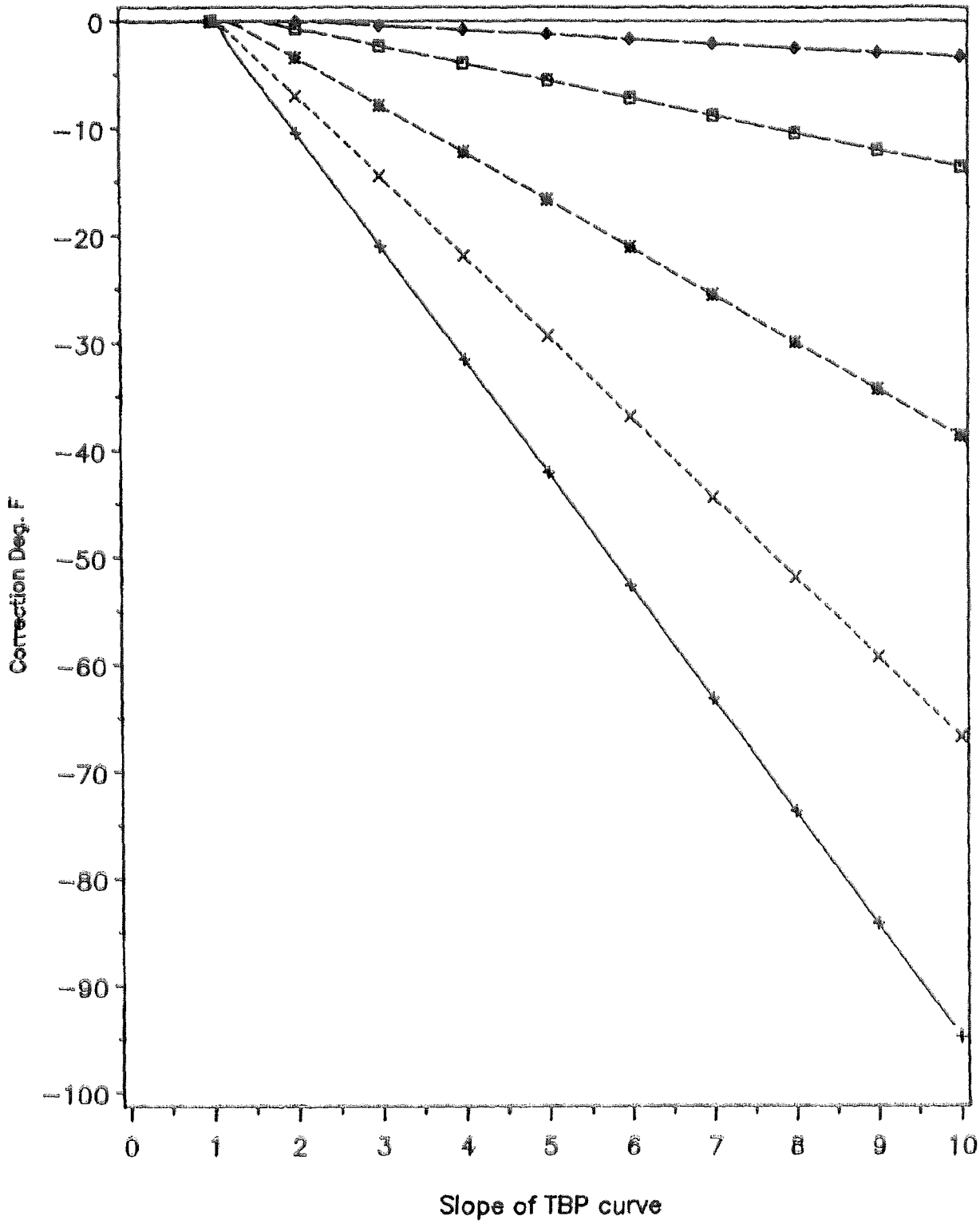


Figure A.5
Correction of cubic average boiling point based on TBP curve



S.E.S. 3/89

Figure A.6
Correction of mean average boiling point based on ASTM D86 curve

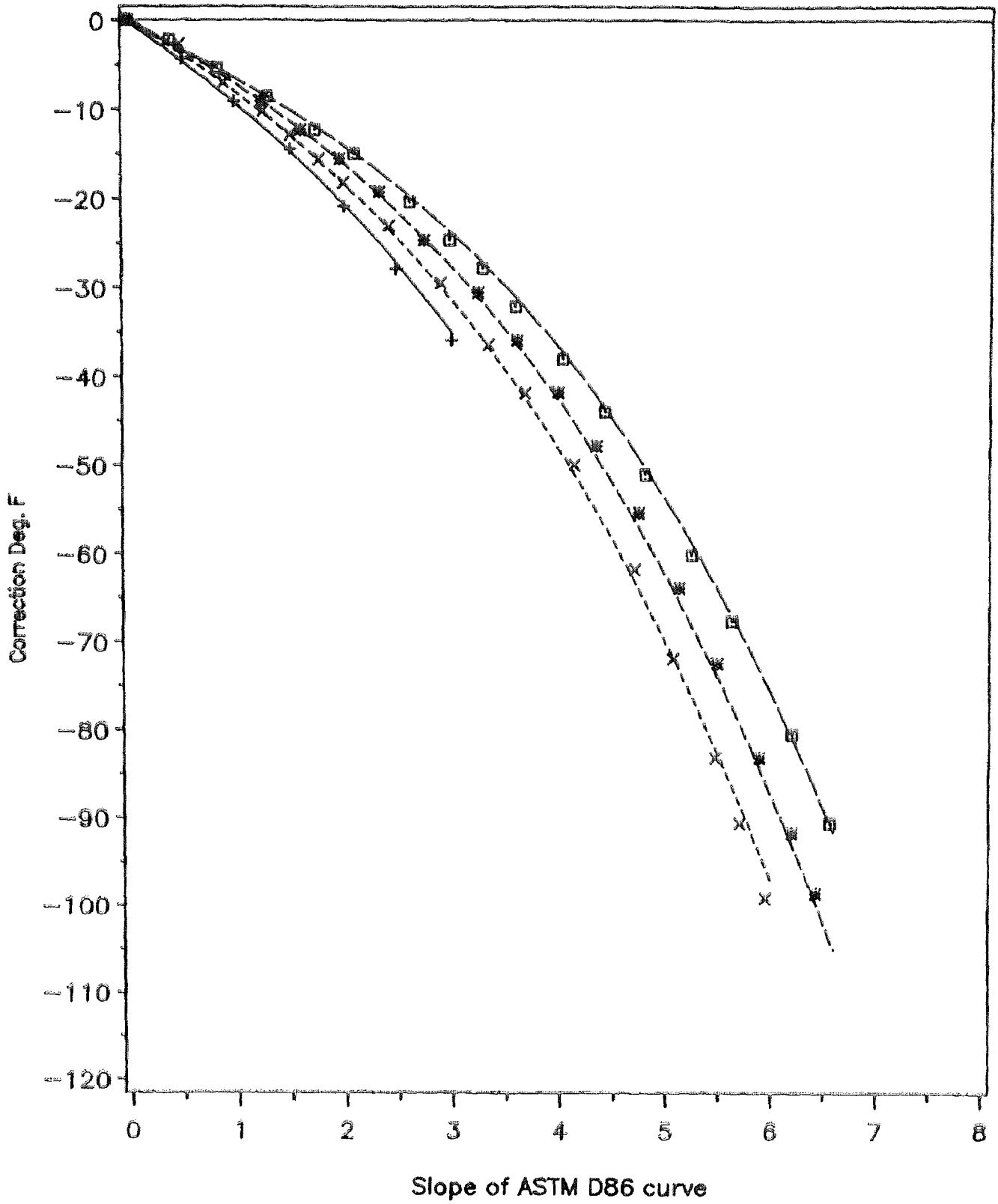


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Figure A.7
Correction of cubic average boiling point based on ASTM D86 curve

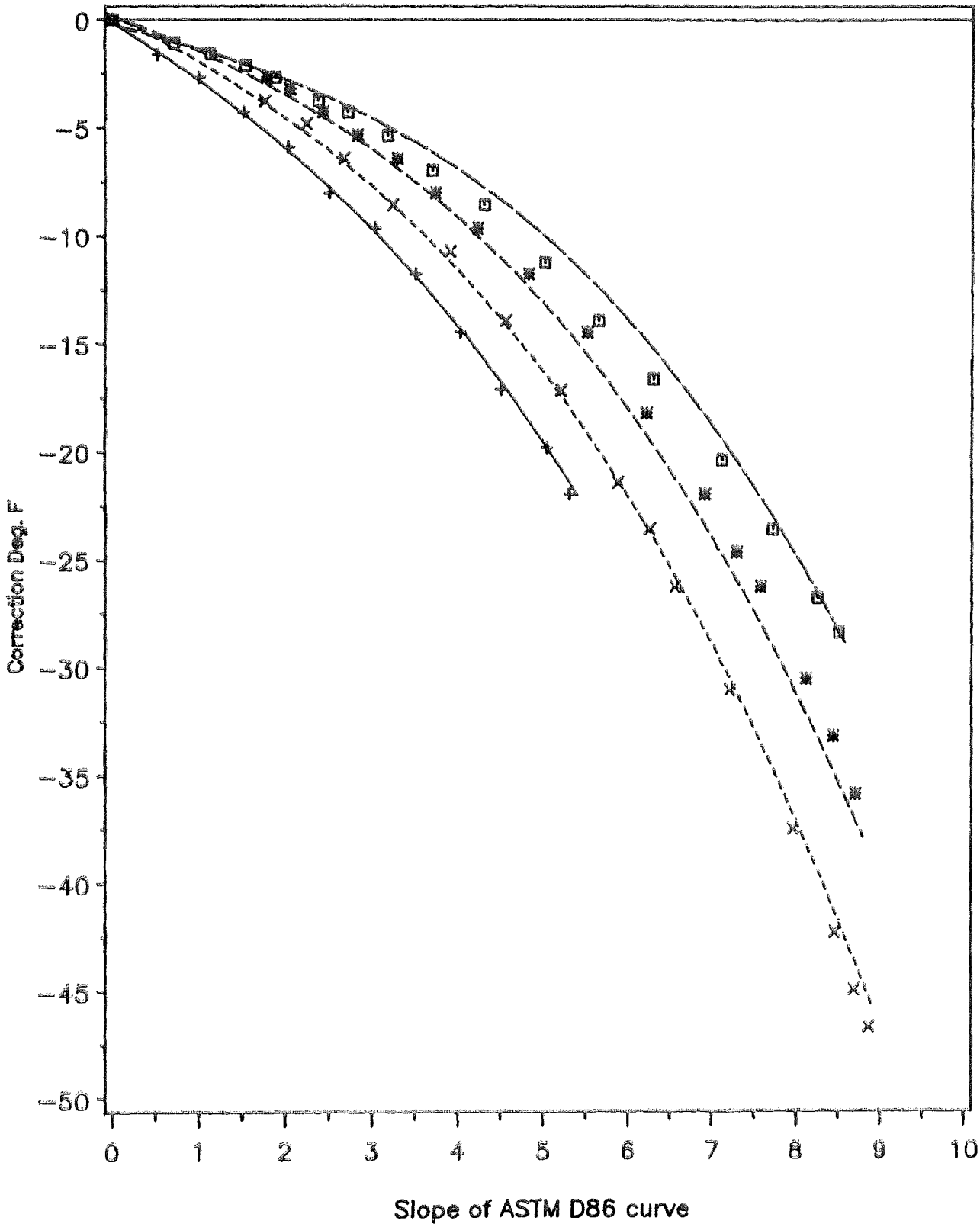

Table A.1
ASPEN pure component data bank summary
For aromatic compounds

Component name	Alias	MW	TC	PC	VC	ZC	OMEGA	PLXANT	CPIG	DHFORM	DGFORM	DHVLWT	RKTZRA	PLCAVT	DHLCVT	VLCVT1	TB	VB	DHVLB	TFP	DELTA	MUP	MULAND	RGYR
BENZENE	C6H6	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
TOLUENE	C7H8	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
ETHYLBENZENE	C8H10-4	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
N-PROPYLBENZENE	C9H12-1	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
ISOPROPYLBENZENE	C9H12-2	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
1-METHYL-2-ETHYLBENZENE	C9H12-3	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	-	X
1-METHYL-3-ETHYLBENZENE	C9H12-4	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	-	X
1-METHYL-4-ETHYLBENZENE	C9H12-5	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
1,2,3-TRIMETHYLBENZENE	C9H12-6	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	-	X
1,2,4-TRIMETHYLBENZENE	C9H12-7	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
1,3,5-TRIMETHYLBENZENE	C9H12-8	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
1,2,3,4-TETRAHYDRONAPHTHALENE	C10H12	X	X	X	X	X	X	X	-	X	X	X	X	X	X	X	X	X	X	X	X	X	-	X
N-BUTYLBENZENE	C10H14-1	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
ISOBUTYLBENZENE	C10H14-2	X	X	X	X	X	X	X	-	X	-	X	X	X	X	X	X	X	X	X	X	X	-	-
SEC-BUTYLBENZENE	C10H14-3	X	X	X	X	X	X	X	X	X	-	X	X	X	X	X	X	X	X	X	X	X	X	-
TERT-BUTYLBENZENE	C10H14-4	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	-	-
1-METHYL-2-ISOPROPYLBENZENE	C10H14-5	X	X	X	X	X	X	X	-	X	X	-	X	X	-	X	X	X	-	X	X	-	-	-
1-METHYL-3-ISOPROPYLBENZENE	C10H14-6	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	-	-	X
1-METHYL-4-ISOPROPYLBENZENE	C10H14-7	X	X	X	X	X	X	X	-	X	X	-	X	X	-	X	X	X	-	X	X	X	-	X
1,2,4,5-TETRAMETHYLBENZENE	C10H14-9	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	-	-	-	X
1-METHYLNAPHTHALENE	C11H10-1	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
2-METHYLNAPHTHALENE	C11H10-2	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X

note: see table 2.1 for definition of ASPEN pure component parameter names and units.

Table A.2
ASPEN pure component data bank summary
For napthene compounds

Component name	Alias	MW	TC	PC	VC	ZC	OMEGA	PLXANT	CPIG	DHFORM	DGFORM	DHVLWT	RKTZRA	PLCAVT	DHLCVT	VLCVT1	TB	VB	DHVLB	TFP	DELTA	MUP	MULAND	RGYR
CYCLOPENTANE	C5H10-1	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
METHYLCYCLOPENTANE	C6H12-2	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
CYCLOHEPTANE	C7H14-1	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	-	-	-	-
1,1-DIMETHYLCYCLOPENTANE	C7H14-2	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	-	-	-
CIS-1,2-DIMETHYLCYCLOPENTANE	C7H14-3	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	-	-	-	-
TRANS-1,2-DIMETHYLCYCLOPENTANE	C7H14-4	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	-	-	-	-
ETHYLCYCLOPENTANE	C7H14-5	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	-	X	X
METHYLCYCLOHEXANE	C7H14-6	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
1,1-DIMETHTYLCYCLOHEXANE	C8H16-1	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	-	-	X
CIS-1,2-DIMETHYLCYCLOHEXANE	C8H16-2	X	X	X	-	-	X	X	X	X	X	X	X	X	X	X	X	X	X	X	-	-	-	X
TRANS-1,2-DIMETHYLCYCLOHEXANE	C8H16-3	X	X	X	-	-	X	X	X	X	X	X	X	X	X	X	X	X	X	X	-	-	-	X
CIS-1,3-DIMETHYLCYCLOHEXANE	C8H16-4	X	X	X	-	-	X	X	X	X	X	X	X	X	X	X	X	X	X	X	-	-	-	X
TRANS-1,3-DIMETHYLCYCLOHEXANE	C8H16-5	X	X	X	-	-	X	X	X	X	X	X	X	X	X	X	X	X	X	X	-	-	-	X
CIS-1,4-DIMETHYLCYCLOHEXANE	C8H16-6	X	X	X	-	-	X	X	X	X	X	X	X	X	X	X	X	X	X	X	-	-	-	X
TRANS-1,4-DIMETHYLCYCLOHEXANE	C8H16-7	X	X	X	-	-	X	X	X	X	X	X	X	X	X	X	X	X	X	X	-	-	-	X
ETHYLCYCLOHEXANE	C8H16-8	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	-
1,1,2-TRIMETHYLCYCLOPENTANE	C8H16-9	X	X	X	-	-	X	X	-	-	-	X	-	X	X	-	X	-	X	-	X	-	-	-
CIC,CIS,TRANS-1,2,4-TRIMETHYLCYC	C8H16-11	X	X	X	-	-	X	X	-	-	-	X	-	X	X	-	X	-	X	-	-	-	-	-
1-METHYL-1-ETHYLCYCLOPENTANE	C8H16-13	X	X	X	-	-	X	X	-	-	-	X	-	X	X	-	X	-	X	-	-	-	-	-
N-PROPYLCYCLOPENTANE	C8H16-14	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	-	X	X
ISOPROPYLCYCLOPENTANE	C8H16-15	X	X	X	-	-	X	X	-	-	-	X	X	X	X	X	X	X	X	X	X	-	-	-
N-PROPYLCYCLOHEXANE	C9H18-1	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
ISOPROPYLCYCLOHEXANE	C9H18-2	X	X	X	-	-	X	X	-	-	-	-	X	X	-	X	X	X	-	X	X	X	-	-
N-BUTYLCYCLOHEXANE	C10H20-1	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
N-HEXYLCYCLOPENTANE	C11H22-1	X	X	X	-	-	X	X	X	X	X	X	-	X	X	-	X	-	X	-	-	-	X	-
N-HEPTYLCYCLOPENTANE	C12H24-1	X	X	X	-	-	X	X	X	X	X	X	-	X	X	-	X	-	X	-	-	-	X	-
N-OCTYLCYCLOPENTANE	C13H26-1	X	X	X	-	-	X	X	X	X	X	X	-	X	X	-	X	-	X	-	-	-	X	-
N-NONYLCYCLOPENTANE	C14H28-1	X	X	X	-	-	X	X	X	X	X	X	-	X	X	-	X	-	X	-	-	-	X	-
N-DECYLCYCLOPENTANE	C15H30-1	X	X	X	-	-	X	X	X	X	X	X	-	X	X	-	X	-	X	-	-	-	X	-
N-DECYLCYCLOHEXANE	C16H32-1	X	X	X	-	-	X	X	X	-	-	X	-	X	X	-	X	-	X	-	-	-	X	-
N-DODECYLCYCLOPENTANE	C17H34	X	X	X	-	-	X	X	X	X	X	X	-	X	X	-	X	-	X	-	-	-	X	-
N-TRIDECYLCYCLOPENTANE	C18H36-2	X	X	X	-	-	X	X	X	X	X	X	-	X	X	-	X	-	X	-	-	-	X	-
N-TETRADECYLCYCLOPENTANE	C19H38	X	X	X	-	-	X	X	X	X	X	X	-	X	X	-	X	-	X	-	-	-	X	-
N-PENTADECYLCYCLOPENTANE	C20H40	X	X	X	-	-	X	X	X	X	X	X	-	X	X	-	X	-	X	-	-	-	X	-
N-HEXADECYLCYCLOPENTANE	C21H42	X	X	X	-	-	X	X	X	X	X	X	-	X	X	-	X	-	X	-	-	-	X	-

note: see table 2.1 for definition of ASPEN pure component parameter names and units.

Table A.3
ASPEN pure component data bank summary
For paraffin compounds

Component name	Alias	MW	TC	PC	VC	ZC	OMEGA	PLXANT	CPIG	DHFORM	DGFORM	DHVLWT	RKTZRA	PCLVC	DHLVCV	VLCVTL	TB	TVBLB	DHVLBP	TFP	DELTA	MUP	MUNDP	LRGYR
N-PENTANE	C5H12-1	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
2-METHYL-BUTANE	C5H12-2	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
N-HEXANE	C6H14-1	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
2-METHYL-PENTANE	C6H14-2	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
3-METHYL-PENTANE	C6H14-3	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
2,2-DIMETHYL-BUTANE	C6H14-4	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
2,3-DIMETHYL-BUTANE	C6H14-5	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
N-HEPTANE	C7H16-1	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
2-METHYLHEXANE	C7H16-2	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
3-METHYLHEXANE	C7H16-3	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	-	X
2,2-DIMETHYLPENTANE	C7H16-4	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
2,3-DIMETHYLPENTANE	C7H16-5	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	-	X	X	-	X
2,4-DIMETHYLPENTANE	C7H16-6	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	-	X
3,3-DIMETHYLPENTANE	C7H16-7	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	-	X
3-ETHYLPENTANE	C7H16-8	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	-	-
2,2,3-TRIMETHYLBUTANE	C7H16-9	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	-	X
N-OCTANE	C8H18-1	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
2-METHYLHEPTANE	C8H18-2	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	-	X	X
3-METHYLHEPTANE	C8H18-3	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	-	-	X
4-METHYLHEPTANE	C8H18-4	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	-	-	X
2,2-DIMETHYLHEXANE	C8H18-5	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	-	-	X
2,3-DIMETHYLHEXANE	C8H18-6	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	-	X	-	-	X
2,4-DIMETHYLHEXANE	C8H18-7	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	-	X	-	-	X
2,5-DIMETHYLHEXANE	C8H18-8	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	-	-	X
3,3-DIMETHYLHEXANE	C8H18-9	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	-	X	X
3,4-DIMETHYLHEXANE	C8H18-10	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	-	X	-	-	X
3-ETHYLHEXANE	C8H18-11	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	-	X	-	X	-
2,2,3-TRIMETHYLPENTANE	C8H18-12	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	-	X	X
2,2,4-TRIMETHYLPENTANE	C8H18-13	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
2,3,3-TRIMETHYLPENTANE	C8H18-14	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	-	-	X
2,3,4-TRIMETHYLPENTANE	C8H18-15	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	-	-	X
2-METHYL-3-ETHYLPENTANE	C8H18-16	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	-	-	-	-
3-METHYL-3-ETHYLPENTANE	C8H18-17	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	-	-	-	-
N-NONANE	C9H20-1	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X

Table A.3
ASPEN pure component data bank summary
For paraffin compounds (Continued)

Component name	Alias	MW	TC	PC	VC	ZC	OMEGA	PLXANT	CPIG	DHFORM	DGFORM	DHVLWT	RKTZRA	PLCVAT	DHLCVT	VLCVTL	TB	TV	DHVLB	TPT	DELTA	MUP	MULDN	RGYR
2,2,4-TRIMETHYLHEXANE	C9H20-3	X	X	X	–	–	X	X	X	X	X	X	X	X	X	X	X	X	X	X	–	–	–	–
2,2,5-TRIMETHYLHEXANE	C9H20-4	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	–	–	X
3,3-DIETHYLPENTANE	C9H20-5	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	–	X
2,2,3,3-TETRAMETHYLPENTANE	C9H20-6	X	X	X	–	–	X	X	X	X	X	X	–	X	X	–	X	–	X	–	–	–	–	X
2,2,3,4-TETRAMETHYLPENTANE	C9H20-7	X	X	X	–	–	X	X	X	X	X	X	–	X	X	–	X	–	X	–	–	–	–	–
2,2,4,4-TETRAMETHYLPENTANE	C9H20-8	X	X	X	–	–	X	X	X	X	X	X	X	X	X	X	X	X	X	X	–	–	–	–
2,3,3,4-TETRAMETHYLPENTANE	C9H20-9	X	X	X	–	–	X	X	X	X	X	X	–	X	X	–	X	–	X	–	–	–	–	–
N-DECANE	C10H22-1	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
N-UNDECANE	C11H24	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
N-DODECANE	C12H26	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
N-TRIDECANE	C13H28	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
N-TETRADECANE	C14H30	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
N-PENTADECANE	C15H32	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
N-HEXADECANE	C16H34	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
N-HEPTADECANE	C17H36	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	–	–	X	–
N-OCTADECANE	C18H38	X	X	X	–	–	X	X	X	X	X	X	X	X	X	X	X	X	X	X	–	–	X	–
N-NONADECANE	C19H40	X	X	X	–	–	X	X	X	X	X	X	X	X	X	X	X	X	X	X	–	–	X	–
N-EICOSANE	C20H42	X	X	X	–	–	X	X	X	X	X	X	X	X	X	X	X	X	X	X	–	–	X	–

note: see table 2.1 for definition of ASPEN pure component parameter names and units.

Table A.4
Napthene pure compound properties
obtained from
ASPEN pure component data bank summary

Component name	Alias	TFP	DHFORM	DGFORM	RGYR
CYCLOPENTANE	C5H10-1	0.179300E3	-0.772883E8	0.386442E8	0.285000E9
METHYLCYCLOPENTANE	C6H12-2	0.130700E3	-0.106763E9	0.357971E8	0.329900E9
CYCLOHEPTANE	C7H14-1	0.265000E3	-0.119408E9	0.630532E8	
1,1-DIMETHYLCYCLOPENTANE	C7H14-2	0.203400E3	-0.138374E9	0.390628E8	
CIS-1,2-DIMETHYLCYCLOPENTANE	C7H14-3	0.219300E3	-0.129623E9	0.457617E8	
TRANS-1,2-DIMETHYLCYCLOPENTANE	C7H14-4	0.155600E3	-0.136783E9	0.383930E8	
ETHYLCYCLOPENTANE	C7H14-5	0.134700E3	-0.127153E9	0.445894E8	0.373400E9
METHYLCYCLOHEXANE	C7H14-6	0.146600E3	-0.154870E9	0.272979E8	0.374670E9
1,1-DIMETHYLCYCLOHEXANE	C8H16-1	0.239700E3	-0.181121E9	0.352529E8	0.409250E9
CIS-1,2-DIMETHYLCYCLOHEXANE	C8H16-2	0.223100E3	-0.172287E9	0.412400E8	0.406120E9
TRANS-1,2-DIMETHYLCYCLOHEXANE	C8H16-3	0.185000E3	-0.180116E9	0.344992E8	0.418140E9
CIS-1,3-DIMETHYLCYCLOHEXANE	C8H16-4	0.197600E3	-0.184889E9	0.298519E8	0.405490E9
TRANS-1,3-DIMETHYLCYCLOHEXANE	C8H16-5	0.183000E3	-0.176683E9	0.363414E8	0.414620E9
CIS-1,4-DIMETHYLCYCLOHEXANE	C8H16-6	0.185700E3	-0.176767E9	0.379743E8	0.414460E9
TRANS-1,4-DIMETHYLCYCLOHEXANE	C8H16-7	0.236200E3	-0.184722E9	0.317359E8	0.416700E9
ETHYLCYCLOHEXANE	C8H16-8	0.161800E3	-0.171868E9	0.392722E8	
N-PROPYLCYCLOPENTANE	C8H16-14	0.155800E3	-0.148171E9	0.526281E8	0.413500E9
ISOPROPYLCYCLOPENTANE	C8H16-15	0.160500E3			
N-PROPYLCYCLOHEXANE	C9H18-1	0.178700E3	-0.193430E9	0.473527E8	0.436700E9
ISOPROPYLCYCLOHEXANE	C9H18-2	0.183400E3			
N-BUTYLCYCLOHEXANE	C10H20-1	0.198400E3	-0.213317E9	0.564799E8	0.487500E9
N-HEXYLCYCLOPENTANE	C11H22-1		-0.209633E9	0.782513E8	
N-HEPTYLCYCLOPENTANE	C12H24-1		-0.230274E9	0.866668E8	
N-OCTYLCYCLOPENTANE	C13H26-1		-0.250873E9	0.951241E8	
N-NONYLCYCLOPENTANE	C14H28-1		-0.271514E9	0.103498E9	
N-DECYLCYCLOPENTANE	C15H30-1		-0.292155E9	0.111913E9	
N-DODECYLCYCLOPENTANE	C17H34		-0.336116E9	0.126023E9	
N-TRIDECYLCYCLOPENTANE	C18H36-2		-0.353994E9	0.137076E9	
N-TETRADECYLCYCLOPENTANE	C19H38		-0.374635E9	0.145575E9	
N-PENTADECYLCYCLOPENTANE	C20H40		-0.395276E9	0.153991E9	
N-HEXADECYLCYCLOPENTANE	C21H42		-0.415875E9	0.162406E9	

note: TFP = normal freezing point, (deg. K)
DHFORM = standard Enthalpy of formation at 25 deg. C, (J/Kmole)
DGFORM = standard Gibbs free energy of formation at 25 deg. C, (J/Kmole)
RGYR = Radius of gyration (M)

Table A.5
Aromatic pure compound properties
obtained from
ASPEN pure component data bank summary

Component name	Alias	TFP	DHFORM	DGFORM	RGYR
BENZENE	C6H6	0.278700E3	0.829824E8	0.129749E9	0.300370E9
TOLUENE	C7H8	0.178000E3	0.500323E8	0.122087E9	0.344310E9
ETHYLBENZENE	C8H10-4	0.178200E3	0.298100E8	0.130670E9	0.382110E9
N-PROPYLBENZENE	C9H12-1	0.173700E3	0.782932E7	0.137327E9	0.434400E9
ISOPROPYLBENZENE	C9H12-2	0.177100E3	0.393559E7	0.137076E9	0.418700E9
1-METHYL-2-ETHYLBENZENE	C9H12-3	0.192300E3	0.130000E7	0.131172E9	0.412960E9
1-METHYL-3-ETHYLBENZENE	C9H12-4	0.177600E3	-0.180000E7	0.126525E9	0.428450E9
1-METHYL-4-ETHYLBENZENE	C9H12-5	0.210800E3	-0.320000E7	0.126776E9	0.416620E9
1,2,3-TRIMETHYLBENZENE	C9H12-6	0.247700E3	-0.958777E7	0.124641E9	0.409960E9
1,2,4-TRIMETHYLBENZENE	C9H12-7	0.227000E3	-0.139420E8	0.117021E9	0.416780E9
1,3,5-TRIMETHYLBENZENE	C9H12-8	0.228400E3	-0.160773E8	0.118026E9	0.434080E9
1,2,3,4-TETRAHYDRONAPHTHALENE	C10H12	0.237401E3	0.276329E8	0.167053E9	0.416200E9
N-BUTYLBENZENE	C10H14-1	0.185200E3	-0.138164E8	0.144780E9	0.484900E9
ISOBUTYLBENZENE	C10H14-2	0.221700E3	-0.215620E8		
SEC-BUTYLBENZENE	C10H14-3	0.197700E3	-0.174590E8		
TERT-BUTYLBENZENE	C10H14-4	0.215300E3	-0.226925E8	0.142947E9	
1-METHYL-2-ISOPROPYLBENZENE	C10H14-5	0.201640E3	-0.256061E8	0.137359E9	
1-METHYL-3-ISOPROPYLBENZENE	C10H14-6	0.209438E3	-0.293076E8	0.132966E9	0.457900E9
1-METHYL-4-ISOPROPYLBENZENE	C10H14-7	0.205250E3	-0.279909E8	0.132966E9	0.452310E9
1,2,4,5-TETRAMETHYLBENZENE	C10H14-9	0.352000E3	-0.453012E8	0.119533E9	0.445420E9
1-METHYLNAPHTHALENE	C11H10-1	0.242700E3	0.116937E9	0.217839E9	0.443500E9
2-METHYLNAPHTHALENE	C11H10-2	0.307700E3	0.116184E9	0.216290E9	0.442600E9

note: TFP = normal freezing point, (deg. K)
DHFORM = standard Enthalpy of formation at 25 deg. C, (J/Kmole)
DGFORM = standard Gibbs free energy of formation at 25 deg. C, (J/Kmole)
RGYR = Radius of gyration (M)

Table A.6
Paraffin pure compound properties
obtained from
ASPEN pure component data bank summary

Component name	Alias	TFP	DHFORM	DGFORM	RGYR
N-PENTANE	C5H12-1	0.143400E3	-0.146538E9	-0.837360E7	0.338500E9
2-METHYL-BUTANE	C5H12-2	0.113300E3	-0.154577E9	-0.133000E8	0.331300E9
N-HEXANE	C6H14-1	0.177800E3	-0.167305E9	-0.800000E5	0.318200E9
2-METHYL-PENTANE	C6H14-2	0.119500E3	-0.174422E9	-0.547000E7	0.380900E9
3-METHYL-PENTANE	C6H14-3	0.110251E3	-0.171743E9	-0.345000E7	0.367970E9
2,2-DIMETHYL-BUTANE	C6H14-4	0.173300E3	-0.185685E9	-0.801000E7	0.348460E9
2,3-DIMETHYL-BUTANE	C6H14-5	0.144600E3	-0.177897E9	-0.219000E7	0.352090E9
N-HEPTANE	C7H16-1	0.182600E3	-0.187904E9	0.799679E7	0.426650E9
2-METHYLHEXANE	C7H16-2	0.154900E3	-0.195063E9	0.322384E7	0.427790E9
3-METHYLHEXANE	C7H16-3	0.153750E3	-0.192425E9	0.508000E7	0.414540E9
2,2-DIMETHYLPENTANE	C7H16-4	0.149400E3	-0.206284E9	0.837360E5	0.400010E9
2,3-DIMETHYLPENTANE	C7H16-5		-0.199375E9	0.571000E7	0.392100E9
2,4-DIMETHYLPENTANE	C7H16-6	0.154000E3	-0.202139E9	0.340000E7	0.396340E9
3,3-DIMETHYLPENTANE	C7H16-7	0.138700E3	-0.201678E9	0.263768E7	0.379520E9
3-ETHYLPENTANE	C7H16-8	0.154600E3	-0.189788E9	0.110113E8	
2,2,3-TRIMETHYLBUTANE	C7H16-9	0.248300E3	-0.204944E9	0.468000E7	0.369600E9
N-OCTANE	C8H18-1	0.216400E3	-0.208586E9	0.164123E8	0.468040E9
2-METHYLHEPTANE	C8H18-2	0.164000E3	-0.215620E9	0.127697E8	0.474010E9
3-METHYLHEPTANE	C8H18-3	0.152700E3	-0.212773E9	0.137327E8	0.459320E9
4-METHYLHEPTANE	C8H18-4	0.152200E3	-0.212229E9	0.167472E8	0.455810E9
2,2-DIMETHYLHEXANE	C8H18-5	0.152000E3	-0.224873E9	0.107182E8	0.449560E9
2,3-DIMETHYLHEXANE	C8H18-6		-0.214071E9	0.177102E8	0.440840E9
2,4-DIMETHYLHEXANE	C8H18-7		-0.219556E9	0.117230E8	0.434630E9
2,5-DIMETHYLHEXANE	C8H18-8	0.181900E3	-0.222780E9	0.104670E8	0.459320E9
3,3-DIMETHYLHEXANE	C8H18-9	0.147000E3	-0.220268E9	0.132722E8	0.431970E9
3,4-DIMETHYLHEXANE	C8H18-10		-0.213150E9	0.173334E8	0.440000E9
3-ETHYLHEXANE	C8H18-11		-0.211015E9	0.165379E8	
2,2,3-TRIMETHYLPENTANE	C8H18-12	0.160900E3	-0.220268E9	0.171240E8	0.416180E9
2,2,4-TRIMETHYLPENTANE	C8H18-13	0.165800E3	-0.224287E9	0.136908E8	0.417140E9
2,3,3-TRIMETHYLPENTANE	C8H18-14	0.172500E3	-0.216583E9	0.189243E8	0.408590E9
2,3,4-TRIMETHYLPENTANE	C8H18-15	0.163900E3	-0.217588E9	0.189243E8	0.420520E9
2-METHYL-3-ETHYLPENTANE	C8H18-16	0.158200E3	-0.211350E9	0.212689E8	
3-METHYL-3-ETHYLPENTANE	C8H18-17	0.182300E3	-0.215118E9	0.199292E8	
N-NONANE	C9H20-1	0.219700E3	-0.229185E9	0.248277E8	0.512630E9

Table A.6
Paraffin pure compound properties
obtained from
ASPEN pure component data bank summary (Continued)

Component name	Alias	TFP	DHFORM	DGFORM	RGYR
2,2,4-TRIMETHYLHEXANE	C9H20-3	0.153000E3	-0.243379E9	0.225250E8	
2,2,5-TRIMETHYLHEXANE	C9H20-4	0.167400E3	-0.254181E9	0.134396E8	0.465800E9
3,3-DIETHYLPENTANE	C9H20-5	0.240060E3	-0.232116E9	0.417000E8	0.431400E9
2,2,3,3-TETRAMETHYLPENTANE	C9H20-6		-0.237392E9	0.343318E8	0.415560E9
2,2,3,4-TETRAMETHYLPENTANE	C9H20-7		-0.237140E9	0.326570E8	
2,2,4,4-TETRAMETHYLPENTANE	C9H20-8	0.206000E3	-0.242123E9	0.340387E8	
2,3,3,4-TETRAMETHYLPENTANE	C9H20-9		-0.236387E9	0.341224E8	
N-DECANE	C10H22-1	0.243500E3	-0.249826E9	0.332432E8	0.553900E9
N-UNDECANE	C11H24	0.247600E3	-0.270467E9	0.416168E8	0.598670E9
N-DODECANE	C12H26	0.263600E3	-0.291066E9	0.500741E8	0.643210E9
N-TRIDECANE	C13H28	0.267800E3	-0.311707E9	0.584896E8	0.676100E9
N-TETRADECANE	C14H30	0.279000E3	-0.332348E9	0.668632E8	0.735780E9
N-PENTADECANE	C15H32	0.283000E3	-0.352989E9	0.752787E8	0.783870E9
N-HEXADECANE	C16H34	0.291000E3	-0.373588E9	0.837360E8	0.831800E9
N-HEPTADECANE	C17H36	0.295000E3	-0.394187E9	0.921515E8	
N-OCTADECANE	C18H38	0.301300E3	-0.414828E9	0.100567E9	
N-NONADECANE	C19H40	0.305000E3	-0.435427E9	0.108982E9	
N-EICOSANE	C20H42	0.310000E3	-0.456068E9	0.117398E9	

note: TFP = normal freezing point, (deg. K)
DHFORM = standard Enthalpy of formation at 25 deg. C, (J/Kmole)
DGFORM = standard Gibbs free energy of formation at 25 deg. C, (J/Kmole)
RGYR = Radius of gyration (M)

Table A.7
Paraffin regression summary for
enthalpy of formation constants

TYPE OF FIT DESIRED IS Y VS X
FORM: Y = A(1) + A(2)*X + A(3)*X**2 + ...

A(1) = 568031546.
A(2) = -4602700.36
A(3) = 9840.17072
A(4) = -8.23774887

DEG. OF FREEDOM = 47.00000 R-SQUARE = 0.9798177

X-INPUT (TEMPERATURE K)	Y-INPUT (DGFORM J/KMOLE)	Y-CALC (DGFORM J/KMOLE)	% DEVIATION
341.9000	-0.1673050E+09	-0.1845938E+09	-10.33373
336.4000	-0.1717430E+09	-0.1803547E+09	-5.014271
333.4000	-0.1744220E+09	-0.1780040E+09	-2.053627
352.4000	-0.2062840E+09	-0.1924601E+09	6.701394
362.9000	-0.1993750E+09	-0.2000769E+09	-0.3520600
395.4000	-0.2421230E+09	-0.2226878E+09	8.026985
575.2000	-0.3941870E+09	-0.3914796E+09	0.6868192
363.2000	-0.1950630E+09	-0.2002914E+09	-2.680389
386.6000	-0.2175880E+09	-0.2166507E+09	0.4307501
388.8000	-0.2140710E+09	-0.2181628E+09	-1.911444
388.8000	-0.2113500E+09	-0.2181628E+09	-3.223491
382.6000	-0.2195560E+09	-0.2138940E+09	2.578845
365.0000	-0.1924250E+09	-0.2015754E+09	-4.755301
366.6000	-0.1897880E+09	-0.2027122E+09	-6.809808
301.0000	-0.1545770E+09	-0.1505028E+09	2.635715
419.3000	-0.2321160E+09	-0.2391276E+09	-3.020744
322.9000	-0.1856850E+09	-0.1695409E+09	8.694339
469.1000	-0.2704670E+09	-0.2760823E+09	-2.076135
371.6000	-0.1879040E+09	-0.2062399E+09	-9.758127
309.2000	-0.1465380E+09	-0.1578731E+09	-7.735297
385.1000	-0.2202680E+09	-0.2156182E+09	2.110973
359.2000	-0.2016780E+09	-0.1974178E+09	2.112391
399.7000	-0.2433790E+09	-0.2256318E+09	7.291997
392.1000	-0.2127730E+09	-0.2204270E+09	-3.597247
543.8000	-0.3529890E+09	-0.3497233E+09	0.9251630
391.7000	-0.2110150E+09	-0.2201527E+09	-4.330375
382.0000	-0.2248730E+09	-0.2134795E+09	5.066641
406.2000	-0.2371400E+09	-0.2300859E+09	2.974637
617.0000	-0.4560680E+09	-0.4607144E+09	-1.018796
387.9000	-0.2165830E+09	-0.2175446E+09	-0.4439679
526.7000	-0.3323480E+09	-0.3300658E+09	0.6866957
560.0000	-0.3735880E+09	-0.3702836E+09	0.8844967
413.4000	-0.2373920E+09	-0.2350399E+09	0.9908117
589.5000	-0.4148280E+09	-0.4132631E+09	0.3772500
508.6000	-0.3117070E+09	-0.3112772E+09	0.1378996
447.3000	-0.2498260E+09	-0.2591954E+09	-3.750388
603.1000	-0.4354270E+09	-0.4357721E+09	-0.7924802E-01
372.4000	-0.2242870E+09	-0.2068011E+09	7.796200
331.2000	-0.1778970E+09	-0.1762619E+09	0.9191247
390.8000	-0.2156200E+09	-0.2195355E+09	-1.815941
489.5000	-0.2910660E+09	-0.2933836E+09	-0.7962574
414.7000	-0.2363870E+09	-0.2359380E+09	0.1899531
397.3000	-0.2541810E+09	-0.2239887E+09	11.87825
390.9000	-0.2131500E+09	-0.2196041E+09	-3.027973
383.0000	-0.2202680E+09	-0.2141702E+09	2.768370
390.9000	-0.2122290E+09	-0.2196041E+09	-3.475079
424.0000	-0.2291850E+09	-0.2424095E+09	-5.770222
354.0000	-0.2049440E+09	-0.1936354E+09	5.517876
391.4000	-0.2151180E+09	-0.2199470E+09	-2.244831
382.3000	-0.2227800E+09	-0.2136868E+09	4.081705
398.8000	-0.2085860E+09	-0.2250156E+09	-7.876676

AVERAGE ABSOLUTE PERCENT DEVIATION = 3.6160
MAXIMUM ABSOLUTE PERCENT DEVIATION = 11.878
SUM OF RESIDUALS = -.25957823E-04

Table A.8
Napthene regression summary for
enthalpy of formation constants

TYPE OF FIT DESIRED IS Y VS X
FORM: Y = A(1) + A(2)*X + A(3)*X**2 + ...

A(1) = 0.161688484E+10
A(2) = -10641443.5
A(3) = 21793.9633
A(4) = -15.8925712

DEG. OF FREEDOM = 24.00000 R-SQUARE = 0.9754591

X-INPUT (TEMPERATURE K)	Y-INPUT (DGFORM J/KMOLE)	Y-CALC (DGFORM J/KMOLE)	% DEVIATION
516.9000	-0.2508730E+09	-0.2555390E+09	-1.859907
625.0000	-0.3952760E+09	-0.4007727E+09	-1.390601
552.5000	-0.2921550E+09	-0.2901161E+09	0.6978685
535.3000	-0.2715140E+09	-0.2722366E+09	-0.2661223
397.6000	-0.1766830E+09	-0.1677638E+09	5.048137
637.0000	-0.4158750E+09	-0.4262300E+09	-2.489930
598.6000	-0.3539940E+09	-0.3526494E+09	0.3798245
476.3000	-0.2096330E+09	-0.2246788E+09	-7.177208
393.3000	-0.1848890E+09	-0.1640635E+09	11.26381
374.1000	-0.1548700E+09	-0.1460614E+09	5.687714
599.0000	-0.3746350E+09	-0.3533040E+09	5.693809
397.5000	-0.1767670E+09	-0.1676790E+09	5.141250
454.1000	-0.2133170E+09	-0.2094877E+09	1.795102
584.1000	-0.3361160E+09	-0.3303309E+09	1.721154
322.4000	-0.7728830E+08	-0.8118680E+08	-5.044100
402.9000	-0.1722870E+09	-0.1721811E+09	0.6144459E-01
361.0000	-0.1383740E+09	-0.1321452E+09	4.501426
404.9000	-0.1718680E+09	-0.1738096E+09	-1.129680
392.7000	-0.1811210E+09	-0.1635384E+09	9.707679
429.9000	-0.1934300E+09	-0.1927313E+09	0.3612243
391.9000	-0.1194080E+09	-0.1628348E+09	-36.36840
497.3000	-0.2302740E+09	-0.2398614E+09	-4.163492
392.5000	-0.1847220E+09	-0.1633628E+09	11.56287
365.0000	-0.1367830E+09	-0.1365513E+09	0.1693674
396.6000	-0.1801160E+09	-0.1669129E+09	7.330334
345.0000	-0.1067630E+09	-0.1129933E+09	-5.835618
404.1000	-0.1481710E+09	-0.1731606E+09	-16.86539
372.7000	-0.1296230E+09	-0.1446428E+09	-11.58730

AVERAGE ABSOLUTE PERCENT DEVIATION = 5.9035
MAXIMUM ABSOLUTE PERCENT DEVIATION = 11.562
SUM OF RESIDUALS = -.10132790E-04

Table A.9
Aromatic regression summary for
enthalpy of formation constants

TYPE OF FIT DESIRED IS Y VS X
FORM: Y = A(1) + A(2)*X + A(3)*X**2 + ...

A(1) = -0.116028149E+11
A(2) = 88976967.9
A(3) = -223012.655
A(4) = 183.320881

DEG. OF FREEDOM = 17.00000 R-SQUARE = 0.9300178

X-INPUT (TEMPERATURE K)	Y-INPUT (DGFORM J/KMOLE)	Y-CALC (DGFORM J/KMOLE)	% DEVIATION
438.3000	1300000.	-0.1077677E+08	928.9820
456.4000	-0.1381640E+08	-0.1942501E+08	-40.59386
514.2000	0.1161840E+09	0.1076800E+09	7.319462
450.3000	-0.2799090E+08	-0.1823456E+08	34.85541
353.3000	0.8298240E+08	0.8041775E+08	3.090597
448.3000	-0.2930760E+08	-0.1743297E+08	40.51723
434.5000	-1800000.	-7241998.	-302.3332
432.4000	7829320.	-5087141.	164.9755
446.5000	-0.1745900E+08	-0.1655031E+08	5.204701
442.3000	-0.2269250E+08	-0.1393371E+08	38.59774
425.6000	3935590.	2733512.	30.54377
437.9000	-0.1607730E+08	-0.1042817E+08	35.13733
517.8000	0.1169370E+09	0.1266136E+09	-8.275085
383.8000	0.5003230E+08	0.6022387E+08	-20.36999
409.3000	0.2981000E+08	0.2498553E+08	16.18405
480.7000	0.2763290E+08	-1025624.	103.7116
451.5000	-0.2560610E+08	-0.1862147E+08	27.27721
470.0000	-0.4530120E+08	-0.1421161E+08	68.62862
442.5000	-0.1394200E+08	-0.1407514E+08	-0.9549656
449.2000	-9587770.	-0.1781751E+08	-85.83582
435.2000	-3200000.	-7929533.	-147.7979

AVERAGE ABSOLUTE PERCENT DEVIATION = 100.53
MAXIMUM ABSOLUTE PERCENT DEVIATION = 928.98
SUM OF RESIDUALS = 0.11062622E-03

Table A.10
Paraffin regression summary for Gibbs free energy of formation

TYPE OF FIT DESIRED IS Y VS X
FORM: Y = A(1) + A(2)*X + A(3)*X**2 + ...

A(1) = -302503962.
A(2) = 1693237.21
A(3) = -3258.30675
A(4) = 2.61935945

DEG. OF FREEDOM = 47.00000 R-SQUARE = 0.9783215

X-INPUT (TEMPERATURE K)	Y-INPUT (DGFORM J/KMOLE)	Y-CALC (DGFORM J/KMOLE)	% DEVIATION
341.9000	-80000.00	218998.2	373.7478
336.4000	-3450000.	-1909530.	44.65131
333.4000	-5470000.	-3086057.	43.58214
383.0000	0.1712400E+08	0.1520869E+08	11.18497
388.8000	0.1771020E+08	0.1723122E+08	2.704516
372.4000	0.1369080E+08	0.1146691E+08	16.24371
382.0000	0.1071820E+08	0.1485837E+08	-38.62744
359.2000	2637680.	6700965.	-154.0454
365.0000	5080000.	8811620.	-73.45709
382.3000	0.1046700E+08	0.1496351E+08	-42.95896
387.9000	0.1892430E+08	0.1691836E+08	10.59983
366.6000	0.1101130E+08	9389138.	14.73180
603.1000	0.1089820E+09	0.1081414E+09	0.7713233
526.7000	0.6686320E+08	0.6815122E+08	-1.926345
447.3000	0.3324320E+08	0.3738631E+08	-12.46302
406.2000	0.3265700E+08	0.2322913E+08	28.86938
419.3000	0.4170000E+08	0.2771378E+08	33.54010
399.7000	0.2252500E+08	0.2099767E+08	6.780605
352.4000	83736.00	4188718.	-4902.291
382.6000	0.1172300E+08	0.1506862E+08	-28.53892
322.9000	-8010000.	-7297183.	8.899094
386.6000	0.1892430E+08	0.1646583E+08	12.99108
560.0000	0.8373600E+08	0.8390530E+08	-0.2021885
543.8000	0.7527870E+08	0.7596065E+08	-0.9059058
390.8000	0.1276970E+08	0.1792533E+08	-40.37392
398.8000	0.1641230E+08	0.2068801E+08	-26.05188
331.2000	-2190000.	-3956123.	-80.64488
395.4000	0.3403870E+08	0.1951629E+08	42.66442
575.2000	0.9215150E+08	0.9190345E+08	0.2691745
309.2000	-8373600.	-0.1303350E+08	-55.64985
390.9000	0.1733340E+08	0.1795999E+08	-3.614950
391.7000	0.1653790E+08	0.1823718E+08	-10.27506
424.0000	0.2482770E+08	0.2932400E+08	-18.11000
301.0000	-0.1330000E+08	-0.1661312E+08	-24.91068
353.7000	3400000.	4672335.	-37.42161
589.5000	0.1005670E+09	0.9995926E+08	0.6043125
363.2000	3223840.	8159523.	-153.0895
469.1000	0.4161680E+08	0.4517802E+08	-8.557167
391.4000	0.1992920E+08	0.1813326E+08	9.011590
390.9000	0.1674720E+08	0.1795999E+08	-7.241770
388.8000	0.2126890E+08	0.1723122E+08	18.98394
385.1000	0.1527220E+08	0.1594276E+08	-20.12142
489.5000	0.5007410E+08	0.5283457E+08	-5.512779
354.0000	4680000.	4783707.	-2.215970
617.0000	0.1173980E+09	0.1170704E+09	0.2790552
508.6000	0.5848960E+08	0.6044443E+08	-3.342180
414.7000	0.3412240E+08	0.2613940E+08	23.39515
392.1000	0.1373270E+08	0.1837568E+08	-33.80970
413.4000	0.3433180E+08	0.2569453E+08	25.15821
371.6000	7996790.	0.1118171E+08	-39.82753
397.3000	0.1343960E+08	0.2017147E+08	-50.08978

AVERAGE ABSOLUTE PERCENT DEVIATION = 129.52
MAXIMUM ABSOLUTE PERCENT DEVIATION = 4902.2
SUM OF RESIDUALS = -.32186508E-05

Table A.11
Napthene regression summary for Gibbs free energy of formation constants

TYPE OF FIT DESIRED IS Y VS X
FORM: Y = A(1) + A(2)*X + A(3)*X**2 + ...

A(1) = 607352828.
A(2) = -3824503.65
A(3) = 7933.60038
A(4) = -4.75792750

DEG. OF FREEDOM = 24.00000 R-SQUARE = 0.9748045

X-INPUT (TEMPERATURE K)	Y-INPUT (DGFORM J/KMOLE)	Y-CALC (DGFORM J/KMOLE)	% DEVIATION
598.6000	0.1370760E+09	0.1402531E+09	-2.317732
584.1000	0.1260230E+09	0.1320338E+09	-4.769577
476.3000	0.7825130E+08	0.7145757E+08	8.681938
397.5000	0.3797430E+08	0.4183762E+08	-10.17350
535.3000	0.1034980E+09	0.1036286E+09	-0.1262139
391.9000	0.6305320E+08	0.4063609E+08	35.55269
392.5000	0.3173590E+08	0.4075790E+08	-28.42836
376.6000	0.4458940E+08	0.3811628E+08	14.51717
429.9000	0.4735270E+08	0.5141453E+08	-8.577818
454.1000	0.5647990E+08	0.6108289E+08	-8.149791
637.0000	0.1624060E+09	0.1605485E+09	1.143749
625.0000	0.1539910E+09	0.1544973E+09	-0.3287861
516.9000	0.9512410E+08	0.9310175E+08	2.126016
552.5000	0.1119130E+09	0.1136518E+09	-1.553694
322.4000	0.3864420E+08	0.3952317E+08	-2.274520
365.0000	0.3839300E+08	0.3699857E+08	3.631986
404.1000	0.5262810E+08	0.4343527E+08	17.46753
374.1000	0.2729790E+08	0.3781567E+08	-38.52960
497.3000	0.8666680E+08	0.8230630E+08	5.031334
397.6000	0.3634140E+08	0.4186037E+08	-15.18647
599.0000	0.1455750E+09	0.1404766E+09	3.502282
361.0000	0.3906280E+08	0.3678085E+08	5.841735
404.9000	0.3927220E+08	0.4364191E+08	-11.12673
392.7000	0.3525290E+08	0.4079887E+08	-15.73195
396.6000	0.3449920E+08	0.4163482E+08	-20.68345
372.7000	0.4576170E+08	0.3766147E+08	17.70090
345.0000	0.3579710E+08	0.3681810E+08	-2.852197
402.9000	0.4124000E+08	0.4313051E+08	-4.584178

AVERAGE ABSOLUTE PERCENT DEVIATION = 10.378
MAXIMUM ABSOLUTE PERCENT DEVIATION = 38.529
SUM OF RESIDUALS = 0.31292439E-05

Table A.12
Aromatic regression summary for Gibbs free energy of formation constants

TYPE OF FIT DESIRED IS Y VS X
FORM: Y = A(1) + A(2)*X + A(3)*X**2 + ...

A(1) = -0.397615347E+10
A(2) = 31010830.9
A(3) = -77805.3565
A(4) = 64.8352936

DEG. OF FREEDOM = 15.00000 R-SQUARE = 0.9028633

X-INPUT (TEMPERATURE K)	Y-INPUT (DGFORM J/KMOLE)	Y-CALC (DGFORM J/KMOLE)	% DEVIATION
449.2000	0.1246410E+09	0.1309593E+09	-5.069214
432.4000	0.1373270E+09	0.1273373E+09	7.274416
353.3000	0.1297490E+09	0.1274252E+09	1.791028
442.5000	0.1170210E+09	0.1289705E+09	-10.21144
450.3000	0.1329660E+09	0.1313648E+09	1.204216
425.6000	0.1370760E+09	0.1269861E+09	7.360806
517.8000	0.2178390E+09	0.2214706E+09	-1.667111
456.4000	0.1447800E+09	0.1340572E+09	7.406273
448.3000	0.1329660E+09	0.1306448E+09	1.745707
438.3000	0.1311720E+09	0.1281096E+09	2.334677
470.0000	0.1195330E+09	0.1431285E+09	-19.73974
437.9000	0.1180260E+09	0.1280417E+09	-8.486024
514.2000	0.2162900E+09	0.2124552E+09	1.772970
434.5000	0.1265250E+09	0.1275577E+09	-0.8162355
409.3000	0.1306700E+09	0.1277862E+09	2.206955
480.7000	0.1670530E+09	0.1537560E+09	7.959768
451.5000	0.1373590E+09	0.1318342E+09	4.022189
435.2000	0.1267760E+09	0.1276442E+09	-0.6848330
383.8000	0.1220870E+09	0.1303269E+09	-6.749231

AVERAGE ABSOLUTE PERCENT DEVIATION = 5.1843
MAXIMUM ABSOLUTE PERCENT DEVIATION = 19.739
SUM OF RESIDUALS = -.12207031E-03

Table A.13
Paraffin regression summary for
Radius of Gyration constants

FORM: RGYR=EXP(B(1)) * UOPK**B(2) * MW**B(3)
ITERATION: 25

SUM OF SQUARES	=	0.13963532
ANGLE (DEGREES)	=	47.04
NUMBER OF TIMES YSOLVE CALLED	=	31.0
NUMBER OF FUNCTIONAL EVALUATIONS	=	26.0
LAMBDA	=	0.10000000E-07
R-SQUARE	=	0.91456633

B(1) = -26.129
B(2) = 0.30375
B(3) = 0.80725

OBS.	Y-CALC	Y-ACTUAL	DIFFERENCE	% DEVIATION
1	0.30990E-09	0.33850E-09	-0.28596E-10	8.4478
2	0.30995E-09	0.33130E-09	-0.21355E-10	6.4458
3	0.35428E-09	0.31820E-09	0.36084E-10	11.340
4	0.35592E-09	0.38090E-09	-0.24981E-10	6.5584
5	0.35446E-09	0.36797E-09	-0.13511E-10	3.6716
6	0.35542E-09	0.34846E-09	0.69572E-11	1.9966
7	0.35422E-09	0.35209E-09	0.21270E-11	0.60411
8	0.40084E-09	0.42665E-09	-0.25805E-10	6.0484
9	0.40079E-09	0.42779E-09	-0.26997E-10	6.3109
10	0.39958E-09	0.41454E-09	-0.14956E-10	3.6079
11	0.40045E-09	0.40001E-09	0.44369E-12	0.11092
12	0.39796E-09	0.39210E-09	0.58583E-11	1.4941
13	0.40078E-09	0.39634E-09	0.44386E-11	1.1199
14	0.39790E-09	0.37952E-09	0.18377E-10	4.8421
15	0.39783E-09	0.36960E-09	0.28225E-10	7.6367
16	0.44510E-09	0.46804E-09	-0.22941E-10	4.9021
17	0.44499E-09	0.47401E-09	-0.29020E-10	6.1223
18	0.44375E-09	0.45932E-09	-0.15565E-10	3.3888
19	0.44381E-09	0.45581E-09	-0.12004E-10	2.6336
20	0.44468E-09	0.44956E-09	-0.48818E-11	1.0859
21	0.44224E-09	0.44084E-09	0.14030E-11	0.31825
22	0.44379E-09	0.43463E-09	0.91589E-11	2.1073
23	0.44510E-09	0.45932E-09	-0.11221E-10	3.0962
24	0.44210E-09	0.43197E-09	0.10224E-10	2.3669
25	0.44118E-09	0.44000E-09	0.11848E-11	0.26927
26	0.44083E-09	0.41618E-09	0.24649E-10	5.9227
27	0.44411E-09	0.41714E-09	0.26971E-10	6.4657
28	0.43956E-09	0.40859E-09	0.30972E-10	7.5802
29	0.44069E-09	0.42052E-09	0.20170E-10	4.7965
30	0.48867E-09	0.51263E-09	-0.23963E-10	4.6746
31	0.48629E-09	0.46580E-09	0.20487E-10	4.3981
32	0.48135E-09	0.43140E-09	0.49953E-10	11.579
33	0.50779E-09	0.41556E-09	0.92232E-10	22.195
34	0.53044E-09	0.55390E-09	-0.23458E-10	4.2351
35	0.57396E-09	0.59867E-09	-0.24710E-10	4.1275
36	0.61586E-09	0.64321E-09	-0.27348E-10	4.2519
37	0.65694E-09	0.67610E-09	-0.19162E-10	2.8342
38	0.72348E-09	0.73578E-09	-0.12295E-10	1.6710
39	0.73774E-09	0.78387E-09	-0.46132E-10	5.8851

AVERAGE ABSOLUTE PERCENT DEVIATION = 4.7985
MAXIMUM ABSOLUTE PERCENT DEVIATION = 22.194

Table A.14
Napthene regression summary for
Radius of Gyration constants

FORM: RGYR=EXP(B(1)) * UOPK**B(2) * MW**B(3)
ITERATION: 42

SUM OF SQUARES	= 0.96269145E-03
ANGLE (DEGREES)	= 46.02
NUMBER OF TIMES YSOLVE CALLED	= 50.0
NUMBER OF FUNCTIONAL EVALUATIONS	= 43.0
LAMBDA	= 0.10000000
R-SQUARE	= 0.99375960

B(1) = -25.879
B(2) = 0.26866
B(3) = 0.76607

OBS.	Y-CALC	Y-ACTUAL	DIFFERENCE	% DEVIATION
1	0.28584E-09	0.28500E-09	0.84359E-12	0.29600
2	0.33009E-09	0.32990E-09	0.19325E-12	0.58580E-01
3	0.37216E-09	0.37340E-09	-0.12361E-11	0.33103
4	0.37155E-09	0.37467E-09	-0.31151E-11	0.83142
5	0.41180E-09	0.40925E-09	0.25540E-11	0.62408
6	0.41076E-09	0.40612E-09	0.46389E-11	1.1423
7	0.41299E-09	0.41814E-09	-0.51528E-11	1.2323
8	0.41412E-09	0.40549E-09	0.86257E-11	2.1272
9	0.41180E-09	0.41462E-09	-0.28170E-11	0.67941
10	0.41208E-09	0.41446E-09	-0.23836E-11	0.57512
11	0.41448E-09	0.41670E-09	-0.22229E-11	0.53346
12	0.41343E-09	0.41350E-09	-0.70820E-13	0.17127E-01

AVERAGE ABSOLUTE PERCENT DEVIATION = 0.7040
MAXIMUM ABSOLUTE PERCENT DEVIATION = 2.1272

Table A.15
Aromatic regression summary for
Radius of Gyration constants

FORM: RGYR=EXP(B(1)) * UOPK**B(2) * MW**B(3)
ITERATION: 30
SUM OF SQUARES = 0.51015438E-02
ANGLE (DEGREES) = 47.36
NUMBER OF TIMES YSOLVE CALLED = 37.0
NUMBER OF FUNCTIONAL EVALUATIONS = 31.0
LAMBDA = 0.10000000E-07
R-SQUARE = 0.97478680

B(1) = -28.663
B(2) = 2.2211
B(3) = 0.38475

OBS.	Y-CALC	Y-ACTUAL	DIFFERENCE	% DEVIATION
1	0.29660E-09	0.30037E-09	-0.37709E-11	1.2554
2	0.34852E-09	0.34431E-09	0.42094E-11	1.2226
3	0.38623E-09	0.38211E-09	0.41208E-11	1.0784
4	0.42757E-09	0.43440E-09	-0.68291E-11	1.5721
5	0.42253E-09	0.41870E-09	0.38282E-11	0.91431
6	0.41145E-09	0.41296E-09	-0.15058E-11	0.36464
7	0.42561E-09	0.42845E-09	-0.28424E-11	0.66342
8	0.43061E-09	0.41662E-09	0.13990E-10	3.3579
9	0.40584E-09	0.40996E-09	-0.41176E-11	1.0044
10	0.41889E-09	0.41678E-09	0.21052E-11	0.50511
11	0.42823E-09	0.43408E-09	-0.58528E-11	1.3483
12	0.42257E-09	0.41620E-09	0.63706E-11	1.5307
13	0.46692E-09	0.48490E-09	-0.17978E-10	3.7075
14	0.44939E-09	0.45790E-09	-0.85058E-11	1.8576
15	0.46580E-09	0.45231E-09	0.13493E-10	2.9831
16	0.44594E-09	0.44542E-09	0.52155E-12	0.11709
17	0.44492E-09	0.44350E-09	0.14153E-11	0.31912

AVERAGE ABSOLUTE PERCENT DEVIATION = 1.4001
MAXIMUM ABSOLUTE PERCENT DEVIATION = 3.7075

Table A.16
Paraffin regression summary for
Freezing/Melting point constants

FORM: TFP=EXP(B(1)) * TBK**B(2) * SG**B(3)
ITERATION: 25
SUM OF SQUARES = 0.77208779
ANGLE (DEGREES) = 72.09
NUMBER OF TIMES YSOLVE CALLED = 31.0
NUMBER OF FUNCTIONAL EVALUATIONS = 26.0
LAMBDA = 0.10000000E-07
R-SQUARE = 0.76581642

B(1) = -3.3158
B(2) = 1.4185
B(3) = -0.85142E-01

OBS.	Y-CALC	Y-ACTUAL	DIFFERENCE	% DEVIATION
1	128.63	143.40	-14.770	10.300
2	123.92	113.30	10.617	9.3706
3	147.53	177.80	-30.275	17.027
4	142.64	119.50	23.136	19.360
5	144.26	110.25	34.006	30.844
6	136.38	173.30	-36.924	21.306
7	141.14	144.60	-3.4606	2.3933
8	165.72	182.60	-16.883	9.2458
9	160.53	154.90	5.6271	3.6327
10	161.50	153.75	7.7473	5.0389
11	153.89	149.40	4.4938	3.0079
12	154.72	154.00	0.71876	0.46672
13	157.75	138.70	19.054	13.737
14	162.28	154.60	7.6843	4.9704
15	154.58	248.30	-93.720	37.745
16	182.76	216.40	-33.637	15.544
17	177.67	164.00	13.675	8.3382
18	178.36	152.70	25.658	16.803
19	177.61	152.20	25.405	16.692
20	172.10	152.00	20.104	13.226
21	172.34	181.90	-9.5627	5.2571
22	173.78	147.00	26.775	18.214
23	172.31	160.90	11.410	7.0913
24	166.06	165.80	0.26160	0.15778
25	175.24	172.50	2.7406	1.5888
26	174.55	163.90	10.650	6.4979
27	175.96	158.20	17.761	11.227
28	177.47	182.30	-4.8327	2.6510
29	199.01	219.70	-20.694	9.4190
30	183.05	153.00	30.047	19.638
31	181.55	167.40	14.154	8.4553
32	195.12	240.06	-44.940	18.720
33	180.21	206.00	-25.785	12.517
34	214.26	243.50	-29.236	12.006
35	229.11	247.60	-18.493	7.4690
36	243.15	263.60	-20.452	7.7589
37	256.49	267.80	-11.315	4.2251
38	272.09	279.00	-6.9091	2.4764
39	281.62	283.00	-1.3793	0.48738
40	293.56	291.00	2.5620	0.88040
41	304.66	295.00	9.6637	3.2758
42	315.32	301.30	14.023	4.6542
43	325.18	305.00	20.176	6.6152

AVERAGE ABSOLUTE PERCENT DEVIATION = 10.007
MAXIMUM ABSOLUTE PERCENT DEVIATION = 37.744

Table A.17
Napthene regression summary for
Freezing/Melting point constants

FORM: TFP=EXP(B(1)) * TBK**B(2) * SG**B(3)
ITERATION: 30

SUM OF SQUARES	=	0.53945060
ANGLE (DEGREES)	=	71.99
NUMBER OF TIMES YSOLVE CALLED	=	37.0
NUMBER OF FUNCTIONAL EVALUATIONS	=	31.0
LAMBDA	=	0.10000000E-07
R-SQUARE	=	0.21622014

B(1) = 10.396
B(2) = -0.63428
B(3) = 5.6091

OBS.	Y-CALC	Y-ACTUAL	DIFFERENCE	% DEVIATION
1	167.11	179.30	-12.188	6.7973
2	166.24	130.70	35.541	27.193
3	234.46	265.00	-30.541	11.525
4	167.61	203.40	-35.792	17.597
5	187.31	219.30	-31.988	14.587
6	162.78	155.60	7.1757	4.6116
7	178.16	134.70	43.461	32.265
8	182.85	146.60	36.248	24.726
9	191.90	239.70	-47.799	19.941
10	208.87	223.10	-14.230	6.3784
11	182.96	185.00	-2.0359	1.1005
12	171.06	197.60	-26.543	13.433
13	194.87	183.00	11.873	6.4882
14	192.13	185.70	6.4327	3.4640
15	167.55	236.20	-68.652	29.065
16	196.65	161.80	34.854	21.541
17	183.11	155.80	27.313	17.531
18	195.79	178.70	17.095	9.5663

AVERAGE ABSOLUTE PERCENT DEVIATION = 14.878
MAXIMUM ABSOLUTE PERCENT DEVIATION = 32.265

Table A.18
Aromatic regression summary for
Freezing/Melting point constants

```
FORM: TFP=EXP(B(1)) * TBK**B(2) * SG**B(3)
ITERATION:         29
SUM OF SQUARES                                    =   0.45754251
ANGLE (DEGREES)                                   =            71.76
NUMBER OF TIMES YSOLVE CALLED                     =            36.0
NUMBER OF FUNCTIONAL EVALUATIONS                  =            30.0
NUMBER OF ANALYTICAL DERIVATIVE EVALUATIONS       =             0.0
LAMBDA                                            =   0.10000000E-08
R-SQUARE                                          =      0.23732463

B( 1) =     6.2971
B( 2) =  -0.67363E-01
B( 3) =     4.0803
```

OBS.	Y-CALC	Y-ACTUAL	DIFFERENCE	% DEVIATION
1	223.34	278.70	-55.362	19.864
2	207.70	178.00	29.705	16.688
3	206.58	178.20	28.380	15.926
4	200.85	173.70	27.153	15.632
5	201.11	177.10	24.015	13.560
6	219.35	192.30	27.051	14.067
7	203.83	177.60	26.231	14.769
8	199.92	210.80	-10.883	5.1625
9	232.21	247.70	-15.486	6.2520
10	214.89	227.00	-12.111	5.3352
11	203.59	228.40	-24.813	10.864
12	251.74	237.40	14.338	6.0395
13	198.08	185.20	12.882	6.9556
14	191.84	221.70	-29.862	13.470
15	200.22	197.70	2.5227	1.2760
16	205.15	215.30	-10.145	4.7120
17	231.82	201.64	30.181	14.968
18	207.64	209.44	-1.7948	0.85698
19	195.53	205.25	-9.7238	4.7375
20	223.88	352.00	-128.12	36.399
21	265.43	242.70	22.731	9.3658

AVERAGE ABSOLUTE PERCENT DEVIATION = 11.281
MAXIMUM ABSOLUTE PERCENT DEVIATION = 36.398

Table A.19
Tia Juana Crude Assay characterization
regression summary for paraffins

TYPE OF FIT DESIRED IS Y VS X
FORM: Y = A(1) + A(2)*X + A(3)*X**2 + ...
A(1) = 163.474495
A(2) = -0.891752893
A(3) = 0.227401200E-02
A(4) = -0.192727416E-05

DEG. OF FREEDOM = 19.00000 R-SQUARE = 0.9677219

X-INPUT (TEMPERATURE F)	Y-INPUT (% PARAFFINS)	Y-CALC (% PARAFFINS)	% DEVIATION
113.0000	90.40000	88.96242	1.590245
185.0000	62.60000	64.12549	-2.436890
230.0000	52.30000	55.21742	-5.578240
257.0000	52.30000	51.77553	1.002819
275.0000	51.60000	50.13333	2.842389
338.0000	47.50000	47.43357	0.1398526
230.0000	52.30000	55.21742	-5.578240
261.5000	52.60000	51.31973	2.433966
288.5000	50.70000	49.19624	2.965992
311.0000	52.80000	48.11121	8.880288
333.5000	46.30000	47.50799	-2.609044
360.5000	45.20000	47.23466	-4.501459
387.5000	48.70000	47.23786	3.002336
441.5000	48.70000	47.16343	3.155165
468.5000	46.40000	46.63059	-0.4969599
495.5000	44.60000	45.46385	-1.936876
522.5000	43.90000	43.43560	1.057860
549.5000	41.30000	40.31824	2.377142
351.5000	47.80000	47.28380	1.079910
378.5000	46.90000	47.22012	-0.6825562
419.0000	46.20000	47.28745	-2.353794
455.0000	45.70000	46.96202	-2.761540
455.0000	45.40000	46.96202	-3.440581

AVERAGE ABSOLUTE PERCENT DEVIATION = 2.7349
MAXIMUM ABSOLUTE PERCENT DEVIATION = 8.8802
SUM OF RESIDUALS = 0.13145041E-11

Table A.20
Tia Juana Crude Assay characterization
regression summary for napthenes

TYPE OF FIT DESIRED IS Y VS X
FORM: Y = A(1) + A(2)*X + A(3)*X**2 + ...
A(1) = -135.918371
A(2) = 2.18056119
A(3) = -0.100266584E-01
A(4) = 0.196502211E-04
A(5) = -0.139185252E-07

DEG. OF FREEDOM = 18.00000 R-SQUARE = 0.9472170

X-INPUT (TEMPERATURE F)	Y-INPUT (% NAPTHENES)	Y-CALC (% NAPTHENES)	% DEVIATION
113.0000	8.100000	8.538508	-5.413675
185.0000	32.80000	32.43742	1.105421
230.0000	37.20000	35.33497	5.013517
257.0000	34.30000	35.07044	-2.246191
275.0000	33.30000	34.53110	-3.697001
338.0000	32.30000	32.74836	-1.388113
230.0000	37.20000	35.33497	5.013517
261.5000	34.20000	34.95249	-2.200263
288.5000	32.50000	34.06113	-4.803470
311.0000	31.40000	33.32379	-6.126707
333.5000	32.20000	32.81190	-1.900302
360.5000	33.10000	32.65368	1.348404
387.5000	34.80000	33.02293	5.106514
441.5000	35.80000	34.61275	3.316351
468.5000	34.10000	35.02393	-2.709481
495.5000	32.80000	34.34385	-4.706862
522.5000	29.60000	31.72400	-7.175681
549.5000	28.10000	26.13836	6.980920
351.5000	33.00000	32.64609	1.072457
378.5000	34.80000	32.84613	5.614568
419.0000	33.90000	33.92589	-0.7637988E-01
455.0000	34.60000	34.90865	-0.8920571
455.0000	35.80000	34.90865	2.489800

AVERAGE ABSOLUTE PERCENT DEVIATION = 6.0125
MAXIMUM ABSOLUTE PERCENT DEVIATION = 7.1756
SUM OF RESIDUALS = -.76791906E-11

APPENDIX B

ESTPRO program listing

```
C*****************************************************************************
C
      PROGRAM ESTPRO
C
C*****************************************************************************
C
C       NAME OF MODULE - ESTPRO
C       MODULE TITLE - MAIN PROGRAM TO CALC ASPEN PROPERTIES FOR
C                      HYDROCARBON PSEUDOCOMPONENTS
C       PURPOSE - TO CONTROL THE CALCULATION PROCEDURE AND OBTAIN
C                 PROPERTIES OF HYDROCARBON PSEUDOCOMPONENTS
C       MODIFIED - 12-20-88
C
C       COPYWRITE 1989 STEVEN E. SUND
C
C
C      'WARNING'              POSSIBLE PROBLEM
C      '*ERROR**              CONTINUE ON ERROR
C      '***SEVERE ERROR***    STOP ON ERROR
C
C       INTERNAL UNITS = SI
C
C
C      ROUTINE NAME(TYPE)                DESCRIPTION
C
C      ANDRA(S).....................MOD. ANDRADE MODEL LIQ VISC
C      ASTMCF(S)....................CHARA. OF PET. FRAC. BOIL PTS (ASTM)
C      CAPS(S)......................CONVERT INPUT TO CAPITALS
C      CAVENT(S)....................CAVETT ENTHALPY VALUE
C      CAVVP(S).....................CAVETT VAPOR PRESSURE
C      CHKSOP(S)....................CHECK SYSOP NUMBER AND SET CALC VECTOR
C      CONV(S)......................CONVERSION CHAR TO REAL OR INTEGER
C      DGFRM(S).....................GIBBS ENERGY OF FORMATION
C      DHFRM(S).....................ENTHALPHY OF FORMATION
C      DIPOLE(S)....................DIPOLE MOMENT
C      ESTFRA(S)....................ESTIMATE PAR,NAP,AND AROMATIC FRACS
C      EXTOK(S).....................EXTRACT TOKEN
C      FEND(S)......................FIND NON BLANK END OF 80 CHAR RECORD
C      GUNYAM(S)....................LIQUID DENSITY CALC
C      GYKL(S)......................ACENTRIC FACTOR CALC
C      HVABP(S).....................HEAT OF VAPORIZATION AT THE BOILING POINT
C      INEX(F)......................LINEAR INTERPOLATION/EXTRAPOLATION
C      INIT(S)......................INITILIZATION ROUTINE
C      INPT(S)......................INPUT TRANSLATOR
C      LMVABP(S)....................LIQUID MOLAR VOLUME AT BOILING PT
C      MAXBN1(S)....................MAXWELL BONELL FIT TO ANTOINE
C      MAXBN2(S)....................MAXWELL BONELL CALC (ONE PT)
C      MESS(S)......................OUTPUT MESSAGE ROUTINE
C      NEED(S)......................CALC NEEDED VALUES FROM INPUT
C      NFMP(S)......................NORMAL FREEZING/MELTING POINT
C      OPENF(S).....................OPEN FILES
C      OUTP(S)......................OUTPUT RESULTS
C      PCON(S)......................PRESSURE CONVERSION
C      PROPS(S).....................DRIVER FOR CALCULATION OF PURE COMP PROPS
C      RADGYR(S)....................RADIUS OF GYRATION
C      RDCHECK(S)...................CHECK OF RIAZI AND DAUBERT ROUTINES
C      RDCPIG(S)....................RIAZI AND DAUBERT SPEC HEAT
C      RDMW(S)......................RIAZI AND DAUBERT MOLE WT
C      RDPC(S)......................RIAZI AND DAUBERT CRIT PRES
C      RDTC(S)......................RIAZI AND DAUBERT CRIT TEMP
C      RDVC(S)......................RIAZI AND DAUBERT CRIT VOLUME
C      REFLV(S).....................RACKET LIQUID VOLUME PARAMETER CALC
C      SECOND(S)....................CALCS CPU TIME IN SECONDS (VAX DEPENDENT)
C      SOLPAR(S)....................SOLUBILITY PARAMETER
C      STRIP(S).....................RECORD TRAILING BLANK STRIPPER
C      TBCALC(S)....................NORMAL BOILING POINT CALC
C      TBPCF(S).....................CHARA. OF PET. FRAC. BOIL PTS (TBP)
```

```
C       TCON(S).....................TEMPERATURE CONVERSION
C       TIME_INIT(S)................INIT. FOR SUB. SECOND (VAX DEPENDENT)
C       VC(F).......................CORRECTION TO VABP VALUE FOR CABP(TBP)
C       VFSH(S).....................CHARACTERISTIC MOLAR VOLUME PAR. CALC
C       VM(F).......................CORRECTION TO VABP VALUE FOR MABP(TBP)
C       WATHOV(S)...................WATSON HEAT OF VAPORIZATION PARAM
C       YSOLVE(S)...................MARQUARDTS METHOD OF NONLIN EST AND EQ SOLV
C       ZCCAL(S)....................CRITICAL COMPRESS FACTOR CALC
C
        IMPLICIT REAL*8 (A-H,O-Z)
        IMPLICIT INTEGER(I-N)
C
        REAL*8 MULAND,MULREG,MABP,MEABP,MUP
C
        PARAMETER         (MNC=25)
C
        CHARACTER*32      CNAME,FILE
C
C         NIN = INPUT LOGICAL UNIT
C         NOUT = OUTPUT LOGICAL UNIT (NOT USED)
C         NHSTRY = HISTORY LOGICAL UNIT
C         NREPT = REPORT LOGICAL UNIT
C
        COMMON /IO     / NIN,NOUT,NHSTRY,NREPT
C
C         IWARN = NUMBER OF WARNING PRINTED
C         INERR = NUMBER OF ERRORS PRINTED
C         ISERR = NUMBER OF SEVERE ERRORS PRINTED
C
        COMMON /ERRC   / IWARN,INERR,ISERR
C
C         FILE = FILE NAME (IE FILE.INP, FILE.REP, FILE.HIS)
C
        COMMON /FILES / FILE
C
C         RMISS = MISSING VALUE FOR PARMAETERS
C
        COMMON /SYS1   / RMISS
C
C         NSYSOP = DESIRED SYSOP NUMBER
C         NPCVEC = VECTOR OF PROPERTIES REQUIRED FOR NSYSOP
C
        COMMON /SYS2   / NSYSOP,NPCVEC(22)
C
C        IERCAL = ERROR IN PROPS SAVE
C
        COMMON /SYS3   / IERCAL(22)
C
C         LDBUG = CALCUATION DEBUG LEVEL (0-8)
C         LDBUGR = REPORT DEBUG LEVEL (0-8)
C
        COMMON /DEBUG / LDBUG,LDBUGR
C
C         TREF = ASPEN REFERENCE TEMP (DEG K)
C         PREF = ASPEN REFERENCE PRES (PASCALS)
C         RGAS = GAS CONSTANT (M**3*PA/KMOLE K)
C
        COMMON /REFS   / TREF,PREF,RGAS
C
C         NCOMP = NUMBER OF COMPOUNDS
C         CNAME = NAMES OF COMPOUNDS
C         ICF   = CHARACTERIZE FRACTION FLAG
C
        COMMON /NPROP1/ NCOMP,CNAME(MNC),ICF
C
C         VABP = VOLUME AVERAGE BOILING POINT (DEG K)
C         SLOP = SLOPE OF CHAR CURVE
C         CABP = CUBIC AVERAGE BOILING POINT (DEG K)
```

```
C         MABP = MOLAL AVERAGE BOILING POINT (DEG K)
C         MEABP = MEAN AVERAGE BOILING POINT (DEG K)
C
      COMMON /NPROP2/ VABP(MNC),SLOP(MNC),CABP(MNC),MABP(MNC),MEABP(MNC)
C
C         UOPK = UOP CHARACTERIZATION FACTOR (WATSON K) MEABP**1/3 / SG
C         API = API GRAVITY
C         SG = SPECIFIC GRAVITY (60/60F)
C         AMW = AVERAGE MOLE WT.
C
      COMMON /NPROP3/ UOPK(MNC),API(MNC),SG(MNC),AMW(MNC)
C
C        PP = PERCENT PARAFFINS
C        PN = PERCENT NAPTHENES
C        PA = PERCENT AROMATICS
C        IPF = PERCENT FLAG
C
      COMMON /NPROP4/ PA(MNC),PN(MNC),PP(MNC),IPF
C
C        XPAR = FRACTION PARAFFINS
C        XNAP = FRACTION NAPTHENES
C        XARO = FRACTION AROMATICS
C
      COMMON /EPROP1/ XPAR(MNC),XNAP(MNC),XARO(MNC)
C
C         NDAT = NUMBER OF DATA POINTS FOR MAXWELL BONEL
C         ST = LOWER TEMP FOR MAX BON.
C         BT = UPPER TEMP FOR MAX BON.
C
      COMMON /EPROP2/ NDAT(MNC),ST(MNC),BT(MNC)
C
C         TC = CRITICAL TEMP (DEG K)
C
      COMMON /CPRP01/ TC(MNC)
C
C         PC = CRITICAL PRESSURE (PA)
C
      COMMON /CPRP02/ PC(MNC)
C
C         VC = CRITICAL VOLUME (M**3/KG-MOLE)
C
      COMMON /CPRP03/ VC(MNC)
C
C         ZC = CRITICAL COMPRESSIBILITY FACTOR
C
      COMMON /CPRP04/ ZC(MNC)
C
C         OMEGA = ACENTRIC FACTOR
C
      COMMON /CPRP05/ OMEGA(MNC)
C
C         PLXANT = EXTENDED ANTOINE VAPOR PRESSURE CONSTS.(LN(PA) VS. DEG K)
C         PLXREG = SUMMARY OF VALUES FOR REGRESSION OF PLXANT
C
      COMMON /CPRP06/ PLXANT(5,MNC),PLXREG(3,MNC)
C
C         CPIG = IDEAL GAS HEAT CAPACITY (J/KMOLE DEG K)
C
      COMMON /CPRP07/ CPIG(11,MNC),CPREG(3,MNC)
C
C         DHVLWT = WATSON EQUATION FOR HEAT OF VAPORIZATION
C
      COMMON /CPRP08/ DHVLWT(5,MNC)
C
C         MULAND = VISCOSITY BY MODIFIED ANDRADE MODEL(LOG(NOL)=A+B/T+C*LOG(T)
C
      COMMON /CPRP09/ MULAND(5,MNC),MULREG(3,MNC)
C
```

```
C         DHFORM = STANDARD HEAT OF FORMATION (J/KMOLE)
C
      COMMON /CPRP10/ DHFORM(MNC)
C
C         DGFORM = STANDARD FREE ENERGY OF FORMATION (J/KMOLE)
C
      COMMON /CPRP11/ DGFORM(MNC)
C
C         RKTZRA = RACKET EQUATION FOR LIQUID VOLUME
C
      COMMON /CPRP12/ RKTZRA(MNC),RKTREG(3,MNC)
C
C         DHLCVT = CAVETT EQUATION FOR ENTHALPY
C
      COMMON /CPRP13/ DHLCVT(MNC)
C
C         TB = ATMOSPHERIC BOILING POINT (DEG K)
C
      COMMON /CPRP14/ TB(MNC)
C
C         VB = LIQUID MOLAR VOLUME AT TB (M**3/KMOLE)
C
      COMMON /CPRP15/ VB(MNC)
C
C         DHVLB = HEAT OF VAPORIZATION AT TB (J/KMOLE)
C
      COMMON /CPRP16/ DHVLB(MNC)
C
C         TFP = NORMAL FREEZING/MELTING POINT (DEG K)
C
      COMMON /CPRP17/ TFP(MNC)
C
C         DELTA = SOLUBILITY PARAM AT 25 DEG C ((J/M**3)**1/2)
C
      COMMON /CPRP18/ DELTA(MNC)
C
C         MUP = DIPOLE MOMENT (COULOMB*M)
C
      COMMON /CPRP19/ MUP(MNC)
C
C         RGYR = RADIUS OF GYRATION (M)
C
      COMMON /CPRP20/ RGYR(MNC)
C
C         PLCAVT = CAVETT EQUATION PARAMS
C         PLCREG = SUMMARY OF VALUES FOR REGRESSION OF PLCAVT
C
      COMMON /CPRP21/ PLCAVT(4,MNC),PLCREG(3,MNC)
C
C         VLCVT1 = CHARACTERISTIC MOLAR VOLUME PARAMETER
C
      COMMON /CPRP22/ VLCVT1(MNC)
C
C       WARNINGS,ERRORS,SEVERE ERRORS
C
      IWARN=0
      INERR=0
      ISERR=0
C
C       IO LOGICAL
C
      NIN=    2
      NOUT=   3
      NHSTRY=4
      NREPT=  5
C
C       REFERENCE CONDITIONS
C
```

```
      TREF=298.15D0
      PREF=101325D0
      RGAS=8314.33D0
C
      RMISS=1.0D30
C
C       CPU TIME SUMMARY INFORMATION
C
      SECO=0.0
      CALL SECOND(SECO)
      TSTART=SECNDS(0.0)
C
C       ASK FOR INPUT DATA FILE NAME
C
      WRITE(*,100)
      READ(*,200)FILE
C
      CALL OPENF(1,IER1)
      IF(IER1.GT.0)GOTO 9999
      WRITE(*,250)
      WRITE(*,300)
C
      CALL OPENF(2,IER2)
      IF(IER2.GT.0)GOTO 9999
      WRITE(*,400)
C
C       CALL INPUT TRANSLATOR
C
      CALL INPT(IER3)
C
      WRITE(*,500)
C
      IF(IER3.LT.0)THEN
       WRITE(*,510)
      ELSE IF(IER3.GT.0)THEN
       WRITE(*,520)
      ENDIF
C
C       OPEN REP FILE
C
      CALL OPENF(3,IER4)
      IF(IER4.GT.0)GOTO 9999
      WRITE(*,600)
C
C       INITILIZE
C
      CALL INIT(IER5)
      WRITE(*,700)
      IF(IER5.LT.0)THEN
       WRITE(*,710)
      ENDIF
C
C       BEGIN CALCULATIONS
C
      CALL NEED(IER6)
      WRITE(*,800)
      IF(IER6.LT.0)THEN
       WRITE(*,810)
      ENDIF
      WRITE(*,900)
      WRITE(*,250)
      WRITE(*,210)
C
C       CALC PROPS
C
      CALL PROPS(IER7)
      IF(IER7.GT.0)THEN
       WRITE(*,1000)IER7
```

```
      ENDIF
C
C       WRITE FINAL FLAG
C
      CALL SECOND(TIME)
C
      WRITE(NHSTRY,2000)NCOMP,TIME,IWARN,INERR,ISERR
C
C        FORMATS
C
100   FORMAT(2X,'Enter input data file name ',$)
200   FORMAT(A32)
210   FORMAT(/)
250   FORMAT(5X,'**************************************')
300   FORMAT(5X,'* SUCCESSFUL OPEN OF INPUT FILE         *')
400   FORMAT(5X,'* SUCCESSFUL OPEN OF HISTORY FILE       *')
500   FORMAT(5X,'* INPUT READ COMPLETE                   *')
510   FORMAT(5X,'*** WARNING IN READ (SEE .HIS FILE)    ***')
520   FORMAT(5X,'*** ERR IN READ (SEE .HIS FILE)        ***')
600   FORMAT(5X,'* SUCCESSFUL OPEN OF REPORT FILE        *')
700   FORMAT(5X,'* INITIALIZATION OF VARIABLES COMPLETE *')
710   FORMAT(5X,'*** WARNING/ERROR IN INIT',
     1          ' ROUTINE (SEE .HIS FILE) ***')
800   FORMAT(5X,'* CALCULATE NEEDED VALUES COMPLETE      *')
810   FORMAT(5X,'*** ERROR/WARNING IN NEED ROUTINE (SEE .HIS FILE) ***')
900   FORMAT(5X,'* BEGIN PROPERTY CALCULATION            *')
1000  FORMAT(5X,'*** ERROR/WARNING COUNT IN ROUTINE PROPS = ',I6,' ***')
1100  FORMAT(5X,'*** ERROR IN ROUTINE = ',I6,' ERROR NUMBER = ',I6)
2000  FORMAT(///,
     1 T5,'*****************************************************',
     2 T5,'*                                                   *',
     3 T5,'*                  ESTPRO ENDS EXECUTION            *',
     4 T5,'*                                                   *',
     5 T5,'*  NUMBER OF COMPOUNDS.....................',I10,   '  *',
     6 T5,'*  CPU TIME ...............................',2X,G12.6,'  *',/
     7 T5,'*  NUMBER OF WARNINGS PRINTED..............',I10,   '  *',/
     8 T5,'*  NUMBER OF ERRORS PRINTED.................',I10,   '  *',
     9 T5,'*  NUMBER OF SEVERE ERRORS PRINTED..........',I10,   '  *',/
     T T5,'*                                                   *',/
     1 T5,'*****************************************************')
C
9999  STOP
      END
C*************************************************************************
C
      SUBROUTINE ANDRA(JC,IERR)
C
C*************************************************************************
C
C        NAME OF MODULE - ANDRA
C        MODULE TITLE - CALCULATE MODIFIED ANDRADE MODEL PARAMETERS
C        PURPOSE - TO CALC PARAMETERS FOR MODIFIED ANDRADE MODEL
C          FOR LIQ VISCOSITY FROM DATA OBTAINED FROM LETSOU-STIEL(1973)
C          MODEL.
C        MODIFIED - 10-15-88
C
C          FOR 0.76<TR<0.98
C
C        VARIABLES USED
C
C VARIABLE I/O TYPE-SPEC DIMENSION      DESCRIPTION AND RANGE
C      JC     I       I          -      COMPONENT ARRAY ID
C    IERR     O       I          -      ERROR CODE
C                                        0 = OK
C                                       -1 = NO IMPROVEMENT POSSIBLE IN
C                                       THE VALUE OF PH EVEN THOUGH
C                                       CONVERGENCE HAS NOT BEEN REACHED.
C                                       -2 = MORE UNKNOWNS THAN FUNCTIONS AND
```

```
C                                       UNIQUE SOLUTION GENERALLY IS IMPOSSIBLE.
C                                       -3 = TOTAL NUMBER OF VARIABLES TO BE
C                                       VARIED IS ZERO
C                                       -4 = CONVERGENCE CRITERION MET BUT FLA
C                                       STILL LARGE
C                                       -5 = IC NOT A VALID NUMBER ON ENTRY
C                                       -6 = X(I) IS NOT WITHIN XMIN(I) TO
C                                        XMAX(I)
C                                       -7 = ZERO DIAGONAL ELEMENT IN EQUATION
C                                       SOLVE
C                                       -10 = TRY TO CALC. DERIVATIVE
C                                       ANALYTICALY
C                                       -11 = RUN EXCEEDED MAXIT SPECIFIED
C
      IMPLICIT REAL*8 (A-H,O-Z)
      IMPLICIT INTEGER(I-N)
C
      REAL*8            MULAND,MULREG
C
      PARAMETER         (MNC=25)
C
      COMMON /IO     / NIN,NOUT,NHSTRY,NREPT
C
      COMMON /NPROP3/ UOPK(MNC),API(MNC),SG(MNC),AMW(MNC)
C
      COMMON /CPRP01/ TC(MNC)
      COMMON /CPRP02/ PC(MNC)
      COMMON /CPRP05/ OMEGA(MNC)
      COMMON /CPRP09/ MULAND(5,MNC),MULREG(3,MNC)
C
      DIMENSION         NDATA(26),DATA(16),OUTPUT(6)
C
      DIMENSION         X(50),XV(50),XMAX(50),XMIN(50),Y(50),
     1                  Z(100),PJ(50),P(206),A(15),AC(15)
      DIMENSION         B(6),BV(3),BMAX(3),BMIN(3)
C
C       CONSTANTS
C
      OS=1.D0/6.D0
      OH=1.D0/2.D0
      TT=2.D0/3.D0
C
      XI=2.173566*TC(JC)**OS  + AMW(JC)**OH  * PC(JC)**TT
C
C       SET UP RANGE FOR LETSOU-STEIL
C
      TRL=0.76D0
      TRH=0.98D0
      TRD=(TRH-TRL)/50.D0
      TR=TRL-TRD
C
C         MARQUARDT SET DEFAULTS
C
C         NUMBER OF UNKNOWNS
      K=3
C         NUMBER OF DATA POINTS
      N=50
C
      IF(LDBUG.GE.5)THEN
       DEGFR=FLOAT(N-K)
      ENDIF
C
      ITER = 0
      IF(MAXIT.LE.0)MAXIT=10000
C
C       SET EQUAL TO 1 FOR INITAL CALL
      NDATA(1)=1
C
```

```
C        SET INPUT PARAMETER DATA
C                  DATA(1) - FNU, FACTOR USED TO CHANGE FLA.  SET INTER-
C                            NALLY TO 10.0  IF ZERO ON INITIAL CALL.
C                  DATA(2) - FLA, FACTOR USED TO COMBINE GRADIENT AND
C                            NEWTON-RAPHSON METHODS.  SET INTERNALLY TO
C                            .01 IF ZERO ON INITIAL CALL.
C                  DATA(3) - TAU, USED IN CONVERGENCE TEST.  SET INTER-
C                            NALLY TO 0.001 IF ZERO ON INITIAL CALL.
C                  DATA(4) - EPS, USED IN CONVERGENCE TEST.  SET INTER-
C                            NALLY TO 0.00002 IF ZERO ON INITIAL CALL.
C                  DATA(5) - PHMIN, WHEN PH .LT. PHMIN, PARTIAL DERIV-
C                            ITIVES FROM THE PREVIOUS ITERATION ARE USED
C                            INSTEAD OF COMPUTING THEM AGAIN.
C                  DATA(6) THRU DATA(16) - VARIABLES USED INTERNALLY
C
      DO 10 I=1,5
       DATA(I)=0.0D0
10    CONTINUE
C
C       BV = VARY VECTOR (0=HOLD PARAMETER CONST,1=ALLOW TO VARY)
C
      DO 20 I=1,K
       BV(I)=1.D0
20    CONTINUE
C
C       INITAL VALUES OF PARMS
C
      B(1)=1.D0
      B(2)=1.D0
      B(3)=0.D0
C
C       MIN AND MAX VALUES
C
      BMAX(1)=2000.D0
      BMIN(1)=-2000.D0
      BMAX(2)=200000.D0
      BMIN(2)=-900000.D0
      BMAX(3)=20000.D0
      BMIN(3)=-20000.D0
C
      IF(LDBUG.GE.7)THEN
       WRITE(NHSTRY,1008)K,N
       DO 30 I=1,K
        WRITE(NHSTRY,1009)B(I),BMIN(I),BMAX(I),BV(I)
30     CONTINUE
       WRITE(NHSTRY,1010)
       WRITE(NHSTRY,1100)
       XSUM=0.0D0
       XSUM2=0.0D0
       YSUM=0.0D0
       YSUM2=0.0D0
      ENDIF
C
C       BEGIN CALC (CALC 50 POINTS TO BE FIT)
C        LOG(ETA)=A+B/TEMP(K) + C*LOG(TEMP(K))
C
C       UNIVERAL FUNCTIONS FOR LETSOU-STIEL MODEL
C                 L    (0)                  I    (1)
C       UF0 = (N XI)            UF1 = (N XI)
C
      DO 40 I=1,50
       TR=TR+TRD
       UF0=0.015174D0-0.02145D0*TR+0.0075D0*TR*TR
       UF1=0.042552D0-0.07674D0*TR+0.0340D0*TR*TR
       Y(I)=LOG((UF0+UF1*OMEGA(JC))/XI)
       X(I)=TR*TC(JC)
C
       IF(LDBUG.GE.7)THEN
```

```
          WRITE(NHSTRY,1020)X(I),Y(I)
          XSUM=XSUM+X(I)
          XSUM2=XSUM2+X(I)**2
          YSUM=YSUM+Y(I)
          YSUM2=YSUM2+Y(I)**2
         ENDIF
40      CONTINUE
C
C        MEANS, VARIANCES AND STANDARD DEV.
C
        IF(LDBUG.GE.7)THEN
         XMEAN=XSUM/FLOAT(N)
         XVAR=(FLOAT(N)*XSUM2-XSUM*XSUM)/FLOAT(N)/FLOAT(N-1)
         XSD=SQRT(XVAR)
         YMEAN=YSUM/FLOAT(N)
         YVAR=(FLOAT(N)*YSUM2-YSUM*YSUM)/FLOAT(N)/FLOAT(N-1)
         YSD=SQRT(YVAR)
         WRITE(NHSTRY,1120)XMEAN,YMEAN,XVAR,YVAR,XSD,YSD
        ENDIF
C
C        BEGIN REGRESSION
C
50      ITER=ITER+1
        IF(ITER.GT.MAXIT)THEN
         IERR=-11
         WRITE(NHSTRY,1015)MAXIT,ITER
         GOTO 9000
        ENDIF
C
C          EVALUATE Z VECTOR (FUNCTION VALUE)
C
C       REGRESS TO MODIFIED ANDRADE MODEL
C        Y=B(1)+B(2)/X+B(3)*LOG(X)+B(4)*LN(T)
C
        DO 60 I=1,N
         Z(I)=B(1)+B(2)/X(I)+B(3)*LOG(X(I))
60      CONTINUE
C
C       CALC ANALYTICAL DERIVATIVES (PJ VECTOR)
C
70      CONTINUE
C
C          CALC DERIVATIVE
C
        IF(NDATA(2).GT.0)THEN
         IERR=-10
         WRITE(NHSTRY,1090)IERR
         GOTO 9000
        ENDIF
C
C
        IF(LDBUG.GE.7)THEN
         WRITE(NHSTRY,1000)ITER,NDATA(3),(COEFF(J),J=1,5)
         YMYC =0.0D0
         SS   =0.0D0
         SSSAS=0.0D0
         DO 90 I=1,N
          YMYC=YMYC+(Y(I)-Z(I))**2
          SS=SS+(Z(I)-YMEAN)**2
          SSSAS=SSSAS+(Y(I)**2 - YMEAN**2)
90       CONTINUE
C
C        CALC R-SQUARE(SAS VERSION) AND ADJ R-SQUARE
C             1-VARIANCE OF FULL MODEL/VARIANCE OF MEAN MODEL
C
         RSQU=SS/(SS+YMYC)
         IF(SSSAS.NE.0.D0)THEN
          RSQUSAS=1.D0-YMYC/(SSSAS)
```

```
      ELSE
       RSQUSAS=0.D0
      ENDIF
      IF(DEGFR.EQ.0.D0)THEN
       ADJRSQU=0.0D0
      ELSE
       ADJRSQU=1.D0-(1.D0-RSQU)*(FLOAT(N)-1.D0)/DEGFR
      ENDIF
      IF(ABS(RSQU-RSQUSAS).GT.1.D8)THEN
       WRITE(NHSTRY,1112)RSQU,ADJRSQU,RSQUSAS,ADJRSQUSAS
      ELSE
       WRITE(NHSTRY,1110)RSQU,ADJRSQU
      ENDIF
C
      DO 100 J=1,K
       WRITE(NHSTRY,1030)J,B(J)
100   CONTINUE
C
      IF(LDBUG.EQ.8)THEN
       WRITE(NHSTRY,1040)
       DO 110 I=1,N
        YMYC=YMYC+(Y(I)-Z(I))**2
        SS=SS+(Z(I)-YMEAN)**2
        PERERR=ABS(Z(I)-Y(I))*ABS(Y(I))*100.D0
        WRITE(NHSTRY,1095)I,Z(I),Y(I),Z(I)-Y(I),PERERR
110    CONTINUE
       ENDIF
      ENDIF
C
120   CALL YSOLVE (K, N, NDATA, DATA, B, BV, BMAX, BMIN, Y, Z, PJ,
     1             OUTPUT, P, A, AC)
C
C                    NDATA(2) = NFCTDR, USED FOR CONTROL IN CALLING PROG
C                       IF = 0, CALCULATE FUNCTION
C                       IF = 1, CALCULATE DERIVATIVE
C                       IF =-1, EXAMINE IERR FOR WHAT TO DO NEXT
C
      IF(NDATA(2))130,50,70
C
C                    NDATA(3) = IERR, MAY TAKE ON VARIOUS VALUES
C                       IF POSITIVE, CONTAINS THE NUMBER OF VARIABLES NO
C                                    SATISFYING CONVERGENCE CRITERION
C                       IF =  0, CONVERGENCE SATISFIED AND SOLUTION RETU
C                       IF = -1, NO IMPROVEMENT POSSIBLE IN THE VALUE OF
C                                PH EVEN THOUGH CONVERGENCE HAS NOT BEEN
C                                REACHED.
C                       IF = -2, MORE UNKNOWNS THAN FUNCTIONS AND UNIQUE
C                                SOLUTION GENERALLY IS IMPOSSIBLE.
C                       IF = -3, TOTAL NUMBER OF VARIABLES TO BE VARIED
C                                IS ZERO
C                       IF = -4, CONVERGENCE CRITERION NET BUT PLA STILL
C                                LARGE
C                       IF = -5, IC NOT A VALID NUMBER ON ENTRY
C                       IF = -6, B(I) IS NOT WITHIN BMIN(I) TO BMAX(I)
C                       IF = -7, ZERO DIAGONAL ELEMENT IN EQUATION SOLVE
C
130   IF(NDATA(3))140,140,120
C
C      FINAL STATISTICAL RESULTS
C
140   CONTINUE
      IF(LDBUG.GE.6)THEN
       WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
       YMYC  =0.0D0
       SS    =0.0D0
       SSSAS =0.0D0
       DO 150 I=1,N
        YMYC=YMYC+(Y(I)-Z(I))**2
```

```
          SS=SS+(Z(I)-YMEAN)**2
          SSSAS=SSSAS+(Y(I)**2-YMEAN**2)
150      CONTINUE
C
C        CALC R-SQUARE(SAS VERSION) AND ADJ R-SQUARE
C
C         RSQUSAS=1-VARIANCE (FULL MODEL)/VARIANCE (MEAN MODEL)
C
         RSQU=SS/(SS+YMYC)
         RSQUSAS=1.D0-YMYC/(SSSAS)
         IF(DEGFR.EQ.0.0D0)THEN
          ADJRSQU=0.0D0
          ADJRSQUSAS=0.0D0
         ELSE
          ADJRSQU=1.D0-(1.D0-RSQU)*(FLOAT(N)-1.D0)/DEGFR
          ADJRSQUSAS=1.D0-(1.D0-RSQUSAS)*(FLOAT(N)-1.D0)/DEGFR
         ENDIF
         IF(ABS(RSQU-RSQUSAS).GT.1.D6)THEN
          WRITE(NHSTRY,1112)RSQU,ADJRSQU,RSQUSAS,ADJRSQUSAS
         ELSE
          WRITE(NHSTRY,1110)RSQU,ADJRSQU
         ENDIF
C
C        FINAL PARAMETERS
C
        DO 160 J=1,K
         WRITE(NHSTRY,1030)J,B(J)
160     CONTINUE
C
C        FINAL SUMMARY
C
        WRITE(NHSTRY,1040)
        DO 170 I=1,N
         PERERR=ABS(Z(I)-Y(I))/ABS(Y(I))*100.D0
         WRITE(NHSTRY,1095)I,Z(I),Y(I),Z(I)-Y(I),PERERR
170     CONTINUE
       ENDIF
C
C       LOAD DATA INTO MULAND ARRAY
C
       IERR=NDATA(3)
       DO 900 JJ=1,5
         MULAND(JJ,JC)=0.0D0
900    CONTINUE
C
       IF(IERR.EQ.0)THEN
C
C        CONVERGED
C
         MULAND(1,JC)=B(1)
         MULAND(2,JC)=B(2)
         MULAND(3,JC)=B(3)
         MULAND(4,JC)=TRL*TC(JC)
         MULAND(5,JC)=TRH*TC(JC)
C
         IF(LDEBUG.GE.1)WRITE(NHSTRY,1000)IERR,NDATA(3),(OUTPUT(I),I=1,5)
       ELSE IF(IERR.EQ.-1)THEN
         MULAND(1,JC)=B(1)
         MULAND(2,JC)=B(2)
         MULAND(3,JC)=B(3)
         MULAND(4,JC)=TRL*TC(JC)
         MULAND(5,JC)=TRH*TC(JC)
         WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
         WRITE(NHSTRY,1004)
       ELSE IF(IERR.EQ.-2)THEN
         MULAND(1,JC)=B(1)
         MULAND(2,JC)=B(2)
         MULAND(3,JC)=B(3)
```

```
        MULAND(4,JC)=TRL*TC(JC)
        MULAND(5,JC)=TRH*TC(JC)
        WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
        WRITE(NHSTRY,1002)
       ELSE IF(IERR.EQ.-3)THEN
        WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
        WRITE(NHSTRY,1003)
       ELSE IF(IERR.EQ.-4)THEN
        MULAND(1,JC)=B(1)
        MULAND(2,JC)=B(2)
        MULAND(3,JC)=B(3)
        MULAND(4,JC)=TRL*TC(JC)
        MULAND(5,JC)=TRH*TC(JC)
        WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
        WRITE(NHSTRY,1004)
       ELSE IF(IERR.EQ.-5)THEN
        WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
        WRITE(NHSTRY,1005)
       ELSE IF(IERR.EQ.-6)THEN
        WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
        WRITE(NHSTRY,1006)
       ELSE IF(IERR.EQ.-7)THEN
        WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
        WRITE(NHSTRY,1007)
       ENDIF
       MULREG(1,JC)=FLOAT(ITER)
       MULREG(2,JC)=FLOAT(NDATA(3))
       MULREG(3,JC)=OUTPUT(1)
C
C         FORMATS
C
1000   FORMAT(/,1X,'IN MODULE ANDRA',/,
      1     1X,'ITERATION:  ',I9,/,
      2     1X,'IERR                                          = ',I15,/,
      3     1X,'SUM OF SQUARES                                = ',G15.8,/,
      4     1X,'ANGLE (DEGREES)                               = ',F15.2,/,
      5     1X,'NUMBER OF TIMES YSOLVE CALLED                 = ',F15.1,/,
      6     1X,'NUMBER OF FUNCTIONAL EVALUATIONS              = ',F15.1,/,
      7     1X,'NUMBER OF ANALYTICAL DERIVATIVE EVALUATIONS   = ',F15.1,/)
1001   FORMAT(1X,'NO IMPROVEMENT POSSIBLE IN THE VALUE OF',/,
      1        1X,'PH EVEN THOUGH CONVERGENCE HAS NOT BEEN REACHED.',/)
1002   FORMAT(1X,'MORE UNKNOWNS THAN FUNCTIONS AND UNIQUE',/)
1003   FORMAT(1X,'TOTAL NUMBER OF VARIABLES TO BE VARIED = 0',/)
1004   FORMAT(1X,'CONVERGENCE CRITERION MET BUT FLA STILL LARGE',/)
1005   FORMAT(1X,'IC NOT A VALID NUMBER ON ENTRY',/)
1006   FORMAT(1X,'X(I) IS NOT WITHIN XMIN(I) TO XMAX(I)',/)
1007   FORMAT(1X,'ZERO DIAGONAL ELEMENT IN EQUATION SOLVE',/)
1008   FORMAT(//,5X,'*****MARQUARDT METHOD REGRESSION*****',//,
      1 5X,'K (NUMBER OF PARAMETERS TO BE VARIED) = ',I4,  ,
      2 5X,'N (NUMBER OF DATA POINTS)             = ',I4,  ,
      3 5X,'INITAL B            B-MIN            B-MAX',
      4'VARY FLAG',  )
1009   FORMAT(2X,4(G15.5,1X))
1010   FORMAT(5X,'VARY FLAG:',/,
      1 10X,'0 = HOLD PARAMETER CONSTANT',,
      2 10X,'1 = VARY PARAMETER USING NUMERICAL DERIVATIVE',,
      3 9X,'-1 = VARY PARAMETER USING ANALYTICAL DERIVATIVE')
1020   FORMAT(1X,3G15.8)
1030   FORMAT(1X,'B(',I2,') = ',G13.5)
1040   FORMAT(/,1X,'OBS.   Y-CALC          Y-ACTUAL        DIFF.          ',
      1 '% ERROR',/)
1095   FORMAT(  1X,I4,  4(1X,G13.5))
1100   FORMAT(/,10X,'INPUT DATA',//,
      1 5X,'X-VALUE          Y-VALUE ',/,
      2 5X,'-------          ------- ',/)
1110   FORMAT(
      1 1X,'R-SQUARE                                        = ',F15.8,/,
      2 1X,'ADJ R-SQUARE                                    = ',F15.8,/)
```

```
1112  FORMAT(
     1 1X,'R-SQUARE                                          = ',F15.8,/,
     2 1X,'ADJ R-SQUARE                                      = ',F15.8,/,
     3 1X,'R-SQUARE(I-VAR.FM/VAR.MM)                         = ',F15.8,/,
     4 1X,'ADJ R-SQUARE(FOR 2ND R-SQUARE)                    = ',F15.8,/)
1120  FORMAT(//,10X,'STATISTICS',//,
     1 5X,'X-VALUES ',26X,'Y-VALUES',/,
     2 5X,'----------',26X,'----------',/,
     3 5X,'MEAN       = ',G15.5,8X,'MEAN       = ',G15.5,/
     4 5X,'VARIANCE   = ',G15.5,8X,'VARIANCE   = ',G15.5,/
     5 5X,'STD. DEV.  = ',G15.5,8X,'STD. DEV.  = ',G15.5,/)
1045  FORMAT(/,1X,'IN ANDRA',/,
     1 1X,'******RUN EXCEEDED MAXIT OF ',I5,' ITER = ',I5,'******'//)
1090  FORMAT(1X,'IN MODULE ANDRA IERR = ',I5,' TRY TO CALC '
     1       ' DERIVATIVE ANALYTICALY, CALC. ABORTED')
9000  CONTINUE
      RETURN
      END
C*************************************************************************
C
      SUBROUTINE ASTMCF(VABP,SASTM,CABP,MABP,IERR)
C
C*************************************************************************
C
C       NAME OF MODULE - ASTMCF
C       MODULE TITLE - PROCEDURE 2B1.1 API DATA BOOK P2-11,12 (1980)
C       PURPOSE - METHOD FOR CHARACTERIZE PETROLEUM FRACTION BOILING
C                 POINTS OF ASTM D86
C       MODIFIED - 1-6-88
C
C       LIMITATIONS:
C          ASTM SLOPE       0-9.0
C          CABP           200-800
C
C       VARIABLES USED-
C
C VARIABLE I/O TYPE-SPEC DIMENSION      DESCRIPTION AND RANGE
C    VABP     I       R          -      VOLUME AVERAGE BOILING POINT (DEG F)
C   SASTM     I       R          -      ASTM D86 10% TO 90% SLOPE
C                                       (DEG F/%OFF)
C    CABP     O       R                 CUBIC AVERAGE BOILING POINT (DEG F)
C    MABP     O       R          -      MOLAL AVERAGE BOILING POINT (DEG F)
C    IERR     O       I          -      ERROR CODE
C                                        0 = OK
C                                       -1 = ASTM NOT IN RANGE ABOVE
C                                       -2 = CABP NOT IN RANGE ABOVE
C
      IMPLICIT REAL*8 (A-H,O-Z)
      IMPLICIT INTEGER(I-N)
C
      REAL*8           MABP,MABPC
C
      COMMON /IO     / NIN,NOUT,NHSTRY,NRSLT
      COMMON /DEBUG  / LDBUG,LDBUGR
C
      DIMENSION CC(6),CW(6),CM(6)
C
      IERR=0
C
      IF(LDBUG.GT.7)WRITE(NHSTRY,900)
C
C       CHECK IF IN RANGE
C
      IF(SASTM.LT.0.D0.OR.SASTM.GT.9.0)THEN
        IERR=-1
        CALL MESS(1)
        WRITE(NHSTRY,900)
        WRITE(NHSTRY,1000)SASTM
```

```
      ENDIF
C
      IF(VABP.LT.200.D0.OR.VABP.GT.800.D0)THEN
        IERR=-2
        CALL MESS(1)
        WRITE(NHSTRY,900)
        WRITE(NHSTRY,2000)VABP
      ENDIF
C
C       CUBIC AVERAGE BOILING PT (F)
C
      IF(SASTM.GT.0.D0)THEN
       CC(1)=-0.90618D0
       CC(2)=-2.9959D0
       CC(3)=0.47688D-2
       CC(4)=0.24128D-2
       CC(5)=-0.15742D0
       CC(6)=-0.49144D-5
       CC(7)=0.16337D-6
       CC(8)=-0.24640D-1
C
       CABPC=CC(1)
     1       + CC(2)*SASTM     + CC(3)*VABP     + CC(4)*SASTM     * VABP
     2       + CC(5)*SASTM**2 + CC(6)*VABP**2 + CC(7)*SASTM**2 * VABP**2
     3       + CC(8)*SASTM**3
       CABP=VABP+CABPC
      ELSE
       CABP=VABP
      ENDIF
C
C   MOLAL AVERAGE BOILING POINT (F)
C
      IF(SASTM.GT.0.D0)THEN
       CM(1)=-0.88301D0
       CM(2)=-9.3967D0
       CM(3)=0.46643D-2
       CM(4)=0.41984D-2
       CM(5)=-0.59240D0
       CM(6)=-0.47915D-5
       CM(7)=0.68208D-6
       CM(8)=-0.15537D0
C
       MABPC=CM(1)
     1       + CM(2)*SASTM     + CM(3)*VABP     + CM(4)*SASTM     * VABP
     2       + CM(5)*SASTM**2 + CM(6)*VABP**2 + CM(7)*SASTM**2 * VABP**2
     3       + CM(8)*SASTM**3
       MABP=VABP+MABPC
      ELSE
       MABP=VABP
      ENDIF
C
C   WEIGHT AVERAGE BOILING POINT (F)
C
      IF(SASTM.GT.0.D0)THEN
       CW(1)=0.24102D0
       CW(2)=2.8301D0
       CW(3)=-0.13291D-2
       CW(4)=-0.24737D-2
       CW(5)=0.42851D-1
       CW(6)=0.14071D-5
       CW(7)=-0.63621D-7
       CW(8)=0.22497D-1
C
       WABPC=CW(1)
     1       + CW(2)*SASTM     + CW(3)*VABP     + CW(4)*SASTM     * VABP
     2       + CW(5)*SASTM**2 + CW(6)*VABP**2 + CW(7)*SASTM**2 * VABP**2
     3       + CW(8)*SASTM**3
       WABP=VABP+WABPC
```

```
      ELSE
       WABP=VABP
      ENDIF
C
C       FORMATS
C
900   FORMAT(1X,'IN MODULE ASTMCF')
1000  FORMAT(1X,'ASTM SLOPE VALUE IS NOT IN RANGE 0-9.0',/,
     1       1X,'ASTM SLOPE-VALUE = ',G12.6,' CALC. CONTINUES')
2000  FORMAT(1X,'VABP VALUE IS NOT IN RANGE 200-800',/,
     1       1X,'VABP-VALUE = ',G12.6,' CALC. CONTINUES')
C
      RETURN
C
      END
C*****************************************************************
C
      SUBROUTINE CAPS(INCASE,UPCASE)
C
C*****************************************************************
C
C       NAME OF MODULE - CAPS
C       MODULE TITLE - INPUT TRANSLATOR FILTER
C       PURPOSE - TO CONVERT ONE INPUT CHARACTER TO VALID OUTPUT
C                 CHARACTER
C       MODIFIED - 3-29-88
C
C       VARIABLES USED-
C
C VARIABLE I/O TYPE-SPEC DIMENSION      DESCRIPTION AND RANGE
C  INCASE   I       C          -        INPUT CHARACTER
C  UPCASE   O       C          -        OUTPUT CHARACTER
C
C
      CHARACTER*1      INCASE,UPCASE,ABLANK
      PARAMETER        (ABLANK = ' ')
C
C       CONVERT LOWERCASE LETTERS TO UPPERCASE LETTERS
C
      IF(ICHAR(INCASE).GE.97.AND.
     1   ICHAR(INCASE).LE.122)THEN
       UPCASE=CHAR(ICHAR(INCASE)-32)
C
C       CHECK FOR UPPER CASE LETTERS
C
       ELSE IF(ICHAR(INCASE).GE.65.AND.
     1     ICHAR(INCASE).LE.90)THEN
        UPCASE=INCASE
C
C       CHECK FOR NUMBERS
C
      ELSE IF(ICHAR(INCASE).GE.48 .AND.
     1        ICHAR(INCASE).LE.57 )THEN
       UPCASE=INCASE
C
C       CHECK FOR =,+,-,$,.,;
C
      ELSE IF(ICHAR(INCASE).EQ.61 .OR.
     1        ICHAR(INCASE).EQ.43 .OR.
     2        ICHAR(INCASE).EQ.45 .OR.
     3        ICHAR(INCASE).EQ.36 .OR.
     3        ICHAR(INCASE).EQ.46 .OR.
     4        ICHAR(INCASE).EQ.59       )THEN
       UPCASE=INCASE
C
      ELSE
       UPCASE=ABLANK
      ENDIF
```

```
      RETURN
      END
C*********************************************************************
C
      SUBROUTINE CAVENT(JC,IERR)
C
C*********************************************************************
C
C       NAME OF MODULE - CAVENT
C       MODULE TITLE - CAVETT EQUATION FOR ENTHALPY
C       PURPOSE - TO SUPPLY DEFAULT VALUE FOR CAVETT ENTHALPY PARAMETER
C       MODIFIED - 10-5-88
C       METHOD - DEFAULT VALUE
C
C
C       VARIABLES USED-
C
C VARIABLE I/O TYPE-SPEC DIMENSION      DESCRIPTION AND RANGE
C      JC    I       I         -        COMPONENT ARRAY ID
C    IERR    O       I         -        ERROR CODE
C                                       0 = OK
C
      IMPLICIT REAL*8 (A-H,O-Z)
      IMPLICIT INTEGER(I-N)
C
      PARAMETER        (MNC=25)
C
      COMMON /IO     / NIN,NOUT,NHSTRY,NREPT
      COMMON /DEBUG  / LDBUG,LDBUGR
C
      COMMON /CPRP04/ ZC(MNC)
      COMMON /CPRP13/ DHLCVT(MNC)
C
      IERR=0
C
C       USES DEFAULT SUGGESTED IN ASPEN
C
      DHLCVT(JC)=ZC(JC)
C
C       FORMATS
C
      RETURN
      END
C*********************************************************************
C
      SUBROUTINE CAVVP(JC,ICALC,IERR)
C
C*********************************************************************
C
C       NAME OF MODULE - CAVVP
C       MODULE TITLE - CAVETT EQUATION FOR VAPOR PRESSURE
C       PURPOSE - TO CALC. CHARACTERISTIC PARAMETERS AND TEMP RANGE
C                 FOR CAVETT EQUATION PURE COMP. LIQ VAPRO PRESSURE
C       MODIFIED - 10-27-88
C       METHOD - MARQUARDT REGRESSION
C
C
C       VARIABLES USED-
C
C VARIABLE I/O TYPE-SPEC DIMENSION      DESCRIPTION AND RANGE
C      JC    I       I         -        COMPONENT ARRAY ID
C   ICALC    I       I         -        CALC TYPE
C                                        0 = FIT 1 CONST
C                                        1 = FIT 2 CONSTS.
C    IERR    O       I         -        ERROR CODE
C                                        0 = OK
C                                       -1 = NO IMPROVEMENT POSSIBLE IN
C                                            THE VALUE OF PH EVEN THOUGH
```

```
C                                          CONVERGENCE HAS NOT BEEN REACHED.
C                                       -2 = MORE UNKNOWNS THAN FUNCTIONS AND
C                                          UNIQUE SOLUTION GENERALLY IS
C                                          IMPOSSIBLE.
C                                       -3 = TOTAL NUMBER OF VARIABLES TO BE
C                                          VARIED IS ZERO
C                                       -4 = CONVERGENCE CRITERION MET BUT FLA
C                                          STILL LARGE
C                                       -5 = IC NOT A VALID NUMBER ON ENTRY
C                                       -6 = X(I) IS NOT WITHIN XMIN(I) TO
C                                          XMAX(I)
C                                       -7 = ZERO DIAGONAL ELEMENT IN EQUATION
C                                          SOLVE
C                                       -10 = TRY TO CALC. DERIVATIVE
C                                            ANALYTICALY
C                                       -11 = RUN EXCEEDED MAXIT SPECIFIED
C
C
      IMPLICIT REAL*8 (A-H,O-Z)
      IMPLICIT INTEGER(I-N)
C
      PARAMETER        (MNC=25)
C
      COMMON /IO     / NIN,NOUT,NHSTRY,NREPT
      COMMON /DEBUG  / LDBUG,LDBUGR
C
      COMMON /CPRP01/ TC(MNC)
      COMMON /CPRP02/ PC(MNC)
      COMMON /CPRP05/ OMEGA(MNC)
      COMMON /CPRP06/ PLXANT(9,MNC),PLXREG(3,MNC)
      COMMON /CPRP21/ PLCAVT(4,MNC),PLCREG(3,MNC)
C
      DIMENSION        NDATA(26),DATA(16),OUTPUT(6)
C
      DIMENSION        X(50),XV(50),XMAX(50),XMIN(50),Y(50),
     1                 Z(100),PJ(50),P(206),A(15),AC(15)
      DIMENSION        B(4),BV(2),BMAX(2),BMIN(2)
C
      DIMENSION        AS(14)
C
      DATA AS        /  8.6956145D0,  -4.3610863D0,    2.3312886D0,
     1                 -0.3744596 4D0,  0.41089072D0,  -0.065391702D0,
     2                  0.3319399 4D0, -0.080981301D0, -9.7687809D0,
     3                 -1.5850550D0,  -6.9238773D0,    -1.1705661D0,
     4                  4.7820604D0,  -4.6670294D0 /
C
      IERR=0
C
      IF(LDBUG.GT.0)WRITE(NHSTRY,900)
C
C       MARQUARDT SET DEFAULTS
C
C       NUMBER OF UNKNOWNS
      K=2
C       NUMBER OF DATA POINTS
      N=50
C
      IF(LDBUG.GE.5)THEN
       DEGFR=FLOAT(N-K)
      ENDIF
C
      ITER = 0
      IF(MAXIT.LE.0)MAXIT=10000
C
C       SET EQUAL TO 1 FOR INITAL CALL
      NDATA(1)=1
C
C       SET INPUT PARAMETER DATA
```

```
C                     DATA(1) - FNU, FACTOR USED TO CHANGE FLA.  SET INTER-
C                               NALLY TO 10.0  IF ZERO ON INITIAL CALL.
C                     DATA(2) - FLA, FACTOR USED TO COMBINE GRADIENT AND
C                               NEWTON-RAPHSON METHODS.  SET INTERNALLY TO
C                               .01 IF ZERO ON INITIAL CALL.
C                     DATA(3) - TAU, USED IN CONVERGENCE TEST.  SET INTER-
C                               NALLY TO 0.001 IF ZERO ON INITIAL CALL.
C                     DATA(4) - EPS, USED IN CONVERGENCE TEST.  SET INTER-
C                               NALLY TO 0.00002 IF ZERO ON INITIAL CALL.
C                     DATA(5) - PHMIN, WHEN PH .LT. PHMIN, PARTIAL DERIV-
C                               ITIVES FROM THE PREVIOUS ITERATION ARE USED
C                               INSTEAD OF COMPUTING THEM AGAIN.
C                     DATA(6) THRU DATA(16) - VARIABLES USED INTERNALLY
C
      DO 10 I=1,5
       DATA(I)=0.0D0
10    CONTINUE
C
C      BV = VARY VECTOR (0=HOLD PARAMTER CONST,1=ALLOW TO VARY)
C
      IF(ICALC.EQ.0)THEN
       BV(1)=0.0D0
       BV(2)=1.0D0
      ELSE
       DO 20 I=1,K
        BV(I)=1.0D0
20     CONTINUE
      ENDIF
C
C      INITAL VALUES OF PARMS
C
      B(1)=OMEGA(JC)/0.14123357D0
      B(2)=0.D0
C
C      MIN AND MAX VALUES
C
      BMAX(1)=2000.D0
      BMIN(1)=-2000.D0
      BMAX(2)=200000.D0
      BMIN(2)=-900000.D0
C
      IF(LDBUG.GE.7)THEN
       WRITE(NHSTRY,1008)K,N
       DO 30 I=1,K
        WRITE(NHSTRY,1009)B(I),BMIN(I),BMAX(I),BV(I)
30     CONTINUE
       WRITE(NHSTRY,1010)
       WRITE(NHSTRY,1100)
       XSUM=0.0D0
       XSUM2=0.0D0
       YSUM=0.0D0
       YSUM2=0.0D0
      ENDIF
C
C      BEGIN CALC (CALC 50 POINTS TO BE FIT)
C       CAVETT EQUATION
C
C      CALC 50 DATA POINTS BY EXTENDED ANTOINE EQUATION
C
      TD=(PLXANT(9,JC)-PLXANT(8,JC))/50.D0
      TT=PLXANT(8,JC)-TD
C
      DO 40 I=1,50
       TT=TT+TD
       X(I)=TT
       Y(I)=PLXANT(1,JC) +
     1       PLXANT(2,JC)/(TT+PLXANT(3,JC))
C    2       +  PLXANT(4,JC)*TT
```

```
C     3      +   PLXANT(5,JC)*LOG(TT)
C     4      +   PLXANT(6,JC)*TT**PLXANT(7,JC)
C
       IF(LDBUG.GE.7)THEN
        WRITE(NHSTRY,1020)X(I),Y(I)
        XSUM=XSUM+X(I)
        XSUM2=XSUM2+X(I)**2
        YSUM=YSUM+Y(I)
        YSUM2=YSUM2+Y(I)**2
       ENDIF
40     CONTINUE
C
C       MEANS, VARIANCES AND STANDARD DEV.
C
       IF(LDBUG.GE.7)THEN
        XMEAN=XSUM/FLOAT(N)
        XVAR=(FLOAT(N)*XSUM2-XSUM*XSUM)/FLOAT(N)/FLOAT(N-1)
        XSD=SQRT(XVAR)
        YMEAN=YSUM/FLOAT(N)
        YVAR=(FLOAT(N)*YSUM2-YSUM*YSUM)/FLOAT(N)/FLOAT(N-1)
        YSD=SQRT(YVAR)
        WRITE(NHSTRY,1120)XMEAN,YMEAN,XVAR,YVAR,XSD,YSD
       ENDIF
C
C       BEGIN REGRESSION
C
50     ITER=ITER+1
       IF(ITER.GT.MAXIT)THEN
        IERR=-11
        WRITE(NHSTRY,1045)MAXIT,ITER
        GOTO 9000
       ENDIF
C
C         EVALUATE Z VECTOR (FUNCTION VALUE)
C
C      REGRESS TO MODIFIED CAVETT EQUATION
C
       DO 60 I=1,N
        TR=X(I)/TC(JC)
        RTR=1.D0/TR
        IF(TR.LT.0.4D0)THEN
         Z(I)=AS(9) + (B(1)-1.D0)*AS(10)
     1               + (RTR-2.5D0)*(AS(11)+(B(1)-1.D0)*AS(12)
     2               + B(2)*(AS(13)+AS(14)*TR)*(TR-0.7D0)*(TR-1.D0))
     3               + LOG(PC(JC))
        ELSE IF(TR.GE.0.4D0)THEN
         Z(I)=(1.D0-1.D0/TR) * (AS(1)+AS(2)/TR+AS(3)/TR/TR
     1        +AS(4)/TR/TR/TR + (B(1)-1.D0)*(AS(5)+AS(6)/TR
     2        +AS(7)/TR/TR+AS(8)/TR/TR/TR))
     3               + B(2)*(AS(13)+AS(14)*TR)*(TR-0.7D0)*(TR-1.D0)
     4               + LOG(PC(JC))
        ENDIF
60     CONTINUE
C
C      CALC ANALYTICAL DERIVATIVES (PJ VECTOR)
C
70     CONTINUE
C
C         CALC DERIVATIVE
C
       IF(NDATA(2).GT.0)THEN
        IERR=-10
        WRITE(NHSTRY,1090)IERR
        GOTO 9000
       ENDIF
C
C
       IF(LDBUG.GE.7)THEN
```

```
      WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
      YMYC =0.0D0
      SS   =0.0D0
      SSSAS=0.0D0
      DO 90 I=1,N
       YMYC=YMYC+(Y(I)-Z(I))**2
       SS=SS+(Z(I)-YMEAN)**2
       SSSAS=SSSAS+(Y(I)**2 - YMEAN**2)
90    CONTINUE
C
C     CALC R-SQUARE(SAS VERSION) AND ADJ R-SQUARE
C          1-VARIANCE OF FULL MODEL/VARIANCE OF MEAN MODEL
C
      RSQU=SS/(SS+YMYC)
      IF(SSSAS.NE.0.D0)THEN
       RSQUSAS=1.D0-YMYC/(SSSAS)
      ELSE
       RSQUSAS=0.D0
      ENDIF
      IF(DEGFR.EQ.0.D0)THEN
       ADJRSQU=0.0D0
      ELSE
       ADJRSQU=1.D0-(1.D0-RSQU)*(FLOAT(N)-1.D0)/DEGFR
      ENDIF
      IF(ABS(RSQU-RSQUSAS).GT.1.D8)THEN
       WRITE(NHSTRY,1112)RSQU,ADJRSQU,RSQUSAS,ADJRSQUSAS
      ELSE
       WRITE(NHSTRY,1110)RSQU,ADJRSQU
      ENDIF
C
      DO 100 J=1,K
       WRITE(NHSTRY,1030)J,B(J)
100   CONTINUE
C
      IF(LDBUG.EQ.8)THEN
       WRITE(NHSTRY,1040)
       DO 110 I=1,N
        YMYC=YMYC+(Y(I)-Z(I))**2
        SS=SS+(Z(I)-YMEAN)**2
        PERERR=ABS(Z(I)-Y(I))/ABS(Y(I))*100.D0
        WRITE(NHSTRY,1095)I,Z(I),Y(I),Z(I)-Y(I),PERERR
110    CONTINUE
       ENDIF
      ENDIF
C
120   CALL YSOLVE (K, N, NDATA, DATA, B, BV, BMAX, BMIN, Y, Z, PJ,
     1             OUTPUT, P, A, AC)
C
C                     NDATA(2) - NFCTDR, USED FOR CONTROL IN CALLING PROG
C                        IF = 0, CALCULATE FUNCTION
C                        IF = 1, CALCULATE DERIVATIVE
C                        IF =-1, EXAMINE IERR FOR WHAT TO DO NEXT
C
      IF(NDATA(2))130,50,70
C
C                     NDATA(3) - IERR, MAY TAKE ON VARIOUS VALUES
C                        IF POSITIVE, CONTAINS THE NUMBER OF VARIABLES NO
C                                     SATISFYING CONVERGENCE CRITERION
C                        IF =  0, CONVERGENCE SATISFIED AND SOLUTION RETU
C                        IF = -1, NO IMPROVEMENT POSSIBLE IN THE VALUE OF
C                                 PH EVEN THOUGH CONVERGENCE HAS NOT BEEN
C                                 REACHED.
C                        IF = -2, MORE UNKNOWNS THAN FUNCTIONS AND UNIQUE
C                                 SOLUTION GENERALLY IS IMPOSSIBLE.
C                        IF = -3, TOTAL NUMBER OF VARIABLES TO BE VARIED
C                                 IS ZERO
C                        IF = -4, CONVERGENCE CRITERION MET BUT FLA STILL
C                                 LARGE
```

```
C                          IF = -5, IC NOT A VALID NUMBER ON ENTRY
C                          IF = -6, B(I) IS NOT WITHIN BMIN(I) TO BMAX(I)
C                          IF = -7, ZERO DIAGONAL ELEMENT IN EQUATION SOLVE
C
130     IF(NDATA(3))140,140,120
C
C        FINAL STATISTICAL RESULTS
C
140     CONTINUE
        IF(LDBUG.GE.6)THEN
         WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
         YMYC  =0.0D0
         SS    =0.0D0
         SSSAS =0.0D0
         DO 150 I=1,N
          YMYC=YMYC+(Y(I)-Z(I))**2
          SS=SS+(Z(I)-YMEAN)**2
          SSSAS=SSSAS+(Y(I)**2-YMEAN**2)
150      CONTINUE
C
C        CALC R-SQUARE(SAS VERSION) AND ADJ R-SQUARE
C
C         RSQUSAS=1-VARIANCE (FULL MODEL)/VARIANCE (MEAN MODEL)
C
         RSQU=SS/(SS+YMYC)
         RSQUSAS=1.D0-YMYC/(SSSAS)
         IF(DEGFR.EQ.0.0D0)THEN
          ADJRSQU=0.0D0
          ADJRSQUSAS=0.0D0
         ELSE
          ADJRSQU=1.D0-(1.D0-RSQU)*(FLOAT(N)-1.D0)/DEGFR
          ADJRSQUSAS=1.D0-(1.D0-RSQUSAS)*(FLOAT(N)-1.D0)/DEGFR
         ENDIF
         IF(ABS(RSQU-RSQUSAS).GT.1.D8)THEN
          WRITE(NHSTRY,1112)RSQU,ADJRSQU,RSQUSAS,ADJRSQUSAS
         ELSE
          WRITE(NHSTRY,1110)RSQU,ADJRSQU
         ENDIF
C
C        FINAL PARAMETERS
C
        DO 160 J=1,K
         WRITE(NHSTRY,1030)J,B(J)
160     CONTINUE
C
C        FINAL SUMMARY
C
        WRITE(NHSTRY,1040)
        DO 170 I=1,N
         PERERR=ABS(Z(I)-Y(I))/ABS(Y(I))*100.D0
         WRITE(NHSTRY,1095)I,Z(I),Y(I),Z(I)-Y(I),PERERR
170     CONTINUE
       ENDIF
C
C        LOAD DATA INTO PLCAVT ARRAY
C
       IERR=NDATA(3)
       DO 800 JJ=1,4
         PLCAVT(JJ,JC)=0.0D0
800    CONTINUE
C
       IF(IERR.EQ.0)THEN
C
C        CONVERGED
C
         PLCAVT(1,JC)=B(1)
         PLCAVT(2,JC)=B(2)
         PLCAVT(3,JC)=PLXANT(8,JC)
```

```
        PLCAVT(4,JC)=PLXANT(9,JC)
C
        IF(LDBUG.GE.1)WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
       ELSE IF(IERR.EQ.-1)THEN
        PLCAVT(1,JC)=B(1)
        PLCAVT(2,JC)=B(2)
        PLCAVT(3,JC)=PLXANT(8,JC)
        PLCAVT(4,JC)=PLXANT(9,JC)
        WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
        WRITE(NHSTRY,1001)
       ELSE IF(IERR.EQ.-2)THEN
        PLCAVT(1,JC)=B(1)
        PLCAVT(2,JC)=B(2)
        PLCAVT(3,JC)=PLXANT(8,JC)
        PLCAVT(4,JC)=PLXANT(9,JC)
        WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
        WRITE(NHSTRY,1002)
       ELSE IF(IERR.EQ.-3)THEN
        WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
        WRITE(NHSTRY,1003)
       ELSE IF(IERR.EQ.-4)THEN
        PLCAVT(1,JC)=B(1)
        PLCAVT(2,JC)=B(2)
        PLCAVT(3,JC)=PLXANT(8,JC)
        PLCAVT(4,JC)=PLXANT(9,JC)
        WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
        WRITE(NHSTRY,1004)
       ELSE IF(IERR.EQ.-5)THEN
        WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
        WRITE(NHSTRY,1005)
       ELSE IF(IERR.EQ.-6)THEN
        WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
        WRITE(NHSTRY,1006)
       ELSE IF(IERR.EQ.-7)THEN
        WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
        WRITE(NHSTRY,1007)
       ENDIF
       PLCREG(1,JC)=FLOAT(ITER)
       PLCREG(2,JC)=FLOAT(NDATA(3))
       PLCREG(3,JC)=OUTPUT(1)
C
C       CHECK AGAINST FLOWTRAN ESTIMATES
C
       IF(ABS(PLCAVT(1,JC)-OMEGA(JC)/0.14123357D0).GT.0.1D0)THEN
        CALL MESS(1)
        WRITE(NHSTRY,900)
        WRITE(NHSTRY,1130)PLCAVT(1,JC),OMEGA(JC)/0.14123357D0
       ENDIF
       IF(PLCAVT(2,JC).GT.0.2D0.OR.PLCAVT(2,JC).LT.-0.2D0)THEN
        CALL MESS(1)
        WRITE(NHSTRY,900)
        WRITE(NHSTRY,1140)PLCAVT(2,JC)
       ENDIF
C
C       FORMATS
C
900    FORMAT(1X,'IN MODULE CAVVP')
1000   FORMAT(/,
     1     1X,'ITERATION: ',I9,/,
     2     1X,'IERR                                          = ',I15,/,
     3     1X,'SUM OF SQUARES                                = ',G15.8,/,
     4     1X,'ANGLE (DEGREES)                               = ',F15.2,/,
     5     1X,'NUMBER OF TIMES YSOLVE CALLED                 = ',F15.1,/,
     6     1X,'NUMBER OF FUNCTIONAL EVALUATIONS              = ',F15.1,/,
     7     1X,'NUMBER OF ANALYTICAL DERIVATIVE EVALUATIONS   = ',F15.1,/)
1001   FORMAT(1X,'NO IMPROVEMENT POSSIBLE IN THE VALUE OF',/,
     1       1X,'PH EVEN THOUGH CONVERGENCE HAS NOT BEEN REACHED.',/)
1002   FORMAT(1X,'MORE UNKNOWNS THAN FUNCTIONS AND UNIQUE',/)
```

```
1003  FORMAT(1X,'TOTAL NUMBER OF VARIABLES TO BE VARIED = 0',/)
1004  FORMAT(1X,'CONVERGENCE CRITERION MET BUT FLA STILL LARGE',/)
1005  FORMAT(1X,'IC NOT A VALID NUMBER ON ENTRY',/)
1006  FORMAT(1X,'X(I) IS NOT WITHIN XMIN(I) TO XMAX(I)',/)
1007  FORMAT(1X,'ZERO DIAGONAL ELEMENT IN EQUATION SOLVE',/)
1008  FORMAT(1H1,/,5X,'*****MARQUARDT METHOD REGRESSION*****',//,
     1 5X,'K (NUMBER OF PARAMETERS TO BE VARIED) = ',I4,/,
     2 5X,'N (NUMBER OF DATA POINTS)             = ',I4,//,
     3 5X,'INITAL B            B-MIN            B-MAX',
     4'VARY FLAG',/)
1009  FORMAT(2X,4(G15.5,1X))
1010  FORMAT(5X,'VARY FLAG:',/,
     1 10X,'0 = HOLD PARAMETER CONSTANT',/,
     2 10X,'1 = VARY PARAMETER USING NUMERICAL DERIVATIVE',/,
     3 9X,'-1 = VARY PARAMETER USING ANALYTICAL DERIVATIVE')
1020  FORMAT(1X,3G15.6)
1030  FORMAT(1X,'B(',I2,') = ',G13.5)
1040  FORMAT(/,1X,'OBS.  Y-CALC         Y-ACTUAL        DIFF.          ',
     1 '% ERROR',/)
1045  FORMAT(/,1X,'IN ANDRA',/,
     1             1X,'*****RUN EXCEEDED MAXIT OF ',I5,' ITER = ',I5,
     2             '******'//)
1090  FORMAT(1X,'IN MODULE ANDRA IERR = ',I5,' TRY TO CALC.',
     1       ' DERIVATIVE ANALYTICALY, CALC. ABORTED')
1095  FORMAT(  1X,I4,  4(1X,G13.5))
1100  FORMAT(/,10X,'INPUT DATA',//,
     1 5X,'X-VALUE         Y-VALUE ',/,
     2 5X,'-------         ------- ',/)
1110  FORMAT(
     1 1X,'R-SQUARE                                          = ',F15.8,/,
     2 1X,'ADJ R-SQUARE                                      = ',F15.8,/)
1112  FORMAT(
     1 1X,'R-SQUARE                                          = ',F15.8,/,
     2 1X,'ADJ R-SQUARE                                      = ',F15.8,/,
     3 1X,'R-SQUARE(1-VAR.FM/VAR.MM)                         = ',F15.8,/,
     4 1X,'ADJ R-SQUARE(FOR 2ND R-SQUARE)                    = ',F15.8,/)
1120  FORMAT(//,10X,'STATISTICS',//,
     1 5X,'X-VALUES ',26X,'Y-VALUES',/,
     2 5X,'----------',26X,'---------',/,
     3 5X,'MEAN       = ',G15.5,8X,'MEAN       = ',G15.5,/
     4 5X,'VARIANCE   = ',G15.5,8X,'VARIANCE   = ',G15.5,/
     5 5X,'STD. DEV.  = ',G15.5,8X,'STD. DEV.  = ',G15.5,/)
1130  FORMAT(1X,'1ST VALUE FOR PLCAVT = ',G13.6,
     1          ' NOT CLOSE TO OMEGA/0.14123357 = ',G13.6,/,
     2       1X,'CALC CONTINUES')
1140  FORMAT(1X,'2ND VALUE FOR PLCAVT = ',F13.6,
     1          ' NOT IN BEST RANGE (-0.2 TO 0.2)',/,
     2       1X,'CALC CONTINUES')
C
9000  CONTINUE
      RETURN
      END
C*************************************************************************
C
      SUBROUTINE CHKSOP(IERR)
C
C*************************************************************************
C
C       NAME OF MODULE - CHKSOP
C       MODULE TITLE - CHECK SYSOP NUMBER AND SET CALC VECTOR
C       PURPOSE - TO SET UP NPCVEC VECTOR OF SIZE 22 WHICH SPECIFIES
C                 WHAT PROPERTIES MUST BE CALCULATED FOR EACH SYSOP
C                 IN SUBROUTINE PROPS(IF NPCVEC=1 CALC PROP)
C       MODIFIED - 11-16-88
C
C       VARIABLES USED-
C
C VARIABLE I/O TYPE-SPEC DIMENSION     DESCRIPTION AND RANGE
```

```
C    IERR     O       I          -           ERROR FLAG
C                                             0 = OK
C                                            -1 = INVALID SYSOP
C
      IMPLICIT REAL*8 (A-H,O-Z)
      IMPLICIT INTEGER(I-N)
C
      PARAMETER        (MNC=25)
C
      COMMON /IO     / NIN,NOUT,NHSTRY,NREPT
      COMMON /DEBUG  / LDBUG,LDBUGR
C
      COMMON /SYS2   / NSYSOP,NPCVEC(22)
C
C      DEFAULT PROPERTY CALC BASED ON SYSOP0
C
      DIMENSION NPDEF(22)
C
C        CALC ORDER
C
C            1          2          3          4          5
C         TC       , PC       ,VC        , ZC       , OMEGA    ,
C            6          7          8          9          10
C         PLXANT   , CPIG     , DHFORM   , DGFORM   , DHLCVT   ,
C           11         12         13         14         15
C         TB       , VB       , DHVLWT   , RKTZRA   , DHVLB    ,
C           16         17         18         19         20
C         TFP      , DELTA    , MUP      , MULAND   , RGYR     ,
C           21         22
C         PLCAVT   , VLCVT1
C
      DATA     NPDEF /
     1        1    ,     1    ,     1    ,     1    ,     1    ,
     2        1    ,     1    ,     1    ,     1    ,     0    ,
     3        1    ,     1    ,     1    ,     1    ,     0    ,
     4        0    ,     0    ,     1    ,     1    ,     0    ,
     5        0    ,     0    /
C
      IF(LDBUG.GT.7)WRITE(NHSTRY,900)
C
      IERR=0
C
C      PROPERTIES WHICH ARE CONSIDERED EXTRA PROPERTIES:
C         ARRAY ELEMENT     1       2       3       4       5       6     7
C                         TFP,DELTA,DHVLB,PLCAVT,DHLCVT,VLCVT1,RGYR
C
C      FOR SYSOP0 ,SYSOP3 ,SYSOP4,SYSOP5,SYSOP8,SYSOP9,SYSOP10,SYSOP11,
C          SYSOP12,SYSOP14 DO NOT CALC ALL 7 EXTRA PROPS
C      FOR SYSOP1,SYSOP2 DO NOT CALC NUMBERS 1,2,4,7
C
C     LOAD NPCVEC VECTOR WITH DEFAULT VALUES (SYSOP0)
C
      DO 10 KS=1,22
       NPCVEC(KS)=NPDEF(KS)
10    CONTINUE
C
C      CHANGE DEFAULT VALUES FOR SYSOP1 AND SYSOP2
C
      IF(NSYSOP.EQ.1.OR.NSYSOP.EQ.2)THEN
       NPCVEC(10)=1
       NPCVEC(17)=1
       NPCVEC(22)=1
      ELSE IF(NSYSOP.EQ. 6.OR.NSYSOP.EQ. 7.OR.
     1        NSYSOP.EQ.13.OR.NSYSOP.GT.14)THEN
C
C        NONEXISTANT SYSOPS
C
       IERR=-1
```

```
        CALL MESS(2)
        WRITE(NHSTRY,900)
        WRITE(NHSTRY,1000)NSYSOP
        NSYSOP=0
       ELSE IF(NSYSOP.LT.0)THEN
C
C         TO FORCE CALC OF ALL PROPS
C
        NPCVEC(10)=1
        NPCVEC(15)=1
        NPCVEC(16)=1
        NPCVEC(17)=1
        NPCVEC(20)=1
        NPCVEC(21)=1
        NPCVEC(22)=1
       ENDIF
C
C         FORMATS
C
900    FORMAT(1X,'IN MODULE CHKSOP')
1000   FORMAT(1X,'ASPEN SYSOP SELECTED IS INVALID: ',I2,/,
     1         1X,'SYSOP IS SET TO SYSOP0')
C
       RETURN
C
       END
C*****************************************************************************
C
       SUBROUTINE CONV(IFLAG,RECORD,IS,IE,RVAL,IVAL,IERR)
C
C*****************************************************************************
C
C         NAME OF MODULE - CONV
C         MODULE TITLE - EXTRACT NUMBER FROM STRING
C         PURPOSE - TO EXTRACT NUMBER TOKEN VALUE FROM INPUT RECORD
C         MODIFIED - 10-11-88
C
C         VARIABLES USED-
C
C VARIABLE I/O TYPE-SPEC DIMENSION      DESCRIPTION AND RANGE
C   IFLAG     I       I          -      INTEGER/REAL FLAG 0 = INTEGER 1=REAL
C RECORD    I/O       C          -      INPUT RECORD
C      IS     I       I          -      START BYTE OF TOKEN
C      IE     I       I          -      END BYTE OF TOKEN
C    RVAL     O       R          -      OUTPUT REAL NUMBER
C    IVAL     O       I          -      OUTPUT INTEGER NUMBER
C    IERR     O       I          -      ERROR CODE
C                                       0=OK
C                                       1=ERROR ON CONVERT TO REAL
C                                       2=ERROR ON CONVERT TO INTEGER
C
       IMPLICIT REAL*8 (A-H,O-Z)
       IMPLICIT INTEGER(I-N)
C
       CHARACTER*80 RECORD
C
       COMMON /IO     / NIN,NOUT,NHSTRY,NREPT
C
       IERR=0
C
       IDEL=IE-IS+1
       IF(IFLAG.EQ.0)THEN
         DECODE(IDEL,1000,RECORD(IS:IE),ERR=10)IVAL
       ELSE
         DECODE(IDEL,2000,RECORD(IS:IE),ERR=20)RVAL
       ENDIF
       GOTO 9990
C
```

```
10     WRITE(NHSTRY,900)
       CALL MESS(3)
       WRITE(NHSTRY,3000)RECORD(IS:IE)
       IERR=2
       GOTO 9990
C
20     WRITE(NHSTRY,900)
       CALL MESS(3)
       WRITE(NHSTRY,4000)RECORD(IS:IE)
       IERR=1
       GOTO 9990
C
C       FORMATS
C
900    FORMAT(1X,'IN MODULE CONV')
1000   FORMAT(I<IDEL+1>)
2000   FORMAT(F<IDEL+1>.0)
3000   FORMAT(1X,'ERROR ON CONVERT TO INTEGER FROM',/,A)
4000   FORMAT(1X,'ERROR ON CONVERT TO REAL FROM',/,A)
C
9990   RETURN
       END
C*******************************************************************************
C
       SUBROUTINE DGFRM(TB,XP,XN,XA,DGF,IERR)
C
C*******************************************************************************
C
C         NAME OF MODULE - DGFRM
C         MODULE TITLE - ESTIMATION OF GIBBS ENERGY OF FORMATION
C         PURPOSE - EST OF GIBSS ENERGY OF FORMATION (J/KMOL)
C         MODIFIED - 11-23-88
C         METHOD - REGRESSION OF ASPEN DATA BANK FOR PARAFFINS,NAPTHENES,
C                  AND AROMATICS
C
C         VARIABLES USED-
C
C VARIABLE I/O TYPE-SPEC DIMENSION      DESCRIPTION AND RANGE
C      TB     I       R          -      BOILING POINT (DEG K)
C      XP     I       R          -      MOLE FRACTION PARAFFINS
C      XN     I       R          -      MOLE FRACTION NAPTHENES
C      XA     I       R          -      MOLE FRACTION AROMATICS
C      DGF    O       R          -      GIBBS ENERGY OF FORMATION
C     IERR    O       I          -      ERROR CODE
C                                        0 = OK
C                                       -1 = TB OUT OF RANGE FOR PARA.
C                                       -2 = TB OUT OF RANGE FOR NAPT.
C                                       -3 = TB OUT OF RANGE FOR AROM.
C
       IMPLICIT REAL*8 (A-H,O-Z)
       IMPLICIT INTEGER(I-N)
C
       COMMON /IO     / NIN,NOUT,NHSTRY,NBEPT
C
C       CHECK IF TB IS OUT OF RANGE
C
C       PARAFFINS
C
       IF(XP.GT.0.D0)THEN
        IF(TB.LT.301.D0)THEN
         IERR=-1
         CALL MESS(1)
         WRITE(NHSTRY,900)
         WRITE(NHSTRY,1000)TB
         TB=301.D0
        ENDIF
        IF(TB.GT.617.D0)THEN
         IERR=-1
```

```
          CALL MESS(1)
          WRITE(NHSTRY,900)
          WRITE(NHSTRY,1000)TB
          TB=617.D0
          ENDIF
         ENDIF
C
C         NAPTHENES
C
        IF(XN.GT.0.D0)THEN
         IF(TB.LT.322.4D0)THEN
          IERR=-2
          CALL MESS(1)
          WRITE(NHSTRY,900)
          WRITE(NHSTRY,2000)TB
          TB=322.4D0
         ENDIF
         IF(TB.GT.637.D0)THEN
          IERR=-2
          CALL MESS(1)
          WRITE(NHSTRY,900)
          WRITE(NHSTRY,2000)TB
         TB=637.D0
         ENDIF
        ENDIF
C
C         AROMATICS
C
        IF(XA.GT.0.D0)THEN
         IF(TB.LT.353.3D0)THEN
          IERR=-3
          CALL MESS(1)
          WRITE(NHSTRY,900)
          WRITE(NHSTRY,3000)TB
          TB=353.3D0
         ENDIF
         IF(TB.GT.517.8D0)THEN
          IERR=-3
          CALL MESS(1)
          WRITE(NHSTRY,900)
          WRITE(NHSTRY,3000)TB
          TB=517.8D0
         ENDIF
        ENDIF
C
C         DATA REGRESSED FOR PARAFFINS
C
        AP=-302503962.D0
        BP=1693237.21D0
        CP=-3258.30675D0
        DP=2.61935945D0
C
        DGFIP=AP + BP*TB + CP*TB*TB + DP*TB*TB*TB
C
C         DATA REGRESSED FOR NAPTHENES
C
        AN=607352826.D0
        BN=-3824503.65D0
        CN=7933.60038D0
        DN=-4.75792750D0
C
        DGFIN=AN + BN*TB + CN*TB*TB + DN*TB*TB*TB
C
C         DATA REGRESSED FOR AROMATICS
C
        AA=-0.397615347D10
        BA=31010830.9D0
        CA=-77805.3565D0
```

```
      DA=64.8352936D0
C
      DGFIA=AA + BA*TB + CA*TB*TB + DA*TB*TB*TB
C
C       EST. FOR FRACTION
C
      DGF=DGFIP*XP+DGFIN*XN+DGFIA*XA
C
C       FORMATS
C
900   FORMAT(1X,'IN MODULE DGFRM')
1000  FORMAT(1X,'TB(K) VALUE OF ',G13.6,/,
     1       2X,' IS NOT IN PARAFFIN CORRELATION RANGE 301-617',/,
     2       2X,'CORRECTIVE ACTION TAKEN AND CALC. CONTINUES')
2000  FORMAT(1X,'TB(K) VALUE OF ',G13.6,/,
     1       2X,'IS NOT IN NAPTHENE CORRELATION RANGE 322.4-637',/,
     2       2X,'CORRECTIVE ACTION TAKEN AND CALC. CONTINUES')
3000  FORMAT(1X,'TB(K) VALUE OF ',G13.6,/,
     1       2X,'IS NOT IN AROMATIC CORRELATION RANGE 353.3-517.8',/,
     2       2X,'CORRECTIVE ACTION TAKEN AND CALC. CONTINUES')
      RETURN
      END
C*****************************************************************
C
      SUBROUTINE DHFRM(TB,XP,XN,XA,DHF,IERR)
C
C*****************************************************************
C
C       NAME OF MODULE - DHFRM
C       MODULE TITLE - ESTIMATION OF ENTHALPY OF FORMATION
C       PURPOSE - EST OF ENTHALPY OF FORMATION (J/KMOL)
C       MODIFIED - 11-23-88
C       METHOD - REGRESSION OF ASPEN DATA BANK FOR PARAFFINS,NAPTHENES,
C                AND AROMATICS TO FORM: B1 + B2*TB + B3*TB**2 + B4*TB**3
C
C
C       VARIABLES USED-
C
C VARIABLE I/O TYPE-SPEC DIMENSION      DESCRIPTION AND RANGE
C      TB     I       R          -      BOILING POINT (DEG K)
C      XP     I       R          -      MOLE FRACTION PARAFFINS
C      XN     I       R          -      MOLE FRACTION NAPTHENES
C      XA     I       R          -      MOLE FRACTION AROMATICS
C      DHF    O       R          -      ENTHALPY OF FORMATION
C     IERR    O       I          -      ERROR CODE
C                                        0 = OK
C                                       -1 = TB OUT OF RANGE FOR PARA.
C                                       -2 = TB OUT OF RANGE FOR NAPT.
C                                       -3 = TB OUT OF RANGE FOR AROM.
C
      IMPLICIT REAL*8 (A-H,O-Z)
      IMPLICIT INTEGER(I-N)
C
      COMMON /IO     / NIN,NOUT,NHSTRY,NREPT
C
C       CHECK IF TB IS OUT OF RANGE
C
C       PARAFFINS
C
      IF(XP.GT.0.D0)THEN
       IF(TB.LT.301.D0)THEN
        IERR=-1
        CALL MESS(1)
        WRITE(NHSTRY,900)
        WRITE(NHSTRY,1000)TB
        TB=301.D0
       ENDIF
       IF(TB.GT.617.D0)THEN
```

```
          IERR=-1
          CALL MESS(1)
          WRITE(NHSTRY,900)
          WRITE(NHSTRY,1000)TB
          TB=617.D0
          ENDIF
         ENDIF
C
C         NAPTHENES
C
        IF(XN.GT.0.D0)THEN
         IF(TB.LT.322.4D0)THEN
          IERR=-2
          CALL MESS(1)
          WRITE(NHSTRY,900)
          WRITE(NHSTRY,2000)TB
          TB=322.4D0
         ENDIF
         IF(TB.GT.637.D0)THEN
          IERR=-2
          CALL MESS(1)
          WRITE(NHSTRY,900)
          WRITE(NHSTRY,2000)TB
          TB=637.D0
         ENDIF
        ENDIF
C
C         AROMATICS
C
        IF(XA.GT.0.D0)THEN
         IF(TB.LT.353.3D0)THEN
          IERR=-3
          CALL MESS(1)
          WRITE(NHSTRY,900)
          WRITE(NHSTRY,3000)TB
          TB=353.3D0
         ENDIF
         IF(TB.GT.517.8D0)THEN
          IERR=-3
          CALL MESS(1)
          WRITE(NHSTRY,900)
          WRITE(NHSTRY,3000)TB
          TB=517.6D0
         ENDIF
        ENDIF
C
C         DATA REGRESSED FOR PARAFFINS
C
        AP=568031546.D0
        BP=-4602700.36D0
        CP=9840.17072D0
        DP=-8.237748877D0
C
        DHFIP=AP + BP*TB + CP*TB*TB + DP*TB*TB*TB
C
C         DATA REGRESSED FOR NAPTHENES
C
        AN=0.161688484D10
        BN=-10641443.5D0
        CN=21793.9633D0
        DN=-15.8925712D0
C
        DHFIN=AN + BN*TB + CN*TB*TB + DN*TB*TB*TB
C
C         DATA REGRESSED FOR AROMATICS
C
        AA=-0.116028149D11
        BA=88976967.9D0
```

```
      CA=-223012.655D0
      DA=183.320881D0
C
      DHFIA=AA + BA*TB + CA*TB*TB + DA*TB*TB*TB
C
C       EST. FOR FRACTION
C
      DHF=DHFIA*XA+DHFIN*XN+DHFIP*XP
C
C       FORMATS
C
900   FORMAT(1X,'IN MODULE DHFRM')
1000  FORMAT(1X,'TB(K) VALUE OF ',G13.6,/,
     1       2X,'IS NOT IN PARAFFIN CORRELATION RANGE 301-617',/,
     2       2X,'CORRECTIVE ACTION TAKEN AND CALC. CONTINUES')
2000  FORMAT(1X,'TB(K) VALUE OF ',G13.6,/,
     1       2X,'IS NOT IN NAPTHENE CORRELATION RANGE 322.4-637',/,
     2       2X,'CORRECTIVE ACTION TAKEN AND CALC. CONTINUES')
3000  FORMAT(1X,'TB(K) VALUE OF ',G13.6,/,
     1       2X,'IS NOT IN AROMATIC CORRELATION RANGE 353.3-517.8',/,
     2       2X,'CORRECTIVE ACTION TAKEN AND CALC. CONTINUES')
      RETURN
      END
C*****************************************************************
C
      SUBROUTINE DIPOLE(JC,IERR)
C
C*****************************************************************
C
C       NAME OF MODULE - DIPOLE
C       MODULE TITLE - ESTIMATION OF DIPOLE MOMENT
C       PURPOSE - EST OF DIPOLE MOMENT (COULOMB*M)
C       MODIFIED - 1-22-88
C
C
C       VARIABLES USED-
C
C VARIABLE I/O TYPE-SPEC DIMENSION     DESCRIPTION AND RANGE
C      JC    I      I         -        COMPONENT ARRAY ID
C    IERR    O      I         -        ERROR CODE
C                                     0 = OK
C
      IMPLICIT REAL*8 (A-H,O-Z)
      IMPLICIT INTEGER(I-N)
C
      REAL*8           MUP
C
      PARAMETER        (MNC=25)
C
      COMMON /CPRP19/ MUP(MNC)
C
      IERR=0
C
C       SET TO DEFAULT SUGGESTED BY ASPEN AND DIPPR
C
      MUP(JC)=0.D0
C
C       FORMATS
C
      RETURN
      END
C*****************************************************************
C
      SUBROUTINE ESTFRA(TB,JC,IERR)
C
C*****************************************************************
C
C       NAME OF MODULE - ESTFRA
```

```
C        MODULE TITLE - ESTIMATE PERCENT PARAFFINS,NAPTHENES, AND AROMATICS
C        PURPOSE - TO ESTIMATE PERCENT PARAFFINS,NAPTHENES, AND AROMATICS
C                  FOR A GIVEN TEMPERATURE BASED ON TIA JUANA LIGHT
C                  (VENEZUELA)
C
C        VARIABLES USED-
C
C VARIABLE I/O TYPE-SPEC DIMENSION      DESCRIPTION AND RANGE
C      TB     I       R         -       BOILING POINT (DEG F)
C      JC     I       I         -       COMPONENT ARRAY ID
C    IERR     O       I         -       ERROR CODE
C                                        0 = OK
C                                       -1 = TB OUT OF RANGE
C
       IMPLICIT REAL*8 (A-H,O-Z)
       IMPLICIT INTEGER(I-N)
C
       PARAMETER        (MNC=25)
C
       COMMON /IO     / NIN,NOUT,NHSTRY,NREPT
       COMMON /DEBUG  / LDBUG,LDBUGR
C
       COMMON /NPROP4/ PA(MNC),PN(MNC),PP(MNC),IPF
C
       COMMON /EPROP1/ XPAR(MNC),XNAP(MNC),XARO(MNC)
C
       IF(LDBUG.GT.7)WRITE(NHSTRY,900)
C
       IERR=0
C
C        CHECK TB
C
       IF(TB.LE.113.D0)THEN
        IERR=-1
        CALL MESS(1)
        WRITE(NHSTRY,900)
        WRITE(NHSTRY,1000)TB
        TB=113.D0
       ENDIF
       IF(TB.GE.549.D0)THEN
        IERR=-1
        CALL MESS(1)
        WRITE(NHSTRY,900)
        WRITE(NHSTRY,1000)TB
        TB=549.D0
       ENDIF
C
C        EST. PERCENT PARAFFINS,NAPTHENES, AND AROMATICS
C          REGRESSION OF PARIFINS VOL% VS TEMP (F)
C          ADJ. R-SQUARE    =       0.9511488
C
       AP =      161.361491
       BP =    -0.063582267
       CP =     0.216788391E-02
       DP =    -0.181295213E-05
C
       VP=AP+BP*TB+CP*TB*TB+DP*TB*TB*TB
       PP(JC)=VP
C
C          REGRESSION OF NAPTHAS VOL% VS TEMP (F)
C          ADJ. R-SQUARE    =       0.8799234
C
       AN =     -134.126283
       BN =      2.15899658
       CN =    -0.996716079E-02
       DN =     0.196670981E-04
       EN =    -0.140405351E-07
C
```

```
      VN=AN+BN*TB+CN*TB*TB+DN*TB*TB*TB+EN*TB*TB*TB*TB
      PN(JC)=VN
C
C          AROMATICS BY DIFFERENCE
C
      PA(JC)=100.D0-PP(JC)-PN(JC)
C
C          CORRECT FOR IMPOSSIBLE CASE
C
      IF(PA(JC).LE.0.D0)THEN
       PA(JC)=0.0D0
       PSUM=PN(JC)+PP(JC)
       PN(JC)=PN(JC)/PSUM*100.D0
       PP(JC)=PP(JC)/PSUM*100.D0
      ENDIF
C
C        CALC MOLE FRACTION PARAFFINS,NAPTHENES, AND AROMATICS
C
       XARO(JC)=PA(JC)/100.D0
       XNAP(JC)=PN(JC)/100.D0
       XPAR(JC)=PP(JC)/100.D0
C
C        FORMATS
C
900   FORMAT(1X,'IN MODULE ESTFRA')
1000  FORMAT(1X,'TB(F) VALUE OF ',G13.6,' IS NOT IN CORRELATION'
     1        ' RANGE 113-549',/,
     2        1X,'CORRECTIVE ACTION TAKEN AND CALC. CONTINUES')
C
      RETURN
C
      END
C*******************************************************************************
C
      SUBROUTINE EXTOK(ISTART,IEND,RECORD,ICNT)
C
C*******************************************************************************
C
C        NAME OF MODULE - EXTOK
C        MODULE TITLE - EXTRACT TOKEN BETWEEN DELIMS.
C        PURPOSE - TO EXTRACT TOKEN VALUES FROM INPUT RECORD
C        MODIFIED - 12-15-88
C
C        VARIABLES USED-
C
C VARIABLE I/O TYPE-SPEC DIMENSION      DESCRIPTION AND RANGE
C ISTART     I       I         10          START BYTE OF TOKEN
C   IEND     I       I         10          END BYTE OF TOKEN
C RECORD   I/O       C          -          INPUT RECORD
C   ICNT     O       I          -          COUNT OF TOKENS FOUND
C
      CHARACTER*1  DELMS(2)
      CHARACTER*80 RECORD
C
      INTEGER ISTART(10),IEND(10)
C
      DATA DELMS/' ','='/
C
C       INITALIZE
C
      K=1
      IWIDE=80
C
      DO 10 JJ=1,10
       ISTART(JJ)=0
       IEND(JJ)=0
10    CONTINUE
C
```

```
20     CONTINUE
C
C       BEGIN COUNT OF TOKENS
C
       ICNT=ICNT+1
C
C         FIND BEGIN OF TOKEN
C
       DO 30 IS=K,IWIDE
        IF(RECORD(IS:IS).NE.DELMS(1) .AND.
      1     RECORD(IS:IS).NE.DELMS(2) )GOTO 40
30     CONTINUE
       ICNT=ICNT-1
       RETURN
C
C       FIND END OF TOKEN
C
40     CONTINUE
       DO 50 IE=IS,IWIDE
        IF(RECORD(IE:IE).EQ.DELMS(1) .OR.
      1     RECORD(IE:IE).EQ.DELMS(2) )GOTO 60
50     CONTINUE
       RETURN
C
C       FOUND START AND END OF TOKEN
C
60     CONTINUE
C
       IES=IE-1
       IDELT=IES-IS
       IF(IDELT.LT.0)THEN
        ICNT=ICNT-1
        GOTO 80
       ENDIF
C
C       LOAD START AND END OF TOKENS
C
       ISTART(ICNT)=IS
       IEND(ICNT)=IES
80     CONTINUE
       K=IES+1
       GOTO 20
C
9999   RETURN
       END
C*****************************************************************************
C
       SUBROUTINE GUNYAM(VR,TR,OMEGA,TRD,ICALC,VD,IERR)
C
C*****************************************************************************
C
C         NAME OF MODULE - GUNYAM
C         MODULE TITLE - TO ESTIMATE LIQ DENSITIES
C         PURPOSE - TO ESTIMATE LIQ. DENSITIES USING THE GUNN YAMADA
C         MODIFIED - 11-10-88
C         METHOD - REF: AICHE J 17:P 1341 (1967)
C                        GUNN & YAMADA
C                        J CHEM ENG. DATA 16: 596 (1971)
C                        YAMADA & GUNN
C
C         VARIABLES USED-
C
C VARIABLE I/O TYPE-SPEC DIMENSION      DESCRIPTION AND RANGE
C     VR       I       R          -     REFERENCE VOLUME(M**3/KMOLE)
C     TR       I       R          -     REFERENCE TEMP REDUCED
C  OMEGA       I       R          -     ACENTRIC FACTOR
C    TRD       I       R          -     REDUCED TEMP OF VOL DESIRED
C  ICALC       I       I          -     CALC TYPE
```

```
C                                                  0 = GUNN YAMADA
C                                                  1 = YAMADA GUNN
C     VD      O       R           -                VOLUME AT DESIRED TEMP(M**3/KMOLE)
C   IERR      I       I           -                ERROR CODE
C                                                  0 = OK
C                                                 -1 = REDUCED TEMP > 0.99
C                                                 -2 = REDUCED TEMP < 0.2
C
      IMPLICIT REAL*8 (A-H,O-Z)
      IMPLICIT INTEGER(I-N)
C
      COMMON /IO     / NIN,NOUT,NHSTRY,NREPT
      COMMON /DEBUG / LDBUG,LDBUGR
C
      IERR=0
      IF(LDBUG.GT.7)WRITE(NHSTRY,900)
C
      IF(ICALC.LE.0)ICALC=0
      IF(ICALC.GT.1)ICALC=1
C
C       WRITE WARNINGS
C
      IF(TR.GT.0.99D0)THEN
       CALL MESS(1)
       WRITE(NHSTRY,900)
       WRITE(NHSTRY,1000)TR
       TR=.99D0
       IERR=-1
      ENDIF
      IF(TRD.GT.0.99D0)THEN
       CALL MESS(1)
       WRITE(NHSTRY,900)
       WRITE(NHSTRY,1010)TRD
       TRD=.99D0
       IERR=-1
      ENDIF
C
      IF(TR.LT.0.2D0)THEN
       CALL MESS(1)
       WRITE(NHSTRY,900)
       WRITE(NHSTRY,1020)TR
       TR=0.2D0
       IERR=-2
      ENDIF
      IF(TRD.LT.0.2D0)THEN
       CALL MESS(1)
       WRITE(NHSTRY,900)
       WRITE(NHSTRY,1030)TRD
       TRD=0.2D0
       IERR=-2
      ENDIF
C
      IF(ICALC.EQ.0)THEN
       IF(TR.LE.0.8D0)THEN
        VR0ATR=0.33593D0-0.33953D0*TR+1.51941D0*TR*TR
     1         -2.02512D0*TR**3+1.11422D0*TR**4
       ELSE
        VR0ATR=1.0D0+1.3D0*(1.D0-TR)**0.5D0*LOG10(1.D0-TR)
     1         -0.50879D0*(1.D0-TR)-0.91534*(1.D0-TR)**2
       ENDIF
C
       IF(TRD.LE.0.8D0)THEN
        VR0ADT=0.33593D0-0.33953D0*TRD+1.51941D0*TRD*TRD
     1         -2.02512D0*TRD**3+1.11422D0*TRD**4
       ELSE
        VR0ADT=1.0D0+1.3D0*(1.D0-TRD)**0.5D0*LOG10(1.D0-TRD)
     1         -0.50879D0*(1.D0-TRD)-0.91534*(1.D0-TRD)**2
       ENDIF
```

```
C
        GAMATR=0.29607D0-0.09045*TR-0.04842*TR**2
        GAMADT=0.29607D0-0.09045*TRD-0.04842*TRD**2
C
        VD=VR * (VR0ADT*(1.D0-OMEGA*GAMADT))/
     1           (VR0ATR*(1.D0-OMEGA*GAMATR))
       ELSE
        TS=2.D0/7.D0
        ZCR=0.29056D0-0.08775D0*OMEGA
        PHI=(1.D0-TR)**TS-(1.D0-TRD)**TS
        VD=VR * ZCR**PHI
       ENDIF
C
C       FORMATS
C
900    FORMAT(1X,'IN MODULE GUNYAM')
1000   FORMAT(1X,'TR VALUE IS GREATER THAN 0.99 ',/,
     1         1X,'TR-VALUE OF ',G15.6,' SET TO 0.99 CALC. CONTINUES')
1010   FORMAT(1X,'TRD VALUE IS GREATER THAN 0.99',/,
     1         1X,'TRD-VALUE OF ',G15.6,' SET TO 0.99 CALC. CONTINUES')
1020   FORMAT(1X,'TR VALUE IS LESS THAN 0.2',/,
     1         1X,'TR-VALUE OF ',G15.6,' SET TO 0.2 CALC. CONTINUES')
1030   FORMAT(1X,'TRD VALUE IS LESS THAN 0.2',/,
     1         1X,'TRD-VALUE OF ',G15.6,' SET TO 0.2 CALC. CONTINUES')
C
       RETURN
       END
C*********************************************************************
C
       SUBROUTINE GYKL(TBR,TC,PC,UOPK,API,OMEGA,IERR)
C
C*********************************************************************
C
C         NAME OF MODULE - GYKL
C         MODULE TITLE - GUNN YAMADA/ KESLER LEE CALC OF ACENTRIC FACTOR
C         PURPOSE - TO CALC ACENTRIC FACTOR USING KESLER LEE METHOD
C         MODIFIED - 11-10-86
C         METHOD - REF: HYDROCARBON PROCESSING VOL 55 NO 3 PP 153-
C                       "IMPROVED PREDICTION OF ENTHALPY OF FRACTIONS"
C                       M.J.KESLER AND B.I.LEE (PAPER 21)
C
C         VARIABLES USED-
C
C VARIABLE I/O TYPE-SPEC DIMENSION      DESCRIPTION AND RANGE
C    TBR     I       R          -       MOLAL AVERAGE POINT TEMP (DEG R)
C     TC     I       R          -       CRITICAL TEMP (DEG R)
C     PC     I       R          -       CRITICAL PRES (PSIA)
C   UOPK     I       R          -       WATSON/UOP CHAR FACTOR
C    API     I       R          -       API VALUE
C OMEGA      O       R          -       ACENTRIC FACTOR
C  IERR      O       I          -       ERROR CODE
C                                       0 = OK
C                                       1 = UOP OUT OF RANGE
C                                       2 = API OUT OF RANGE
C                                       3 = OMEGA
C
       IMPLICIT REAL*8 (A-H,O-Z)
       IMPLICIT INTEGER (I-N)
C
       COMMON /IO     / NIN,NOUT,NHSTRY,NRLPT
       COMMON /DEBUG / LDBUG,LDBUGR
C
       IERR=0
       IF(LDBUG.GT.7)WRITE(NHSTRY,900)
C
C         CHECK IF UOPK IN RANGE(10-13) WARNING
C
       IF(UOPK.LT.10.D0.OR.UOPK.GT.13.D0)THEN
```

```
        IERR=1
        CALL MESS(1)
        WRITE(NHSTRY,900)
        WRITE(NHSTRY,1000)UOPK
       ENDIF
C
C       API (0-80)
C
       IF(API.LT.0.D0.OR.API.GT.80.D0)THEN
        IERR=2
        CALL MESS(1)
        WRITE(NHSTRY,900)
        WRITE(NHSTRY,1000)API
       ENDIF
C
C         REDUCED PROPERTIES
C
       REDT=(TBR/TC)
       BOILP=14.696D0
       REDP=BOILP/PC
C
       IF(REDT.LE.0.8D0)THEN
        OMEGA=(LOG(REDP)-5.92714D0+6.09648D0/REDT+
      1          1.28862D0*LOG(REDT)-0.169347D0*REDT**6)/
      2          (15.2518D0-15.6875D0/REDT-
      3          13.4721D0*LOG(REDT)+0.43577D0*REDT**6)
        ELSE
         OMEGA=-7.904D0+0.1352D0*UOPK-0.007465D0*UOPK**2+8.359D0*REDT+
      1        (1.408D0-0.01063D0*UOPK)/REDT
        ENDIF
C
C       OMEGA
C
       IF(OMEGA.LT.0.2D0.OR.OMEGA.GT.1.4D0)THEN
        IERR=3
        CALL MESS(2)
        WRITE(NHSTRY,900)
        WRITE(NHSTRY,3000)OMEGA
       ENDIF
C
C       FORMATS
C
900    FORMAT(1X,'IN MODULE GYKL')
1000   FORMAT(1X,'UOPK VALUE NOT IN OPTIMAL RANGE (10-13)',/,
      1        1X,'UOPK = ',G13.6,' CALC. CONTINUES')
2000   FORMAT(1X,'API GRAVITY VALUE NOT IN OPTIMAL RANGE (0-80)',/,
      1        1X,'API = ',G13.6,' CALC. CONTINUES')
3000   FORMAT(1X,'OMEGA VALUE NOT IN OPTIMAL RANGE (0.2-1.4)',/,
      1        1X,'OMEGA = ',G13.6,' CALC. CONTINUES')
C
       RETURN
       END
C*******************************************************************************
C
       SUBROUTINE HVABP(JC,IERR)
C
C*******************************************************************************
C
C         NAME OF MODULE - HVABP
C         MODULE TITLE - CALC HEAT OF VAPORIZATION AT THE BOILING POINT
C         PURPOSE - TO CALC HEAT OF VAPORIZATION AT THE BOILING POINT
C                   USING ASPEN'S WATSON EQUATION
C         MODIFIED - 12-19-88
C         METHOD - ASPEN'S WATSON HEAT OF VAPORIZATION EQUATION
C
C         VARIABLES USED-
C
C VARIABLE I/O TYPE-SPEC DIMENSION      DESCRIPTION AND RANGE
```

```
C      JC     I       I         -           COMPONENT ARRAY ID
C    IERR     O       I         -           ERROR CODE
C                                           0 = OK
C
       IMPLICIT REAL*8 (A-H,O-Z)
       IMPLICIT INTEGER(I-N)
C
       PARAMETER        (MNC=25)
C
       COMMON /IO     / NIN,NOUT,NHSTRY,NREPT
       COMMON /DEBUG  / LDBUG,LDBUGR
C
       COMMON /CPRP01/ TC(MNC)
       COMMON /CPRP08/ DHVLWT(5,MNC)
       COMMON /CPRP14/ TB(MNC)
       COMMON /CPRP16/ DHVLB(MNC)
C
       IERR=0
       IF(LDBUG.GT.7)WRITE(NHSTRY,900)
C
       TBUSE=TB(JC)
C
C       CHECK LIMITS OF EQUATION
C
       IF(TB(JC).LT.DHVLWT(5,JC))THEN
        IERR=1
        CALL MESS(2)
        WRITE(NHSTRY,900)
        WRITE(NHSTRY,1000)DHVLWT(5,JC),TB(JC)
        TBUSE=DHVLWT(5,JC)
       ENDIF
C
       IF(TB(JC).GT.TC(JC))THEN
        IERR=2
        CALL MESS(2)
        WRITE(NHSTRY,900)
        WRITE(NHSTRY,1000)TC(JC),TB(JC)
        TBUSE=TC(JC)
       ENDIF
C
C       CALC HEAT OF VAPORIZATION AT BOILING POINT USING ASPEN'S
C       WATSON EQUATION
C
       DHVLB(JC)=DHVLWT(1,JC) *
      1           ((1.D0-TBUSE/TC(JC))/(1.D0-DHVLWT(2,JC)/TC(JC)))**
      2           (DHVLWT(3,JC)+DHVLWT(4,JC)*(1.D0-TBUSE/TC(JC)))
C
C       FORMATS
C
900    FORMAT(1X,'IN MODULE HVABP')
1000   FORMAT(1X,'TB VALUE LESS THAN LOWER LIMIT OF ',G13.6,/,
      1        1X,'TB-VALUE OF ',G15.6,' SET TO LOWER LIMIT ',
      2        'CALC. CONTINUES')
       RETURN
       END
C*******************************************************************
C
       SUBROUTINE INIT(IERR)
C
C*******************************************************************
C
C        NAME OF MODULE - INIT
C        MODULE TITLE - INITILIZE TO DEFAULT VALUE FOR PROPERTIES
C        PURPOSE - TO INITILIZE ALL PROPERTIES
C
C        VARIABLES USED-
C
C VARIABLE I/O TYPE-SPEC DIMENSION     DESCRIPTION AND RANGE
```

```
C    IERR    O       I          -          ERROR CODE
C                                          0 = OK
C                                          -1 = ERROR ON INIT
C
      IMPLICIT REAL*8 (A-H,O-Z)
      IMPLICIT INTEGER(I-N)
C
      REAL*8           MULAND,MULREG,MUP
      CHARACTER*32     CNAME
C
      PARAMETER        (MNC=25)
C
      COMMON /IO     / NIN,NOUT,NHSTRY,NREPT
      COMMON /DEBUG  / LDBUG,LDBUGR
      COMMON /SYS1   / RMISS
C
      COMMON /NPROP1/ NCOMP,CNAME(MNC),ICF
C
      COMMON /CPRP01/ TC(MNC)
      COMMON /CPRP02/ PC(MNC)
      COMMON /CPRP03/ VC(MNC)
      COMMON /CPRP04/ ZC(MNC)
      COMMON /CPRP05/ OMEGA(MNC)
      COMMON /CPRP06/ PLXANT(9,MNC),PLXREG(3,MNC)
      COMMON /CPRP07/ CPIG(11,MNC),CPREG(3,MNC)
      COMMON /CPRP08/ DHVLWT(5,MNC)
      COMMON /CPRP09/ MULAND(5,MNC),MULREG(3,MNC)
      COMMON /CPRP10/ DHFORM(MNC)
      COMMON /CPRP11/ DGFORM(MNC)
      COMMON /CPRP12/ RKTZRA(MNC),RKTREG(3,MNC)
      COMMON /CPRP13/ DHLCVT(MNC)
      COMMON /CPRP14/ TB(MNC)
      COMMON /CPRP15/ VB(MNC)
      COMMON /CPRP16/ DHVLB(MNC)
      COMMON /CPRP17/ TFP(MNC)
      COMMON /CPRP18/ DELTA(MNC)
      COMMON /CPRP19/ MUP(MNC)
      COMMON /CPRP20/ RGYR(MNC)
      COMMON /CPRP21/ PLCAVT(4,MNC),PLCREG(3,MNC)
      COMMON /CPRP22/ VLCVT1(MNC)
C
      IF(LDBUG.GT.7)WRITE(NHSTRY,900)
C
      IERR=0
C
      DO 50 JC=1,NCOMP
C
       TC(JC)=RMISS
       PC(JC)=RMISS
       VC(JC)=RMISS
       ZC(JC)=RMISS
C
       DO 10 IN=1,9
10     PLXANT(IN,JC)=RMISS
C
       DO 20 IN=1,11
20     CPIG(IN,JC)=RMISS
C
       DO 30 IN=1,5
        DHVLWT(IN,JC)=RMISS
        MULAND(IN,JC)=RMISS
        PLCAVT(IN,JC)=RMISS
30     CONTINUE
C
       OMEGA(JC)=RMISS
       DHFORM(JC)=RMISS
       DGFORM(JC)=RMISS
       RKTZRA(JC)=RMISS
```

```
        DHLCVT(JC)=RMISS
        TB(JC)=RMISS
        VB(JC)=RMISS
        DHVLB(JC)=RMISS
        TFP(JC)=RMISS
        DELTA(JC)=RMISS
        MUP(JC)=RMISS
        RGYR(JC)=RMISS
        VLCVT1(JC)=RMISS
C
C         REGRESSION VALUES
C
        DO 40 IN=1,3
         PLXREG(IN,JC)=RMISS
         CPREG(IN,JC)=RMISS
         MULREG(IN,JC)=RMISS
         PLCREG(IN,JC)=RMISS
         RKTREG(IN,JC)=RMISS
40      CONTINUE
50     CONTINUE
C
C         FORMATS
C
900    FORMAT(1X,'IN MODULE INIT')
C
       RETURN
       END
C*******************************************************************************
C
       SUBROUTINE INPT(IERR)
C
C*******************************************************************************
C
C         NAME OF MODULE - INPT
C         MODULE TITLE - INPUT TRANSLATOR
C         PURPOSE - TO READ INPUT FILE AND OBTAIN INPUT VALUES
C         MODIFIED - 12-20-88
C
C         VARIABLES USED-
C
C VARIABLE I/O TYPE-SPEC DIMENSION      DESCRIPTION AND RANGE
C  IERR     I/O      I          -       ERROR CODE
C                                        0 = OK
C                                       -1 = EXTOK ERROR
C                                        1 = TEMP INPUT WARNING
C                                        2 = PRES INPUT WARNING
C                                        3 = TO MANY DESCRIPTION LINES
C                                        4 = SYSOP WARNING
C                                        5 = ASPENOUT WARNING
C                                        6 = PC WARNING
C                                        7 = TC WARNING
C                                        8 = CAL-DBUG WARNING
C                                        9 = REP-DBUG WARNING
C
C
C * * * * * * * * * * * * * INPUT COMMANDS * * * * * * * * * * * * * * * * * * *
C
C       ALL INPUT MUST BE IN CAPS
C       ; FOR COMMENT CARDS
C
C       PKW                          SKW                        TKW
C       TITLE                                              (UP TO 62 CHARACTERS)
C       DESC                                               (UP TO 25 LINES)
C       T-UNITS                      F K C R
C       P-UNITS                      PA MMHG PSIA PSIG ATM
C       PROP-DATA
C                                    COMP-LIST
C                                    CVAL
```

```
C                                                                       API=
C                                                                       SG=
C                                                                       VABP=
C                                                                       UOPK=
C                                                                       STBP=
C                                                                       SASTMD86=
C                                                                       TC=
C                                                                       PC=
C                                                                       PER-PAR=
C                                                                       PER-NAP=
C                                                                       PER-ARO=
C       PRINT-OPT
C                                       CAL-DBUG=1,2,3,4,5,6,7,8
C                                       REP-DBUG=1,2,3,4,5,6,7,8
C                                       PROP-OPT=SYSOP*
C                                       ASPENOUT=DFMS,INPUT
C                                       REP-FILE=FILENAME.EXT
C       END-INPUT
C
C
      IMPLICIT REAL*8 (A-H,O-Z)
      IMPLICIT INTEGER(I-N)
C
      REAL*8            MABP,MEABP
C
      PARAMETER         (MNC=25)
      PARAMETER         (MXDESC=25)
C
      CHARACTER*1       INCHA,OUTCHA
      CHARACTER*32      FILE,CNAME
      CHARACTER*62      TITLE
      CHARACTER*80      REC1,REC2
      CHARACTER*80      DESC(MXDESC),CVALU
C
      INTEGER           IS(10),IE(10)
C
      COMMON /IO     / NIN,NOUT,NHISTRY,NREPT
      COMMON /FILES  / FILE
      COMMON /DEBUG  / LDBUG,LDBUGR
      COMMON /PRINT  / IPTYPE
      COMMON /SYS1   / RMISS
      COMMON /SYS2   / NSYSOP,NPCVEC(22)
      COMMON /INFO   / TITLE,DESC,IDESC
C
      COMMON /NPROP1/ NCOMP,CHABL(MNC),ICF
      COMMON /NPROP2/ VABP(MNC),SLOP(MNC),CABP(MNC),MABP(MNC),MEABP(MNC)
      COMMON /NPROP3/ UOPK(MNC),API(MNC),SG(MNC),AHW(MNC)
      COMMON /NPROP4/ PA(MNC),PB(MNC),PF(MNC),IPF
C
      COMMON /CPRP01/ TC(MNC)
      COMMON /CPRP02/ PC(MNC)
C
C       SET DEFAULTS
C
      IERR=0
C
      ICF=0
      IDESC=0
      IFIL=0
      NCOMP=0
      NSYSOP=0
      IFLAG=1
      ITUNIT=1
      IPUNIT=1
      INUM=0
      IEND=80
      IFP=0
C
```

```
      CALL IDATE(IM,ID,IY)
C
      WRITE(NHSTRY,900)IM,ID,IY
C
C       BEGIN INPUT TRANSLATION
C
100   READ(NIN,1000,END=9000)REC1
101   CONTINUE
C
C       FILTER OUT BAD CHARACTERS AND CAPITALIZE IF NECESSARY
C
      DO 200 IC=1,80
       INCHA=REC1(IC:IC)
       CALL CAPS(INCHA,OUTCHA)
       REC1(IC:IC)=OUTCHA
200   CONTINUE
C
C       ECHO INPUT
C
      CALL STRIP(REC1,INUM,NHSTRY,IERS)
C
C       LOOK FOR ;
C
      IF(REC1(1:1).EQ.';')GOTO 100
C
C       FOUND TITLE PKW
C
      IF(REC1(1:5).EQ.'TITLE')THEN
       TITLE=REC1(6:80)
      ENDIF
C
C       FOUND DESC PKW
C
      IF(REC1(1:4).EQ.'DESC')THEN
       IDESC=IDESC+1
       IF(IDESC.GT.MXDESC)THEN
        CALL MESS(2)
        WRITE(NHSTRY,5000)
        IERR=3
        GOTO 100
       ENDIF
       DESC(IDESC)=REC1(5:80)
      ENDIF
C
C       FOUND T-UNITS PKW
C
      IVAL1=INDEX(REC1,'T-UNITS=')
      IF(IVAL1.EQ.1)THEN
       REC2=REC1(IVAL1+8:80)
       IF(INDEX(REC2,'F').NE.0)THEN
        ITUNIT=1
       ELSE IF(INDEX(REC2,'R').NE.0)THEN
        ITUNIT=2
       ELSE IF(INDEX(REC2,'C').NE.0)THEN
        ITUNIT=3
       ELSE IF(INDEX(REC2,'K').NE.0)THEN
        ITUNIT=4
       ELSE
        ITUNIT=1
        REC1=REC2
        CALL MESS(2)
        WRITE(NHSTRY,5010)
        IERR=1
        GOTO 100
       ENDIF
      ENDIF
C
C       FOUND P-UNITS PKW
```

```
C
      IVAL1=INDEX(REC1,'P-UNITS=')
      IF(IVAL1.EQ.1)THEN
       REC2=REC1(IVAL1+8:80)
       IF(INDEX(REC2,'PSIA').NE.0)THEN
        IPUNIT=1
       ELSE IF(INDEX(REC2,'PSIG').NE.0)THEN
        IPUNIT=2
       ELSE IF(INDEX(REC2,'ATM').NE.0)THEN
        IPUNIT=3
       ELSE IF(INDEX(REC2,'MMHG').NE.0)THEN
        IPUNIT=4
       ELSE IF(INDEX(REC2,'PA').NE.0)THEN
        IPUNIT=5
       ELSE
        IPUNIT=1
        REC1=REC2
        CALL MESS(2)
        WRITE(NHSTRY,5020)
        IERR=2
        GOTO 100
       ENDIF
      ENDIF
C
C       FOUND PROP-DATA PKW
C
      IVAL1=INDEX(REC1,'PROP-DATA ')
C
      IF(IVAL1.EQ.1)THEN
400    ICNT=0
       READ(NIN,1000,END=9000)REC2
C
C       FILTER OUT BAD CHARACTERS AND CAPITALIZE IF NECESSARY
C
      DO 500 IC=1,80
       INCHA=REC2(IC:IC)
       CALL CAPS(INCHA,OUTCHA)
       REC2(IC:IC)=OUTCHA
500   CONTINUE
C
C       ECHO INPUT
C
      CALL STRIP(REC2,INUM,NHSTRY,IERS)
C
C       LOOK FOR ;
C
      IF(REC2(1:1).EQ.';')GOTO 400
C
C       CHECK IF FIRST CHAR IS NON BLANK
C
      IF(REC2(1:1).NE.' ')THEN
       REC1=REC2
       GOTO 101
      ENDIF
C
C        FOUND COMP-LIST SKW
C
       IVAL2=INDEX(REC2,'COMP-LIST ')
       IF(IVAL2.NE.0)THEN
        NCOMP=NCOMP+1
        CNAME(NCOMP)=REC2(IVAL2+10:IVAL2+10+32)
        GOTO 400
       ENDIF
C
C        FOUND CVAL TKW
C
       IVAL2=INDEX(REC2,'CVAL ')
       IF(IVAL2.NE.0)THEN
```

```
      CVALU=REC2(IVAL2+5:80)
C
C     FIND TOKENS
C
      CALL EXTOK(IS,IE,CVALU,ICNT)
      IF(ICNT.LE.0)THEN
       IERR=-1
       GOTO 400
      ENDIF
C
C      FOUND MW
C
      IF(CVALU(IS(1):IE(1)).EQ.'MW')THEN
C
       IFLAG=1
       CALL CONV(IFLAG,CVALU,IS(2),IE(2),AMW(NCOMP),IDUM,IERC)
       GOTO 400
      ENDIF
C
C      FOUND VABP
C
      IF(CVALU(IS(1):IE(1)).EQ.'VABP')THEN
C
       IFLAG=1
       CALL CONV(IFLAG,CVALU,IS(2),IE(2),VABPI,IDUM,IERC)
C
       IF(ITUNIT.EQ.1)THEN
        CALL TCON(VABPI,VABP(NCOMP),14,IERT)
       ELSE IF(ITUNIT.EQ.2)THEN
        CALL TCON(VABPI,VABP(NCOMP),24,IERT)
       ELSE IF(ITUNIT.EQ.3)THEN
        CALL TCON(VABPI,VABP(NCOMP),34,IERT)
       ELSE
        VABP(NCOMP)=VABPI
       ENDIF
C
       GOTO 400
      ENDIF
C
C      FOUND STBP
C
      IF(CVALU(IS(1):IE(1)).EQ.'STBP')THEN
C
       ICF=0
       IFLAG=1
       CALL CONV(IFLAG,CVALU,IS(2),IE(2),SLOP(NCOMP),IDUM,IERC)
       GOTO 400
      ENDIF
C
C      FOUND SASTMD86
C
      IF(CVALU(IS(1):IE(1)).EQ.'SASTMD86')THEN
C
       IFLAG=1
       ICF=1
       CALL CONV(IFLAG,CVALU,IS(2),IE(2),SLOP(NCOMP),IDUM,IERC)
       GOTO 400
      ENDIF
C
C      FOUND API
C
      IF(CVALU(IS(1):IE(1)).EQ.'API')THEN
C
       IFLAG=1
       CALL CONV(IFLAG,CVALU,IS(2),IE(2),API(NCOMP),IDUM,IERC)
       GOTO 400
      ENDIF
C
```

```
C          FOUND SG
C
          IF(CVALU(IS(1):IE(1)).EQ.'SG')THEN
C
           IFLAG=1
           CALL CONV(IFLAG,CVALU,IS(2),IE(2),SG(NCOMP),IDUM,IERC)
           GOTO 400
          ENDIF
C
C          FOUND UOPK
C
          IF(CVALU(IS(1):IE(1)).EQ.'UOPK')THEN
C
           IFLAG=1
           CALL CONV(IFLAG,CVALU,IS(2),IE(2),UOPK(NCOMP),IDUM,IERC)
           GOTO 400
          ENDIF
C
C          FOUND WK
C
          IF(CVALU(IS(1):IE(1)).EQ.'WK')THEN
C
           IFLAG=1
           CALL CONV(IFLAG,CVALU,IS(2),IE(2),UOPK(NCOMP),IDUM,IERC)
           GOTO 400
          ENDIF
C
C          FOUND TC
C
          IF(CVALU(IS(1):IE(1)).EQ.'TC')THEN
C
           IFLAG=1
           CALL CONV(IFLAG,CVALU,IS(2),IE(2),TCI,IDUM,IERC)
           IF(IERC.GT.0)THEN
            CALL MESS(1)
            WRITE(NHSTRY,5040)
            IERR=7
            TC(NCOMP)=RMISS
            GOTO 100
           ENDIF
C
           IF(ITUNIT.EQ.1)THEN
            CALL TCON(TCI,TC(NCOMP),14,IERT)
           ELSE IF(ITUNIT.EQ.2)THEN
            CALL TCON(TCI,TC(NCOMP),24,IERT)
           ELSE IF(ITUNIT.EQ.3)THEN
            CALL TCON(TCI,TC(NCOMP),34,IERT)
           ELSE
            TC(NCOMP)=TCI
           ENDIF
C
           GOTO 400
          ENDIF
C
C          FOUND PC
C
          IF(CVALU(IS(1):IE(1)).EQ.'PC')THEN
C
           IFLAG=1
           CALL CONV(IFLAG,CVALU,IS(2),IE(2),PCI,IDUM,IERC)
C
           IF(IERC.GT.0)THEN
            CALL MESS(1)
            WRITE(NHSTRY,5050)
            PC(NCOMP)=RMISS
            IERR=6
            GOTO 100
           ENDIF
```

```
C
          IF(ITUNIT.EQ.1)THEN
           CALL PCON(PCI,PC(NCOMP),15,IERP)
          ELSE IF(ITUNIT.EQ.2)THEN
           CALL PCON(PCI,PC(NCOMP),25,IERP)
          ELSE IF(ITUNIT.EQ.3)THEN
           CALL PCON(PCI,PC(NCOMP),35,IERP)
          ELSE IF(IPUNIT.EQ.4)THEN
           CALL PCON(PCI,PC(NCOMP),45,IERP)
          ELSE
           PC(NCOMP)=PCI
          ENDIF
          GOTO 400
         ENDIF
C
C          FOUND PER-PAR
C
         IF(CVALU(IS(1):IE(1)).EQ.'PER-PAR')THEN
C
          IFLAG=1
          CALL CONV(IFLAG,CVALU,IS(2),IE(2),PP(NCOMP),IDUM,IERC)
          GOTO 400
         ENDIF
C
C          FOUND PER-ARO
C
         IF(CVALU(IS(1).IE(1)).EQ.'PER-ARO')THEN
C
          IFLAG=1
          CALL CONV(IFLAG,CVALU,IS(2),IE(2),PA(NCOMP),IDUM,IERC)
          GOTO 400
         ENDIF
C
C          FOUND PER-NAP
C
         IF(CVALU(IS(1):IE(1)).EQ.'PER-NAP')THEN
C
          IFLAG=1
          CALL CONV(IFLAG,CVALU,IS(2),IE(2),PN(NCOMP),IDUM,IERC)
          GOTO 400
         ENDIF
        ENDIF
       ENDIF
C
C       FOUND PRINT-OPT PKW
C
       IVAL1=INDEX(REC1,'PRINT-OPT')
       IF(IVAL1.EQ.1)THEN
600     ICNT=0
        READ(NIN,1000,END=9000)REC2
C
C       FILTER OUT BAD CHARACTERS AND CAPITALIZE IF NECESSARY
C
        DO 650 IC=1,80
         INCHA=REC2(IC:IC)
         CALL CAPS(INCHA,OUTCHA)
         REC2(IC:IC)=OUTCHA
650     CONTINUE
C
C       ECHO INPUT
C
       CALL STRIP(REC2,INUM,NHSTRY,IERS)
C
C       LOOK FOR ;
C
       IF(REC2(1:1).EQ.';')GOTO 600
C
C       CHECK IF FIRST CHAR IS NON BLANK
```

```
C
      IF(REC2(1:1).NE.' ')THEN
       REC1=REC2
       GOTO 101
      ENDIF
C
C       FOUND CAL-DBUG SKW
C
       IVAL2=INDEX(REC2,'CAL-DBUG')
       IF(IVAL2.NE.0)THEN
        CVALU=REC2(IVAL2+8:80)
        CALL EXTOK(IS,IE,CVALU,ICNT)
        IF(ICNT.LE.0)THEN
         IERR=-1
         GOTO 600
        ENDIF
        IFLAG=0
        CALL CONV(IFLAG,CVALU,IS(1),IE(1),RDUM,LDBUG,IERC)
        IF(IERC.GT.0)THEN
         CALL MESS(1)
         WRITE(NHSTRY,5060)
         IERR=8
         LDBUG=0
        ENDIF
        IF(LDBUG.LT.0)LDBUG=0
        IF(LDBUG.GT.8)LDBUG=8
        GOTO 600
       ENDIF
C
C       FOUND REP-DBUG SKW
C
       IVAL2=INDEX(REC2,'REP-DBUG')
       IF(IVAL2.NE.0)THEN
        CVALU=REC2(IVAL2+8:80)
        CALL EXTOK(IS,IE,CVALU,ICNT)
        IF(ICNT.LE.0)THEN
         IERR=-1
         GOTO 600
        ENDIF
        IFLAG=0
        CALL CONV(IFLAG,CVALU,IS(1),IE(1),RDUM,LDBUGR,IERC)
        IF(IERC.GT.0)THEN
         CALL MESS(1)
         WRITE(NHSTRY,5070)
         IERR=9
         LDBUGR=0
        ENDIF
        IF(LDBUGR.LT.0)LDBUGR=0
        IF(LDBUGR.GT.8)LDBUGR=8
        GOTO 600
       ENDIF
C
C       FOUND PROP-OPT= SKW
C
       IVAL2=INDEX(REC2,'PROP-OPT')
       IF(IVAL2.NE.0)THEN
        CVALU=REC2(IVAL2+8:80)
        IVAL3=INDEX(CVALU,'SYSOP')
        IF(IVAL3.NE.0)THEN
         IF(INDEX(CVALU,'-1').NE.0)THEN
          NSYSOP=-1
         ELSE
          IS(1)=IVAL3
          IE(2)=IVAL3+4
          IS(2)=IVAL3+5
          IE(2)=IVAL3+5
          IFLAG=0
          CALL CONV(IFLAG,CVALU,IS(2),IE(2),RDUM,NSYSOP,IERC)
```

```
            ENDIF
            GOTO 600
           ELSE
            REC1=REC2
            ISYSOP=0
            CALL MESS(2)
            WRITE(NHSTRY,5030)
            IERR=4
            GOTO 100
           ENDIF
          ENDIF
C
C         FOUND ASPENOUT SKW
C
          IVAL2=INDEX(REC2,'ASPENOUT')
          IF(IVAL2.NE.0)THEN
           CVALU=REC2(IVAL2+8:80)
           IF(INDEX(CVALU,'DFMS').NE.0)THEN
            IPTYPE=1
           ELSE IF(INDEX(CVALU,'IMP').NE.0)THEN
            IPTYPE=0
           ELSE
            CALL MESS(1)
            WRITE(NHSTRY,5080)
            IPTYPE=0
            IERR=5
           ENDIF
           GOTO 600
          ENDIF
C
C         FOUND REP-FILE SKW
C
          IVAL2=INDEX(REC2,'REP-FILE')
          IF(IVAL2.NE.0)THEN
           CVALU=REC2(IVAL2+8:80)
           CALL EXTOK(IS,IE,CVALU,ICNT)
           IF(ICNT.LE.0)THEN
            IERR=-1
            GOTO 600
           ENDIF
           FILE=CVALU(IS(1):IE(1))
           IFP=1
           GOTO 600
          ENDIF
          REC1=REC2
          GOTO 100
         ENDIF
C
C         FOUND END-INPUT  PKW
C
         IVAL1=INDEX(REC1,'END-INPUT')
         IF(IVAL1.NE.0)THEN
          GOTO 9100
         ENDIF
         GOTO 100
C
9000     WRITE(NHSTRY,5200)
C
C         WRITE SUMMARY TO .HIS FILE
C
9100     WRITE(NHSTRY,6000)NCOMP,INUM,LDBUG,LDBUGR,IDESC
         IF(NSYSOP.GE.0)THEN
          WRITE(NHSTRY,6040)NSYSOP
         ELSE
          WRITE(NHSTRY,6050)
         ENDIF
C
         IF(IPTYPE.EQ.0)THEN
```

```
       WRITE(NHSTRY,6010)
      ELSE
       WRITE(NHSTRY,6020)
      ENDIF
C
      IF(ICF.EQ.1)THEN
       WRITE(NHSTRY,6060)
      ELSE
       WRITE(NHSTRY,6070)
      ENDIF
C
      WRITE(NHSTRY,6030)FILE
C
      WRITE(NHSTRY,6100)
      WRITE(NHSTRY,5100)
C
C       FORMATS
C
 900  FORMAT(1H1,//,5X,'ESTPRO BEGINS EXECUTION',/,
     1               5X,'RUN MADE ON ',I2,'/',I2,'/',I2,//,
     2               5X,'INPUT ECHO FOR PROGRAM COMPEST',/,
     3               1X,'----',1X,62('-'))
1000  FORMAT(A80)
2000  FORMAT(2X,'IN READ OF FILE NAME')
5000  FORMAT(2X,'IN READ OF DESC, TOO MANY LINES, MAX=25')
5010  FORMAT(2X,'IN READ OF T-UNITS, DEFAULT T-UNITS=F SET')
5020  FORMAT(2X,'IN READ OF P-UNITS, DEFAULT P-UNITS=PSIA SET')
5030  FORMAT(2X,'IN READ OF SYSOP NUMBER, DEFAULT TO SYSOP0')
5040  FORMAT(2X,'IN READ OF TC, TC WILL BE ESTIMATED')
5050  FORMAT(2X,'IN READ OF PC, PC WILL BE ESTIMATED')
5060  FORMAT(2X,'IN READ OF CAL-DBUG, CAL-DBUG SET TO 0')
5070  FORMAT(2X,'IN READ OF REP-DBUG, REP-DBUG SET TO 0')
5080  FORMAT(2X,'IN READ OF ASPENOUT TYPE (DFMS,INPUT), INPUT ASSUMED')
5100  FORMAT(1H1,//,5X,'COMPONENT ESTIMATION SUMMARY',/)
5200  FORMAT(2X,'END-INPUT NOT FOUND, END-INPUT IS ASSUMED')
C
6000  FORMAT(1H1,//,
     1 T5,'*************************************************************'/
     2 T5,'*                                                           *'/
     3 T5,'*                     INPUT SUMMARY                         *'/
     4 T5,'*                                                           *'/
     5 T5,'*     NUMBER OF COMPOUNDS.................',I10,    '       *'/
     6 T5,'*     NUMBER OF INPUT LINES...............',I10,    '       *'/
     7 T5,'*     SIMULATION DEBUG NUMBER.............',I10,    '       *'/
     8 T5,'*     REPORT DEBUG NUMBER.................',I10,    '       *'/
     9 T5,'*     NUMBER OF DESC. STORED..............',I10,    '       *')
6010  FORMAT(T5,'*     ASPEN PRINT TYPE.....................      INPUT',
     1     '       *')
6020  FORMAT(T5,'*     ASPEN PRINT TYPE.....................       DFMS ',
     1     '       *')
6030  FORMAT(T5,'*     REP FILE NAME: ',A32,
     1     '       *')
6040  FORMAT(T5,'*     SYSOP NUMBER........................',I10,
     1     '       *')
6050  FORMAT(T5,'*     SYSOP NUMBER.........................        ALL',
     1     '       *')
6060  FORMAT(T5,'*     BOILING POINT CONV TYPE..............   ASTHD86',
     1     '       *')
6070  FORMAT(T5,'*     BOILING POINT CONV TYPE..............        TBP',
     1     '       *')
6100  FORMAT(
     1 T5,'*                                                           *'/
     2 T5,'*************************************************************',
     3 /)
C
      RETURN
      END
C*************************************************************************
```

```
C
      SUBROUTINE STRIP(REC,INUM,IOLOG,IERR)
C
C*****************************************************************************
C
C       NAME OF MODULE - STRIP
C       MODULE TITLE - RECORD TRAILING STRIPPER
C       PURPOSE - TO STRIP OFF TRAILING BLANKS FROM A RECORD AND WRITE
C                 OUT (UTILITY FOR INPT)
C       MODIFIED - 12-16-88
C
C
C       VARIABLES USED-
C
C VARIABLE I/O TYPE-SPEC DIMENSION      DESCRIPTION AND RANGE
C     REC    I/O      C         80      RECORD TO BE WRITTEN
C    INUM     I       I          -      INTEGER NUMBER OF RECORD
C   IOLOG     I       I          -      I/O LOGICAL NUMBER
C    IERR     O       I          -      ERROR FLAG
C                                       0 = OK
C                                       1 = NO CHARACTERS IN RECORD
      IMPLICIT INTEGER(I-N)
      CHARACTER*80      REC
C
      IERR=0
      INUM=INUM+1
C
      CALL FEND(REC,IE,IERR)
      IF(IERR.GT.0)GOTO 9990
      WRITE(IOLOG,1000)INUM,REC(1:IE)
C
C      FORMATS
C
1000  FORMAT(1X,I4,1X,A)
C
9990  RETURN
      END
C*****************************************************************************
C
      SUBROUTINE LMVABP(JC,IERR)
C
C*****************************************************************************
C
C       NAME OF MODULE - LMVABP
C       MODULE TITLE - LIQUID MOLAR VOLUME AT BOILING POINT
C       PURPOSE - TO CALC LIQUID MOLAR VOLUME AT THE NORMAL BOILING
C                 POINT
C       MODIFIED - 11-15-88
C       METHOD - ESTIMATE LMV AT 20 C AND 1 ATM BY RAIZI DAUBERT METHOD
C                AND CORRECT TO BOILING POINT BY GUNN & YAMADA METHOD
C
C
C       VARIABLES USED-
C
C VARIABLE I/O TYPE-SPEC DIMENSION      DESCRIPTION AND RANGE
C     JC     I       I          -      COMPONENT ARRAY ID
C   IERR     O       I          -      ERROR CODE
C                                       0 = OK
C                                      -1 = REDUCED TEMP > 0.99
C                                      -2 = REDUCED TEMP < 0.2
C
C
      IMPLICIT REAL*8 (A-H,O-Z)
      IMPLICIT INTEGER(I-N)
C
      PARAMETER        (MNC=25)
C
      COMMON /IO     / NIN,NOUT,NHSTRY,NREPT
```

```
      COMMON /DEBUG / LDBUG,LDBUGR
C
      COMMON /NPROP3/ UOPK(MNC),API(MNC),SG(MNC),AMW(MNC)
C
      COMMON /CPRP01/ TC(MNC)
      COMMON /CPRP05/ OMEGA(MNC)
      COMMON /CPRP14/ TB(MNC)
      COMMON /CPRP15/ VB(MNC)
C
      IERR=0
      IF(LDBUG.GT.7)WRITE(NHSTRY,900)
C
C       LIQUID MOLAR VOLUME AT 20 DEG C AND 1 ATM (CM**3/G-MOLE)
C
      CALL TCON(TB(JC),T1,42,IERRT)
      S1=SG(JC)
C
C       CHECK LIMITS ON VOL CALC
C
      IF(T1.LT.569.67D0.OR.T1.GT.1309.67)THEN
       CALL MESS(1)
       WRITE(NHSTRY,900)
       WRITE(NHSTRY,1000)T1
      ENDIF
C
      IF(S1.LT.0.6247D0.OR.S1.GT.1.0244D0)THEN
       CALL MESS(1)
       WRITE(NHSTRY,900)
       WRITE(NHSTRY,2000)S1
      ENDIF
C
      V=7.6211D-5 * T1**(2.1262D0) * S1**(-1.8688D0)
C
C       LIQUID MOLAR VOLUME AT 20 DEG C AND 1 ATM (M**3/KG-MOLE)
C
      VR=V/1.D6*1000.D0
C
C       CORRECT TO BOILING POINT TEMPERATURE TB
C
      TR=(20.D0+273.15D0)/TC(JC)
      TBKR=TB(JC)/TC(JC)
      ICALC1=0
      OMEGAT=OMEGA(JC)
C
      CALL GUNYAM(VR,TR,OMEGAT,TBKR,ICALC1,VOL,IERR1)
      IERR=IERR1
C
      VB(JC)=VOL
C
C       FORMATS
C
900   FORMAT(1X,'IN MODULE LMVABP')
1000  FORMAT(1X,'TB(DEG R) VALUE IS NOT IN RANGE 569.67-1309.67',/,
     |       1X,'TB-VALUE = ',G12.6,' CALC. CONTINUES')
2000  FORMAT(1X,'SG VALUE IS NOT IN RANGE 0.6247-1.0244',/,
     |       1X,'SG VALUE = ',G12.6,' CALC. CONTINUES')
      RETURN
C
      END
C*********************************************************************
C
      SUBROUTINE MAXBN1(MABPF,UOPK,SG,MAXIT,NDAT,ST,BT,JC,IERR)
C
C*********************************************************************
C
C       NAME OF MODULE - MAXBN1
C       MODULE TITLE - VAPOR PRESSURES USING MAXWELL-BONELL
C       PURPOSE - TO CALCULATE VAPOR PRESSURES USING MAXWELL-BONELL
```

```
C         METHOD OF TRIAL AND ERROR FOR THE ESTIMATION OF PRESSURES BASED
C         UPON BENZENE AS A STANDARD. REFERENCE:I+EC,VOL.49,1187,JULY 1957
C         FIT TO NDAT(50) DATA POINTS IN THE RANGE (ST-BT)
C        MODIFIED - 11-4-88 AND COMPLETED
C
C        VARIABLES USED-
C
C VARIABLE I/O TYPE-SPEC DIMENSION      DESCRIPTION AND RANGE
C  MABPF     I       R          -       MEAN AVG BOILING POINT DEG F
C   UOPK     I       R          -       UOP K OR WATSON K
C     SG     I       R          -       SPECIFIC GRAVITY (60/60F)
C  MAXIT     I       I          -       MAXIMUM ITERATIONS ON CALC
C   NDAT     I       I          -       NUMBER OF DATA POINTS (DEF=50)
C     ST     I       R          -       SMALL TEMP (F) (DEF=-50F FROM VABPF)
C     BT     I       R          -       BIG TEMP (F) (DEF=+50F FROM VABPF)
C     JC     I       I          -       COMPONENT ARRAY ID
C   IERR     O       I          -       ERROR CODE
C                                        0 = OK
C                                       -1 = NO IMPROVEMENT POSSIBLE IN
C                                            THE VALUE OF PH EVEN THOUGH
C                                            CONVERGENCE HAS NOT BEEN REACHED.
C                                       -2 = MORE UNKNOWNS THAN FUNCTIONS AND
C                                            UNIQUE SOLUTION GENERALLY IS
C                                            IMPOSSIBLE.
C                                       -3 = TOTAL NUMBER OF VARIABLES TO BE
C                                            VARIED IS ZERO
C                                       -4 = CONVERGENCE CRITERION MET BUT FLA
C                                            STILL LARGE
C                                       -5 = IC NOT A VALID NUMBER ON ENTRY
C                                       -6 = X(I) IS NOT WITHIN XMIN(I) TO
C                                            XMAX(I)
C                                       -7 = ZERO DIAGONAL ELEMENT IN EQUATION
C                                            SOLVE
C                                      -10 = TRY TO CALC. DERIVATIVE
C                                             ANALYTICALY
C                                      -11 = RUN EXCEEDED MAXIT SPECIFIED
C
      IMPLICIT REAL*8 (A-H,O-Z)
      IMPLICIT INTEGER(I-N)
C
      REAL*8            MABPF
C
      PARAMETER         (MNC=25)
C
      COMMON /IO      / NIN,NOUT,NHSTRY,NREPT
      COMMON /DEBUG   / LDBUG,LDBUGR
C
      COMMON /CPRP06/ PLXANT(9,MNC),PLXREG(3,MNC)
C
      DIMENSION         NDATA(26),DATA(16),OUTPUT(6)
C
      DIMENSION         X(50),Y(50),
     1                  Z(100),PJ(50),P(206),A(15),AC(15)
C     |                   Z(100),PJ(50),P(154),A(15),AC(15)
      DIMENSION         B(6),BV(3),BMAX(3),BMIN(3)
C
      IF(LDBUG.GT.7)WRITE(NHSTRY,900)
C
C       SET DEFAULTS
C
C       NUMBER OF UNKNOWNS
      K=3
C       NUMBER OF DATA POINTS
C
      IF(NDAT.GT.0.AND.NDAT.LE.50)THEN
       N=NDAT
      ELSE
C       DEFAULT
```

```
        NDAT=50
        N=NDAT
       ENDIF
C
       IF(ST.LE.0.0D0)ST=MABPF-40.D0
       IF(BT.LE.0.0D0)BT=MABPF+40.D0
C
       IF(LDBUG.GE.5)THEN
        DEGFR=FLOAT(N-K)
       ENDIF
C
       ITER = 0
       IF(MAXIT.LE.0)MAXIT=10000
C
C       SET EQUAL TO 1 FOR INITAL CALL
       NDATA(1)=1
C
C         SET INPUT PARAMETER DATA
C                    DATA(1) - FNU, FACTOR USED TO CHANGE FLA.  SET INTER-
C                              NALLY TO 10.0  IF ZERO ON INITIAL CALL.
C                    DATA(2) - FLA, FACTOR USED TO COMBINE GRADIENT AND
C                              NEWTON-RAPHSON METHODS.  SET INTERNALLY TO
C                              .01 IF ZERO ON INITIAL CALL.
C                    DATA(3) - TAU, USED IN CONVERGENCE TEST.  SET INTER-
C                              NALLY TO 0.001 IF ZERO ON INITIAL CALL.
C                    DATA(4) - EPS, USED IN CONVERGENCE TEST.  SET INTER-
C                              NALLY TO 0.00002 IF ZERO ON INITIAL CALL.
C                    DATA(5) - PHMIN, WHEN PH .LT. PHMIN, PARTIAL DERIV-
C                              ITIVES FROM THE PREVIOUS ITERATION ARE USED
C                              INSTEAD OF COMPUTING THEM AGAIN.
C                    DATA(6) THRU DATA(16) - VARIABLES USED INTERNALLY
C
       DO 10 I=1,5
        DATA(I)=0.0D0
10     CONTINUE
C
C       BV = VARY VECTOR (0=HOLD PARAMTER CONST,1=ALLOW TO VARY)
C
       DO 20 I=1,K
        BV(I)=1.D0
20     CONTINUE
C
C       INITAL VALUES OF PARMS
C
       B(1)=10.D0
       B(2)=-1000.D0
       B(3)=1.D0
C
C       MIN AND MAX VALUES
C
       BMAX(1)=2000.D0
       BMIN(1)=-2000.D0
       BMAX(2)=200000.D0
       BMIN(2)=-900000.D0
       BMAX(3)=20000.D0
       BMIN(3)=-20000.D0
C
       IF(LDBUG.GE.7)THEN
        WRITE(NHSTRY,1008)K,N
        DO 30 I=1,K
         WRITE(NHSTRY,1009)B(I),BMIN(I),BMAX(I),BV(I)
30      CONTINUE
        WRITE(NHSTRY,1010)
        WRITE(NHSTRY,1100)
        XSUM=0.0D0
        XSUM2=0.0D0
        YSUM=0.0D0
        YSUM2=0.0D0
```

```
      ENDIF
C
C       BEGIN CALC (CALC 5 POINTS TO BE FIT)
C        LOG(PA)=A+B/(C+TEMP(K))
C
      DEL=(BT-ST)/FLOAT(NDAT)
      T=ST-DEL
C
      DO 40 I=1,NDAT
       T=T+DEL
       CALL MAXBN2(MABPF,UOPK,SG,T,MAXIT,PA,IERR2)
C
C        CHECK IERR
C
       IF(IERR2.EQ.0.OR.IERR2.EQ.-1.OR.IERR2.EQ.-4)THEN
        CALL TCON(T,X(I),14,IERT)
        Y(I)=LOG(PA)
       ELSE
        CALL TCON(MABPF,X(I),14,IERT)
        Y(I)=LOG(1.01325D5)
       ENDIF
C
       IF(LDBUG.GE.7)THEN
        WRITE(NHSTRY,1020)X(I),Y(I)
        XSUM=XSUM+X(I)
        XSUM2=XSUM2+X(I)**2
        YSUM=YSUM+Y(I)
        YSUM2=YSUM2+Y(I)**2
       ENDIF
40    CONTINUE
C
C       MEANS, VARIANCES AND STANDARD DEV.
C
      IF(LDBUG.GE.7)THEN
       XMEAN=XSUM/FLOAT(N)
       XVAR=(FLOAT(N)*XSUM2-XSUM*XSUM)/FLOAT(N)/FLOAT(N-1)
       XSD=SQRT(XVAR)
       YMEAN=YSUM/FLOAT(N)
       YVAR=(FLOAT(N)*YSUM2-YSUM*YSUM)/FLOAT(N)/FLOAT(N-1)
       YSD=SQRT(YVAR)
       WRITE(NHSTRY,1120)XMEAN,YMEAN,XVAR,YVAR,XSD,YSD
      ENDIF
C
C       BEGIN REGRESSION
C
50    ITER=ITER+1
      IF(ITER.GT.MAXIT)THEN
       CALL MESS(2)
       WRITE(NHSTRY,900)
       IERR=-11
       WRITE(NHSTRY,1045)MAXIT,ITER
       GOTO 9000
      ENDIF
C
C        EVALUATE Z VECTOR (FUNCTION VALUE)
C        EQUATION OF FORM LN(PRES)=A+B/(C+T)
C
      DO 60 I=1,N
       Z(I)=(B(1)+B(2)/(X(I)+B(3)))
60    CONTINUE
C
C      CALC ANALYTICAL DERIVATIVES (PJ VECTOR)
C
70    CONTINUE
C
C        CALC DERIVATIVE
C
      IF(NDATA(2).GT.0)THEN
```

```
        IERR=-10
        CALL MESS(3)
        WRITE(NHSTRY,900)
        WRITE(NHSTRY,1090)IERR
        GOTO 9000
       ENDIF
C
C
       IF(LDBUG.GE.7)THEN
        WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
        YMYC =0.0D0
        SS   =0.0D0
        SSSAS=0.0D0
        DO 90 I=1,N
         YMYC=YMYC+(Y(I)-Z(I))**2
         SS=SS+(Z(I)-YMEAN)**2
         SSSAS=SSSAS+(Y(I)**2 - YMEAN**2)
90      CONTINUE
C
C       CALC R-SQUARE(SAS VERSION) AND ADJ R-SQUARE
C            1-VARIANCE OF FULL MODEL/VARIANCE OF MEAN MODEL
C
        RSQU=SS/(SS+YMYC)
        IF(SSSAS.NE.0.D0)THEN
         RSQUSAS=1.D0-YMYC/(SSSAS)
        ELSE
         RSQUSAS=0.D0
        ENDIF
        IF(DEGFR.EQ.0.D0)THEN
         ADJRSQU=0.0D0
        ELSE
         ADJRSQU=1.D0-(1.D0-RSQU)*(FLOAT(N)-1.D0)/DEGFR
        ENDIF
        IF(ABS(RSQU-RSQUSAS).GT.1.D8)THEN
         WRITE(NHSTRY,1112)RSQU,ADJRSQU,RSQUSAS,ADJRSQUSAS
        ELSE
         WRITE(NHSTRY,1110)RSQU,ADJRSQU
        ENDIF
C
        DO 100 J=1,K
         WRITE(NHSTRY,1030)J,B(J)
100     CONTINUE
C
        IF(LDBUG.EQ.0)THEN
         WRITE(NHSTRY,1040)
         DO 110 I=1,N
          YMYC=YMYC+(Y(I)-Z(I))**2
          SS=SS+(Z(I)-YMEAN)**2
          PERERR=ABS(Z(I)-Y(I))/ABS(Y(I))*100.D0
          WRITE(NHSTRY,1095)I,Z(I),Y(I),Z(I)-Y(I),PERERR
110      CONTINUE
         ENDIF
       ENDIF
C
120    CALL YSOLVE (K, N, NDATA, DATA, B, BV, BMAX, BMIN, Y, Z, PJ,
     1              OUTPUT, P, A, AC)
C
C                      NDATA(2) - NFCTDR, USED FOR CONTROL IN CALLING PROG
C                         IF = 0, CALCULATE FUNCTION
C                         IF = 1, CALCULATE DERIVATIVE
C                         IF =-1, EXAMINE IERR FOR WHAT TO DO NEXT
C
       IF(NDATA(2))130,50,70
C
C                      NDATA(3) - IERR, MAY TAKE ON VARIOUS VALUES
C                         IF POSITIVE, CONTAINS THE NUMBER OF VARIABLES NO
C                                      SATISFYING CONVERGENCE CRITERION
C                         IF =  0, CONVERGENCE SATISFIED AND SOLUTION RETU
```

```
C                          IF = -1, NO IMPROVEMENT POSSIBLE IN THE VALUE OF
C                                   PH EVEN THOUGH CONVERGENCE HAS NOT BEEN
C                                   REACHED.
C                          IF = -2, MORE UNKNOWNS THAN FUNCTIONS AND UNIQUE
C                                   SOLUTION GENERALLY IS IMPOSSIBLE.
C                          IF = -3, TOTAL NUMBER OF VARIABLES TO BE VARIED
C                                   IS ZERO
C                          IF = -4, CONVERGENCE CRITERION MET BUT FLA STILL
C                                   LARGE
C                          IF = -5, IC NOT A VALID NUMBER ON ENTRY
C                          IF = -6, B(I) IS NOT WITHIN BMIN(I) TO BMAX(I)
C                          IF = -7, ZERO DIAGONAL ELEMENT IN EQUATION SOLVE
C
130     IF(NDATA(3))140,140,120
C
C        FINAL STATISTICAL RESULTS
C
140     CONTINUE
        IF(LDBUG.GE.6)THEN
         WRITE(NHSTRY,900)
         WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
         YMYC  =0.0D0
         SS    =0.0D0
         SSSAS =0.0D0
         DO 150 I=1,N
          YMYC=YMYC+(Y(I)-Z(I))**2
          SS=SS+(Z(I)-YMEAN)**2
          SSSAS=SSSAS+(Y(I)**2-YMEAN**2)
150      CONTINUE
C
C        CALC R-SQUARE(SAS VERSION) AND ADJ R-SQUARE
C
C         RSQUSAS=1-VARIANCE (FULL MODEL)/VARIANCE (MEAN MODEL)
C
         RSQU=SS/(SS+YMYC)
         RSQUSAS=1.D0-YMYC/(SSSAS)
         IF(DEGFR.EQ.0.0D0)THEN
          ADJRSQU=0.0D0
          ADJRSQUSAS=0.0D0
         ELSE
          ADJRSQU=1.D0-(1.D0-RSQU)*(FLOAT(N)-1.D0)/DEGFR
          ADJRSQUSAS=1.D0-(1.D0-RSQUSAS)*(FLOAT(N)-1.D0)/DEGFR
         ENDIF
         IF(ABS(RSQU-RSQUSAS).GT.1.D8)THEN
          WRITE(NHSTRY,1112)RSQU,ADJRSQU,RSQUSAS,ADJRSQUSAS
         ELSE
          WRITE(NHSTRY,1110)RSQU,ADJRSQU
         ENDIF
C
C        FINAL PARAMETERS
C
        DO 160 J=1,K
         WRITE(NHSTRY,1030)J,B(J)
160     CONTINUE
C
C        FINAL SUMMARY
C
        WRITE(NHSTRY,1040)
        DO 170 I=1,N
         PERERR=ABS(Z(I)-Y(I))/ABS(Y(I))*100.D0
         WRITE(NHSTRY,1095)I,Z(I),Y(I),Z(I)-Y(I),PERERR
170     CONTINUE
       ENDIF
C
C       LOAD DATA INTO PLXANT ARRAY
C
       IERR=NDATA(3)
       DO 180 JJ=1,9
```

```
          PLXANT(JJ,JC)=0.0D0
180     CONTINUE
C
        IF(IERR.EQ.0)THEN
C
C        CONVERGED
C
         PLXANT(1,JC)=B(1)
         PLXANT(2,JC)=B(2)
         PLXANT(3,JC)=B(3)
         PLXANT(8,JC)=ST
         PLXANT(9,JC)=BT
C
         IF(LDBUG.GE.1)THEN
          WRITE(NHSTRY,900)
          WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
         ENDIF
        ELSE IF(IERR.EQ.-1)THEN
         PLXANT(1,JC)=B(1)
         PLXANT(2,JC)=B(2)
         PLXANT(3,JC)=B(3)
         PLXANT(8,JC)=ST
         PLXANT(9,JC)=BT
         CALL MESS(1)
         WRITE(NHSTRY,900)
         WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
         WRITE(NHSTRY,1001)
        ELSE IF(IERR.EQ.-2)THEN
         PLXANT(1,JC)=B(1)
         PLXANT(2,JC)=B(2)
         PLXANT(3,JC)=B(3)
         PLXANT(8,JC)=ST
         PLXANT(9,JC)=BT
         CALL MESS(1)
         WRITE(NHSTRY,900)
         WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
         WRITE(NHSTRY,1002)
        ELSE IF(IERR.EQ.-3)THEN
         CALL MESS(2)
         WRITE(NHSTRY,900)
         WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
         WRITE(NHSTRY,1003)
        ELSE IF(IERR.EQ.-4)THEN
         PLXANT(1,JC)=B(1)
         PLXANT(2,JC)=B(2)
         PLXANT(3,JC)=B(3)
         PLXANT(8,JC)=ST
         PLXANT(9,JC)=BT
         CALL MESS(2)
         WRITE(NHSTRY,900)
         WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
         WRITE(NHSTRY,1004)
        ELSE IF(IERR.EQ.-5)THEN
         CALL MESS(2)
         WRITE(NHSTRY,900)
         WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
         WRITE(NHSTRY,1005)
        ELSE IF(IERR.EQ.-6)THEN
         CALL MESS(2)
         WRITE(NHSTRY,900)
         WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
         WRITE(NHSTRY,1006)
        ELSE IF(IERR.EQ.-7)THEN
         CALL MESS(2)
         WRITE(NHSTRY,900)
         WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
         WRITE(NHSTRY,1007)
        ENDIF
```

```
      PLXREG(1,JC)=FLOAT(ITER)
      PLXREG(2,JC)=FLOAT(NDATA(3))
      PLXREG(3,JC)=OUTPUT(1)
C
C       FORMATS
C
900   FORMAT(1X,'IN MODULE MAXBN1')
1000  FORMAT(/,
     1 1X,'ITERATION: ',I9,/,
     2 1X,'IERR                                          = ',I15,/,
     3 1X,'SUM OF SQUARES                                = ',G15.8,/,
     4 1X,'ANGLE (DEGREES)                               = ',F15.2,/,
     5 1X,'NUMBER OF TIMES YSOLVE CALLED                 = ',F15.1,/,
     6 1X,'NUMBER OF FUNCTIONAL EVALUATIONS              = ',F15.1,/,
     7 1X,'NUMBER OF ANALYTICAL DERIVATIVE EVALUATIONS   = ',F15.1,/)
1001  FORMAT(1X,'NO IMPROVEMENT POSSIBLE IN THE VALUE OF',/,
     1 1X,'PH EVEN THOUGH CONVERGENCE HAS NOT BEEN REACHED.',/)
1002  FORMAT(1X,'MORE UNKNOWNS THAN FUNCTIONS AND UNIQUE',/)
1003  FORMAT(1X,'TOTAL NUMBER OF VARIABLES TO BE VARIED = 0',/)
1004  FORMAT(1X,'CONVERGENCE CRITERION MET BUT FLA STILL LARGE',/)
1005  FORMAT(1X,'IC NOT A VALID NUMBER ON ENTRY',/)
1006  FORMAT(1X,'X(I) IS NOT WITHIN XMIN(I) TO XMAX(I)',/)
1007  FORMAT(1X,'ZERO DIAGONAL ELEMENT IN EQUATION SOLVE',/)
1008  FORMAT(1H1,/,5X,1X,'*****MARQUARDT METHOD REGRESSION*****',//,
     1 5X,1X,'K (NUMBER OF PARAMETERS TO BE VARIED) = ',I4,/,
     2 5X,1X,'N (NUMBER OF DATA POINTS)             = ',I4,//,
     3 5X,'INITAL B            B-MIN            B-MAX',
     4'VARY FLAG',/)
1009  FORMAT(2X,4(G15.5,1X))
1010  FORMAT(5X,1X,'VARY FLAG:',/,
     1 10X,'0 = HOLD PARAMETER CONSTANT',/,
     2 10X,'1 = VARY PARAMETER USING NUMERICAL DERIVATIVE',/,
     3 9X,'-1 = VARY PARAMETER USING ANALYTICAL DERIVATIVE')
1020  FORMAT(1X,3G15.6)
1030  FORMAT(1X,'B(',I2,') = ',G13.5)
1040  FORMAT(/,1X,'OBS.  Y-CALC         Y-ACTUAL        DIFF.          ',
     1 '% ERROR',/)
1095  FORMAT(  1X,I4,  4(1X,G13.5))
1100  FORMAT(/,10X,'INPUT DATA',//,
     1 5X,'X-VALUE         Y-VALUE ',/,
     2 5X,'-------         ------- ',/)
1110  FORMAT(
     1 1X,'R-SQUARE                                      = ',F15.8,/,
     2 1X,'ADJ R-SQUARE                                  = ',F15.8,/)
1112  FORMAT(
     1 1X,'R-SQUARE                                      = ',F15.8,/,
     2 1X,'ADJ R-SQUARE                                  = ',F15.8,/,
     3 1X,'R-SQUARE(1-VAR.FM/VAR.MM)                     = ',F15.8,/,
     4 1X,'ADJ R-SQUARE(FOR 2ND R-SQUARE)                = ',F15.8,/)
1120  FORMAT(//,10X,'STATISTICS',//,
     1 5X,'X-VALUES ',26X,'Y-VALUES',/,
     2 5X,'---------',26X,'---------',/,
     3 5X,'MEAN      = ',G15.5,8X,'MEAN      = ',G15.5,/
     4 5X,'VARIANCE  = ',G15.5,8X,'VARIANCE  = ',G15.5,/
     5 5X,'STD. DEV. = ',G15.5,8X,'STD. DEV. = ',G15.5,/)
1045  FORMAT(/,1X,'*****RUN EXCEEDED MAXIT OF ',I5,' ITER = ',I5,
     2          '*****'//)
1090  FORMAT(1X,'IERR = ',I5,' TRY TO CALC.',
     i       ' DERIVATIVE ANALYTICALY, CALC. ABORTED')
9000  CONTINUE
      RETURN
      END
C*******************************************************************************
C
      SUBROUTINE MAXBN2(MABPF,UOPK,SG,TF,MAXIT,PA,IERR)
C
C*******************************************************************************
C
```

```
C        NAME OF MODULE - MAXBN2
C        MODULE TITLE - VAPOR PRESSURES USING MAXWELL-BONELL
C        PURPOSE - TO CALCULATE VAPOR PRESSURES USING MAXWELL-BONELL
C         METHOD OF TRIAL AND ERROR FOR THE ESTIMATION OF PRESSURES BASED
C         UPON BENZENE AS A STANDARD. REFERENCE:I+EC,VOL.49,1187,JULY 1957
C         FOR ONE TEMPERATURE
C        MODIFIED - 11-4-88
C
C        VARIABLES USED-
C
C VARIABLE I/O TYPE-SPEC DIMENSION      DESCRIPTION AND RANGE
C  MABPF     I       R          -       MEAN AVG BOILING POINT DEG F
C   UOPK     I       R          -       UOP K OR WATSON K
C     SG     I       R          -       SPECIFIC GRAVITY (60/60F)
C     TF     I       R          -       TEMPERATURE OF VP (F)
C  MAXIT     I       I          -       MAXIMUM ITERATIONS ON CALC
C     PA     O       R          -       VAPOR PRESSURE (PA)
C   IERR     O       I          -       ERROR CODE
C                                        0 = OK
C                                       -1 = NO IMPROVEMENT POSSIBLE IN
C                                            THE VALUE OF PH EVEN THOUGH
C                                            CONVERGENCE HAS NOT BEEN REACHED.
C                                       -2 = MORE UNKNOWNS THAN FUNCTIONS AND
C                                            UNIQUE SOLUTION GENERALLY IS
C                                            IMPOSSIBLE.
C                                       -3 = TOTAL NUMBER OF VARIABLES TO BE
C                                            VARIED IS ZERO
C                                       -4 = CONVERGENCE CRITERION MET BUT FLA
C                                            STILL LARGE
C                                       -5 = IC NOT A VALID NUMBER ON ENTRY
C                                       -6 = X(I) IS NOT WITHIN XMIN(I) TO
C                                            XMAX(I)
C                                       -7 = ZERO DIAGONAL ELEMENT IN EQUATION
C                                            SOLVE
C                                      -10 = TRY TO CALC. DERIVATIVE
C                                             ANALYTICALY
C                                      -11 = RUN EXCEEDED MAXIT SPECIFIED
C
      IMPLICIT REAL*8 (A-H,O-Z)
      IMPLICIT INTEGER(I-N)
C
      REAL*8           MABPF
C
      COMMON /IO     / NIN,NOUT,NHSTRY,NREPT
      COMMON /DEBUG  / LDBUG,LDBUGH
C
      DIMENSION        NDATA(26),DATA(16),OUTPUT(6)
C
      DIMENSION        X(2),XV(1),XMAX(1),XMIN(1),Y(1),
     1                 Z(2),PJ(1),P(4),A(3),AC(3)
C
      IF(LDBUG.GT.7)WRITE(NHSTRY,900)
C
C       SET DEFAULTS
C
C       NUMBER OF UNKNOWNS
      N=1
C       NUMBER OF EQUATIONS
      N=1
C
      ITER = 0
C
C       INITIAL GUESS
C
C       X(1) = 10.D0**(-2.34D-2*MABPF)
       X(1) = 500.D0
C
      NDATA(1)=1
```

```
C
      DO 10 I=1,5
       DATA(I)=0.0D0
10    CONTINUE
      DO 20 I=1,K
       XV(I)=1.D0
       Y(I)=0.D0
       XMAX(I)= 500000.D0
       XMIN(I)= 1.0D-20
20    CONTINUE
      IF(X(1).LT.XMIN(1))X(1)=XMIN(1)
      IF(X(1).GT.XMAX(1))X(1)=XMAX(1)
C
      TR=459.67D0
C
C      CALC BEGINS
C
      RTP=TF+TR
C
C        IF UOPK LE.0 THEN CALC UOPK FROM BP AND SG
C
      IF(UOPK.LE.0.D0) UOPK=MABPF**(1.D0/3.D0)/SG
C
C         MAX. BON. CONV. LOOP BEGINS
C
50    ITER=ITER+1
      IF(ITER.GT.MAXIT)THEN
       IERR=-11
       CALL MESS(2)
       WRITE(NHSTRY,900)
       WRITE(NHSTRY,1000)MAXIT,ITER
       GOTO 9000
      ENDIF
C
C         CHECK IF MEAN AVE BP IS GE 400
      IF(MABPF.GE.400.D0)THEN
       T=MABPF+TR+(2.5D0*(UOPK-12.D0)*(DLOG(1.D0/X(1))/2.30259D0))
C
C         CHECK IF MEAN AVE BP IS LE 200
      ELSE IF(MABPF.LE.200.D0)THEN
       T=MABPF+TR
      ELSE
C
C         MEAN AVE BP IN RANGE 200+ TO 400-
       EFK=0.005D0*MABPF-1.D0
C
C         FIRST TRIAL FROM BOILING POINT
       T=MABPF+TR+((2.5D0*(UOPK-12.D0)*(DLOG(1.D0/X(1))/2.30259D0))
     |    *EFK)
      ENDIF
C
      AX=T*((1.D0/RTP)-0.0002867D0),(748.1D0-(0.2145D0*T))
C
      IF( AX.GE.0.0021844D0)THEN
C
C        FOR VAPOR PRESSURE BELOW 2 MMHG (AX>0.0021844)
       PRE=(2876.663D0*AX-3.916264D0)/((43.D0*AX)-0.987673D0)
      ELSE IF(AX.LT.0.0013367D0)THEN
C
C         FOR VAPOR PRESSURE GT 760 MMHG (AX<0.0013367)
       PRE=((2666.376D0*AX)-3.56155D0)/((36.D0*AX)-0.989679D0)
      ELSE
C
C         FOR VAPOR PRESSURE IN RANGE 2-760 MMHG (AX=0.0013367-0.002184)
       PRE=((2387.262D0*AX)-3.192572D0)/((95.76D0*AX)-0.972546D0)
      ENDIF
C
C        PSAVE AND X(1) ARE IN ATMS
```

```
C
      PSAV=10.D0**PRE
C
      Z(1)=PSAV-X(1)
C
      CALL YSOLVE (K, N, NDATA, DATA, X, XV, XMAX, XMIN, Y, Z, PJ,
     1             OUTPUT, P, A, AC)
C
      IF(LDBUG.GT.5)THEN
       WRITE(NHSTRY,900)
       WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
      ENDIF
C
C      CALC FUNCTION
C
      IF(NDATA(2).EQ.0)THEN
       GOTO 50
C      CALC DERIVATIVE
      ELSE IF(NDATA(2).GT.0)THEN
       IERR=-10
       CALL MESS(3)
       WRITE(NHSTRY,900)
       WRITE(NHSTRY,1090)IERR
       GOTO 9000
      ENDIF
C      NDATA(2) < 0 CHECK NDATA(3)
C      NDATA(3) = NUMBER OF VARIABLES NOT SATISFYING CONV. CRITERION
      IF(NDATA(3).GT.0)GOTO 50
C
      IERR=NDATA(3)
C
C      CONVERGED OR PROBLEM
C
      IF(IERR.EQ.0)THEN
       CALL PCON(X(1),PA,35,IERP)
      ELSE IF(IERR.EQ.-1)THEN
       CALL PCON(X(1),PA,35,IERP)
       CALL MESS(1)
       WRITE(NHSTRY,900)
       WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
       WRITE(NHSTRY,1001)
      ELSE IF(IERR.EQ.-2)THEN
       CALL PCON(X(1),PA,35,IERP)
       CALL MESS(1)
       WRITE(NHSTRY,900)
       WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
       WRITE(NHSTRY,1002)
      ELSE IF(IERR.EQ.-3)THEN
       CALL MESS(2)
       WRITE(NHSTRY,900)
       WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
       WRITE(NHSTRY,1003)
      ELSE IF(IERR.EQ.-4)THEN
       CALL PCON(X(1),PA,35,IERP)
       CALL MESS(1)
       WRITE(NHSTRY,900)
       WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
       WRITE(NHSTRY,1004)
      ELSE IF(IERR.EQ.-5)THEN
       CALL MESS(2)
       WRITE(NHSTRY,900)
       WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
       WRITE(NHSTRY,1005)
      ELSE IF(IERR.EQ.-6)THEN
       CALL MESS(2)
       WRITE(NHSTRY,900)
       WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
       WRITE(NHSTRY,1006)
```

```
      ELSE IF(IERR.EQ.-7)THEN
       CALL MESS(2)
       WRITE(NHSTRY,900)
       WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
       WRITE(NHSTRY,1007)
      ENDIF
C
      IF(LDBUG.GT.5)THEN
       WRITE(NHSTRY,900)
       WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
       WRITE(NHSTRY,1100)TF,X(1),Z(1),PA
      ENDIF
C
C       FORMATS
C
900   FORMAT(1X,'IN MODULE MAXBN2')
1000  FORMAT(/,
     1     1X,'ITERATION: ',I9,/,
     2     1X,'IERR                                          = ',I15,/,
     3     1X,'SUM OF SQUARES                                = ',G15.8,/
     4     1X,'ANGLE (DEGREES)                               = ',F15.2,/,
     5     1X,'NUMBER OF TIMES YSOLVE CALLED                 = ',F15.1,/,
     6     1X,'NUMBER OF FUNCTIONAL EVALUATIONS              = ',F15.1,/,
     7     1X,'NUMBER OF ANALYTICAL DERIVATIVE EVALUATIONS   = ',F15.1,/)
1001  FORMAT(1X,'NO IMPROVEMENT POSSIBLE IN THE VALUE OF',/,
     1        1X,'PH EVEN THOUGH CONVERGENCE HAS NOT BEEN REACHED.',/)
1002  FORMAT(1X,'MORE UNKNOWNS THAN FUNCTIONS AND UNIQUE',/)
1003  FORMAT(1X,'TOTAL NUMBER OF VARIABLES TO BE VARIED = 0',/)
1004  FORMAT(1X,'CONVERGENCE CRITERION MET BUT FLA STILL LARGE',/)
1005  FORMAT(1X,'IC NOT A VALID NUMBER ON ENTRY',/)
1006  FORMAT(1X,'X(I) IS NOT WITHIN XMIN(I) TO XMAX(I)',/)
1007  FORMAT(1X,'ZERO DIAGONAL ELEMENT IN EQUATION SOLVE',/)
1080  FORMAT(/,
     1        /,1X,'*****RUN EXCEEDED MAXIT OF ',I5,' ITER = ',I5,
     2          '*****',/)
1090  FORMAT(1X,'IERR = ',I5,1X,'TRY TO CALC.',
     1        ' DERIVATIVE ANALYTICALY, CALC. ABORTED')
1100  FORMAT(1X,'TEMPERATURE (DEG F) = ',G12.6,/,
     1        ' PSAV = ' G12.6,' DELTA = ',G12.6,' PRESS(PA) = ',G12.6)
9000  CONTINUE
      RETURN
      END
C*******************************************************************************
C
      SUBROUTINE MESS(IRROR)
C
C*******************************************************************************
C
C        NAME OF MODULE - MESS
C        MODULE TITLE - WRITE OUT CALC MESSAGES
C        PURPOSE - TO WRITE OUT MESSAGES
C        MODIFIED - 10-28-88
C
C        VARIABLES USED-
C
C  VARIABLE I/O TYPE-SPEC DIMENSION      DESCRIPTION AND RANGE
C  IRROR      I       I          -       ERROR FLAG
C                                        0 = NONE
C                                        1 = 'WARNING' (POSSIBLE PROBLEM)
C                                        2 = **ERROR** (CONTINUE ON ERROR)
C                                        3 = ***SEVERE ERROR*** (STOP ON ERROR)
C
      IMPLICIT INTEGER(I-N)
C
      COMMON /IO     / NIN,NOUT,NHSTRY,NREPT
      COMMON /ERRC   / IWARN,INERR,ISERR
C
      IF(IRROR.EQ.0)GOTO 999
```

```
      IF(IRROR.EQ.1)THEN
       IWARN=IWARN+1
       WRITE(NHSTRY,1000)
      ELSE IF(IRROR.EQ.2)THEN
       INERR=INERR+1
       WRITE(NHSTRY,2000)
      ELSE IF(IRROR.EQ.3)THEN
       ISERR=ISERR+1
       WRITE(NHSTRY,3000)
      ENDIF
C
C       FORMATS
C
1000  FORMAT(5X,'*WARNING*')
2000  FORMAT(5X,'**ERROR**')
3000  FORMAT(5X,'***SEVERE ERROR***')
C
999   CONTINUE
      RETURN
      END
C*****************************************************************************
C
      SUBROUTINE NEED(IERR)
C
C*****************************************************************************
C
C        NAME OF MODULE - NEED
C        MODULE TITLE - CALC NEEDED PARAMETERS
C        PURPOSE - TO CALC NEEDED PARMATERS FROM INPUT DATA
C        MODIFIED - 10-28-88
C
C        VARIABLES USED-
C
C VARIABLE I/O TYPE-SPEC DIMENSION      DESCRIPTION AND RANGE
C   IERR     O       I          -       ERROR CODE
C                                        0 = OK
C                                       -1 = BOTH API AND UOP K VALUES SPEC.
C                                       -2 = BOTH API AND UOP K VALUES SPEC.
C                                            LESS THAN ZERO
C                                       -3 = AMW CALC OUT OF SPEC RANGE
C
      IMPLICIT REAL*8 (A-H,O-Z)
      IMPLICIT INTEGER(I-N)
C
      REAL*8           MABP,MEABP,MABPO
C
      PARAMETER        (MNC=25)
C
      CHARACTER*32     CNAME
C
      COMMON /IO     / NIN,NOUT,NHSTRY,NREPT
      COMMON /DEBUG  / LDBUG,LDBUGR
C
      COMMON /NPROP1/ NCOMP,CNAME(MNC),ICF
      COMMON /NPROP2/ VABP(MNC),SLOP(MNC),CABP(MNC),MABP(MNC),MEABP(MNC)
      COMMON /NPROP3/ UOPK(MNC),API(MNC),SG(MNC),AMW(MNC)
      COMMON /NPROP4/ PA(MNC),PN(MNC),PP(MNC),IPF
      COMMON /CALCV / NCALC(MNC)
C
      COMMON /EPROP1/ XPAR(MNC),XNAP(MNC),XARO(MNC)
C
      IF(LDBUG.GT.7)WRITE(NHSTRY,900)
C
      IERR=0
C
      OT=1.D0/3.D0
C
      DO 10 JC=1,NCOMP
```

```
          NCALC(JC)=1
C
C         CALC CABP AND MABP FROM VABP AND SLOPE OF TBP CURVE
C          OR ASTM CURVE
C
          CALL TCON(VABP(JC),VABPI,41,IERT)
          IF(ICF.EQ.1)THEN
           CALL ASTMCF(VABPI,SLOP(JC),CABPO,MABPO,IERC)
          ELSE
           CALL TBPCF(VABPI,SLOP(JC),CABPO,MABPO,IERC)
          ENDIF
          CALL TCON(CABPO,CABP(JC),14,IERT)
          CALL TCON(MABPO,MABP(JC),14,IERT)
C
C         CALC MEAN AVER BP
C
          MEABP(JC)=(CABP(JC)+MABP(JC))/2.D0
C
C         CHECK REST OF INPUT (SG,API,WK)
C
C          ALL SPECIFIED
C
          IF(API(JC).GT.0.D0.AND.UOPK(JC).GT.0.D0.AND.SG(JC).GT.0.0D0)THEN
           UOPK(JC)=0.D0
           SG(JC)=0.0D0
           CALL MESS(1)
           WRITE(NHSTRY,900)
           WRITE(NHSTRY,1000)
           IERR=-1
          ENDIF
C
C          NOT ENOUGH DATA
C
          IF(API(JC).LE.0.D0.AND.UOPK(JC).LE.0.D0.AND.
     1       SG(JC).LE.0.0D0)THEN
           CALL MESS(2)
           WRITE(NHSTRY,900)
           WRITE(NHSTRY,2000)
           NCALC(JC)=0
           IERR=-2
C
C         IF API GIVEN CALC WATSON K AND SG
C
          ELSE IF(API(JC).GT.0.D0.AND.UOPK(JC).LE.0.D0.AND.
     1            SG(JC).LE.0.D0)THEN
           SG(JC)=141.5D0/(API(JC)+131.5D0)
C
           CALL TCON(MEABP(JC),TEMPR,42,IERT)
           UOPK(JC)=TEMPR**OT/SG(JC)
C
C           IF UOPK GIVEN CALC API AND SG
C
          ELSE IF(API(JC).LE.0.D0.AND.UOPK(JC).GT.0.D0.AND.
     1            SG(JC).LE.0.D0)THEN
           CALL TCON(MEABP(JC),TEMPR,42,IERT)
           SG(JC)=TEMPR**OT/UOPK(JC)
           API(JC)=141.5D0/SG(JC)-131.5D0
C
C           IF SG GIVEN CALC API AND UOPK
C
          ELSE IF(API(JC).LE.0.D0.AND.UOPK(JC).LE.0.D0.AND.
     1            SG(JC).GT.0.D0)THEN
           API(JC)=141.5D0/SG(JC)-131.5D0
           CALL TCON(MEABP(JC),TEMPR,42,IERT)
           UOPK(JC)=TEMPR**OT/SG(JC)
C
C           IF API AND SG GIVEN USE API TO CALC SG AND UOPK
C
```

```
      ELSE IF(API(JC).GT.0.D0.AND.UOPK(JC).LE.0.D0.AND.
     1           SG(JC).GT.0.D0)THEN
       SG(JC)=141.5D0/(API(JC)+131.5D0)
C
       CALL TCON(MEABP(JC),TEMPR,42,IERT)
       UOPK(JC)=TEMPR**OT/SG(JC)
C
C        IF UOPK AND SG GIVEN USE SG TO CALC API AND UOPK
C
      ELSE IF(API(JC).LE.0.D0.AND.UOPK(JC).GT.0.D0.AND.
     1           SG(JC).GT.0.D0)THEN
       API(JC)=141.5D0/SG(JC)-131.5D0
       CALL TCON(MEABP(JC),TEMPR,42,IERT)
       UOPK(JC)=TEMPR**OT/SG(JC)
C
C        IF UOPK AND API GIVEN USE API TO CALC SG AND UOPK
C
      ELSE IF(API(JC).GT.0.D0.AND.UOPK(JC).GT.0.D0.AND.
     1           SG(JC).LE.0.D0)THEN
       SG(JC)=141.5D0/(API(JC)+131.5D0)
C
       CALL TCON(MEABP(JC),TEMPR,42,IERT)
       UOPK(JC)=TEMPR**OT/SG(JC)
      ELSE
C
C        ERROR
C
       CALL MESS(2)
       WRITE(NHSTRY,900)
       WRITE(NHSTRY,2010)
       IERR=-2
      ENDIF
C
C        CALC MOLE WT IF NEEDED
C
      IF(AMW(JC).LE.0.D0)THEN
       CALL TCON(MEABP(JC),TEMPR,42,IERT)
       CALL RDMW(TEMPR,API(JC),SG(JC),AMW(JC),IERM)
       IF(IERM.LT.0)IERR=-3
      ENDIF
C
C        CHECK PERCENT PARAFINS ETC
C
      PSUM=PA(JC)+PN(JC)+PP(JC)
C
      IF(PSUM.LE.0.D0.OR.IPF.EQ.0)THEN
C       ESTIMATE % PARF,NAPS, & ARO.
       CALL MESS(1)
       WRITE(NHSTRY,900)
       WRITE(NHSTRY,3000)
       CALL TCON(MEABP(JC),TF,41,IERT)
       CALL ESTFRA(TF,JC,IERI)
      ELSE IF(PSUM.EQ.100.D0)THEN
C       CALC XA,XN AND XP
       XARO(JC)=PA(JC)/PSUM
       XNAP(JC)=PA(JC)/PSUM
       XPAR(JC)=PA(JC)/PSUM
      ELSE
C        WRITE WARNING & NORMALIZE
       XARO(JC)=PA(JC)/PSUM
       PA(JC)=XARO(JC)*100.D0
       XNAP(JC)=PN(JC)/PSUM
       PN(JC)=XNAP(JC)*100.D0
       XPAR(JC)=PP(JC)/PSUM
       PP(JC)=XPAR(JC)*100.D0
       CALL MESS(1)
       WRITE(NHSTRY,900)
       WRITE(NHSTRY,4000)
```

```
        ENDIF
        IF(LDBUG.GE.1)THEN
         WRITE(NHSTRY,5000)PP(JC),PN(JC),PA(JC),
     1                     XPAR(JC),XNAP(JC),XARO(JC)
        ENDIF
10     CONTINUE
C
C       CHECK FOR PROPERTIES NEEDED FOR SYSOP
C
       CALL CHKSOP(IERC)
C
C         FORMATS
C
900    FORMAT(1X,'IN MODULE NEED')
1000   FORMAT(1X,'BOTH API AND UOP K VALUES SPECIFIED',/,
     1        1X,'API VALUE USED AND CALC. CONTINUES')
2000   FORMAT(1X,'BOTH API AND UOP K VALUES SPECIFIED ARE LESS THAN 0.0'
     1     ,/,1X,'CALC. BYPASSED FOR THIS COMPOUND')
2010   FORMAT(1X,'INVALID SPECIFICATION '
     1     ,/,1X,'CALC. BYPASSED FOR THIS COMPOUND')
3000   FORMAT(1X,'PERCENT PARAFFINS,NAPTHENES, AND AROMATICS ARE ALL',/,
     1        1X,'0.0  VALUES WILL BE ESTIMATED.')
4000   FORMAT(1X,'PERCENT PARAFFINS,NAPTHENES, AND AROMATICS INCORRECTLY'
     1     ,/,1X,'SPECIFIED.  VALUES WILL BE NORMALIZED.')
5000   FORMAT(1X,'VALUES FOR PARAFFINS,NAPTHENES, AND AROMATICS',/,
     1        1X,'PERCENT: ',3(1X,G13.6),/,
     2        1X,'FRACTIONS: ',3(1X,G13.6))
C
       RETURN
       END
C*******************************************************************************
C
       SUBROUTINE NFMP(TBK,SG,XP,XN,XA,FPT,IERR)
C
C*******************************************************************************
C
C         NAME OF MODULE - NFMP
C         MODULE TITLE - TO CALC NORMAL FREEZING/MELTING POINT
C         PURPOSE - TO CALC NORMAL FREEZING/MELTING POINT OF A PETROL. FRACT.
C         MODIFIED - 12-19-88
C
C         VARIABLES USED-
C
C VARIABLE I/O TYPE-SPEC DIMENSION      DESCRIPTION AND RANGE
C      TBK    I       R          -      BOILING POINT (DEG K)
C       SG    I       R          -      SPECIFIC GRAVITY (60/60F)
C       XP    I       R          -      MOLE FRACTION PARAFFINS
C       XN    I       R          -      MOLE FRACTION NAPTHENES
C       XA    I       R          -      MOLE FRACTION AROMATICS
C      FPT    O       R          -      NORMAL FREEZING/MELTING POINT DEG K
C     IERR    O       I          -      ERROR CODE
C                                        0 = OK
C
C
       IMPLICIT REAL*8 (A-H,O-Z)
       IMPLICIT INTEGER(I-N)
C
       COMMON /IO     / NIN,NOUT,NHSTRY,NREPT
       COMMON /DEBUG  / LDBUG,LDBUGR
C
       IERR=0
       IF(LDBUG.GT.7)WRITE(NHSTRY,900)
C
C        DATA REGRESSED FOR PARAFFINS
C
       AP=EXP(-3.3158D0)
       BP=1.4185D0
       CP=-0.85142D-1
```

```
C
      FMPP=AP*TBK**BP*SG**CP
C
      IF(FMPP.LT.110.251D0.AND.XP.GT.0.D0)THEN
       CALL MESS(1)
       WRITE(NHSTRY,900)
       WRITE(NHSTRY,1000)FMPP
       FMPP=110.251D0
      ENDIF
      IF(FMPP.GT.310.D0.AND.XP.GT.0.D0)THEN
       CALL MESS(1)
       WRITE(NHSTRY,900)
       WRITE(NHSTRY,1100)FMPP
       FMPP=310.D0
      ENDIF
C
C       DATA REGRESSED FOR NAPTHENES
C
      AN=EXP(10.396D0)
      BN=-0.63428D0
      CN=5.6091D0
C
      FMPN=AN * TBK**BN * SG**CN
C
      IF(FMPN.LT.130.7D0.AND.XN.GT.0.D0)THEN
       CALL MESS(1)
       WRITE(NHSTRY,900)
       WRITE(NHSTRY,2000)FMPN
       FMPP=130.7D0
      ENDIF
      IF(FMPN.GT.265.D0.AND.XN.GT.0.D0)THEN
       CALL MESS(1)
       WRITE(NHSTRY,900)
       WRITE(NHSTRY,2100)FMPN
       FMPP=265.D0
      ENDIF
C
C       DATA REGRESSED FOR AROMATICS
C
      AA=EXP(6.2971D0)
      BA=-0.67363D-1
      CA=4.0803D0
C
      FMPA=AA*TBK**BA*SG**CA
C
      IF(FMPN.LT.173.7D0.AND.XA.GT.0.D0)THEN
       CALL MESS(1)
       WRITE(NHSTRY,900)
       WRITE(NHSTRY,3000)FMPA
       FMPP=173.7D0
      ENDIF
      IF(FMPN.GT.352.D0.AND.XA.GT.0.D0)THEN
       CALL MESS(1)
       WRITE(NHSTRY,900)
       WRITE(NHSTRY,3100)FMPA
       FMPP=352.D0
      ENDIF
C
C       EST. FOR FRACTION
C
      FPT=XP*FMPP + XN*FMPN + XA*FMPA
C
C       FORMATS
C
900   FORMAT(1X,'IN MODULE NFMP')
1000  FORMAT(1X,'FPT VALUE FOR PARAFFINS IS LESS THAN 110.251 ',/,
     1       1X,'FPT-VALUE OF ',G15.6,' SET TO 110.251 CALC. CONTINUES')
1100  FORMAT(1X,'FPT VALUE FOR PARAFFINS IS GREATER THAN 310.0 ',/,
```

```
     1        1X,'FPT-VALUE OF ',G15.6,' SET TO 310 CALC. CONTINUES')
2000  FORMAT(1X,'FPT VALUE FOR NAPTHENES IS LESS THAN 130.71 ',/,
     1        1X,'FPT-VALUE OF ',G15.6,' SET TO 130.7 CALC. CONTINUES')
2100  FORMAT(1X,'FPT VALUE FOR NAPTHENES IS GREATER THAN 265.0 ',/,
     1        1X,'FPT-VALUE OF ',G15.6,' SET TO 265 CALC. CONTINUES')
3000  FORMAT(1X,'FPT VALUE FOR AROMATICS IS LESS THAN 173.7 ',/,
     1        1X,'FPT-VALUE OF ',G15.6,' SET TO 173.7 CALC. CONTINUES')
3100  FORMAT(1X,'FPT VALUE FOR AROMATICS IS GREATER THAN 352.0 ',/,
     1        1X,'FPT-VALUE OF ',G15.6,' SET TO 352 CALC. CONTINUES')
C
      RETURN
      END
C*****************************************************************************
C
      SUBROUTINE OPENF(ITYP,IERR)
C
C*****************************************************************************
C
C       NAME OF MODULE - OPENF
C       MODULE TITLE - OPEN FILES FOR IO
C       PURPOSE - TO OPEN INPUT/OUTPUT FILES FOR RUN
C                 INPUT FILE MUST END IN .INP
C                 HISTORY FILE MUST END IN .HIS
C                 REPORT FILE MAY BE SPECIFIED AS NAME.EXT
C       MODIFIED - 12-15-88
C
C       VARIABLES USED-
C
C VARIABLE I/O TYPE-SPEC DIMENSION      DESCRIPTION AND RANGE
C  ITYP     I       I          -        OPEN CALC FLAG
C                                       0 = ALL (.INP,.HIS,.REP)
C                                       1 = INPUT FILE (.INP)
C                                       2 = HISTORY FILE (.HIS)
C                                       3 = REPORT FILE (.REP)
C  IERR     I/O     I          -        ERROR CODE
C                                       0 = OK
C                                       1 = FILE SPEC ERROR ON .INP FILE
C                                       2 = FILE SPEC ERROR ON .HIS FILE
C                                       3 = FILE SPEC ERROR ON .REP FILE
C
      PARAMETER        (MAXOPE=100)
C
      IMPLICIT INTEGER(I-N)
C
      CHARACTER*32     FILE,FILINP,FILHIS,FILREP
C
      COMMON /IO     / NIN,NOUT,NHSTRY,NREPT
      COMMON /FILES  / FILE
      COMMON /DEBUG  / LDBUG,LDBUGR
C
C         .INP FILE
C
      IF(ITYP.EQ.1.OR.ITYP.EQ.0)THEN
       FILINP=FILE
C
C       INPUT FILE FILINP
C
       IOPINP=0
100    IOPINP=IOPINP+1
       IF(IOPINP.GT.MAXOPE)THEN
        IERR=2
        WRITE(*,5000)
        WRITE(*,900)
        WRITE(*,1000)FILINP
        GOTO 9999
       ENDIF
C
       OPEN(UNIT=NIN,FILE=FILINP,STATUS='OLD',DEFAULTFILE='.INP',
```

```
      ENDIF
C
C       WRITE FINAL FLAG
C
      CALL SECOND(TIME)
C
      WRITE(NHSTRY,2000)NCOMP,TIME,IWARN,INERR,ISERR
C
C        FORMATS
C
100   FORMAT(2X,'Enter input data file name ',$)
200   FORMAT(A32)
210   FORMAT(/)
250   FORMAT(5X,'*****************************************')
300   FORMAT(5X,'* SUCCESSFUL OPEN OF INPUT FILE         *')
400   FORMAT(5X,'* SUCCESSFUL OPEN OF HISTORY FILE       *')
500   FORMAT(5X,'* INPUT READ COMPLETE                   *')
510   FORMAT(5X,'** WARNING IN READ (SEE .HIS FILE)     **')
520   FORMAT(5X,'** ERR IN READ (SEE .HIS FILE)         **')
600   FORMAT(5X,'* SUCCESSFUL OPEN OF REPORT FILE        *')
700   FORMAT(5X,'* INITIALIZATION OF VARIABLES COMPLETE *')
710   FORMAT(5X,'** WARNING/ERROR IN INIT',
     1          ' ROUTINE (SEE .HIS FILE) **')
800   FORMAT(5X,'* CALCULATE NEEDED VALUES COMPLETE      *')
810   FORMAT(5X,'** ERROR/WARNING IN NEED ROUTINE (SEE .HIS FILE) **')
900   FORMAT(5X,'* BEGIN PROPERTY CALCULATION            *')
1000  FORMAT(5X,'** ERROR/WARNING COUNT IN ROUTINE PROPS = ',I6,' **')
1100  FORMAT(5X,'** ERROR IN ROUTINE = ',I6,' ERROR NUMBER = ',I6)
2000  FORMAT(///,
     1 T5,'*****************************************************'/
     2 T5,'*                                                   *'/
     3 T5,'*                 ESTPRO ENDS EXECUTION             *'/
     4 T5,'*                                                   *'/
     5 T5,'*  NUMBER OF COMPOUNDS.....................',I10,    '  *'/
     6 T5,'*  CPU TIME ...............................',2X,G12.6,  '*'/
     7 T5,'*  NUMBER OF WARNINGS PRINTED..............',I10,    '  *'/
     8 T5,'*  NUMBER OF ERRORS PRINTED.................',I10,    '  *'/
     9 T5,'*  NUMBER OF SEVERE ERRORS PRINTED.........',I10,    '  *'/
     T T5,'*                                                   *'/
     1 T5,'*****************************************************')
C
9999  STOP
      END
C*************************************************************************
C
      SUBROUTINE ANDRA(JC,IERR)
C
C*************************************************************************
C
C        NAME OF MODULE - ANDRA
C        MODULE TITLE - CALCULATE MODIFIED ANDRADE MODEL PARAMETERS
C        PURPOSE - TO CALC PARAMETERS FOR MODIFIED ANDRADE MODEL
C         FOR LIQ VISCOSITY FROM DATA OBTAINED FROM LETSOU-STIEL(1973)
C         MODEL
C        MODIFIED - 10-19-88
C
C         FOR 0.76<TR<0.98
C
C        VARIABLES USED-
C
C VARIABLE I/O TYPE-SPEC DIMENSION      DESCRIPTION AND RANGE
C      JC     I       I         -       COMPONENT ARRAY ID
C   IERR      O       I         -       ERROR CODE
C                                        0 = OK
C                                       -1 = NO IMPROVEMENT POSSIBLE IN
C                                       THE VALUE OF PH EVEN THOUGH
C                                       CONVERGENCE HAS NOT BEEN REACHED.
C                                       -2 = MORE UNKNOWNS THAN FUNCTIONS AND
```

```
C                                       UNIQUE SOLUTION GENERALLY IS IMPOSSIBLE.
C                                       -3 = TOTAL NUMBER OF VARIABLES TO BE
C                                       VARIED IS ZERO
C                                       -4 = CONVERGENCE CRITERION MET BUT FLA
C                                       STILL LARGE
C                                       -5 = IC NOT A VALID NUMBER ON ENTRY
C                                       -6 = X(I) IS NOT WITHIN XMIN(I) TO
C                                        XMAX(I)
C                                       -7 = ZERO DIAGONAL ELEMENT IN EQUATION
C                                       SOLVE
C                                       -10 = TRY TO CALC. DERIVATIVE
C                                       ANALYTICALY
C                                       -11 = RUN EXCEEDED MAXIT SPECIFIED
C
      IMPLICIT REAL*8 (A-H,O-Z)
      IMPLICIT INTEGER(I-N)
C
      REAL*8            MULAND,MULREG
C
      PARAMETER         (MNC=25)
C
      COMMON /IO     / NIN,NOUT,NHSTRY,NREPT
C
      COMMON /NPROP3/ UOPK(MNC),API(MNC),SG(MNC),AMW(MNC)
C
      COMMON /CPRP01/ TC(MNC)
      COMMON /CPRP02/ PC(MNC)
      COMMON /CPRP05/ OMEGA(MNC)
      COMMON /CPRP09/ MULAND(5,MNC),MULREG(3,MNC)
C
      DIMENSION         NDATA(26),DATA(16),OUTPUT(6)
C
      DIMENSION         X(50),XV(50),XMAX(50),XMIN(50),Y(50),
     1                  Z(100),PJ(50),P(206),A(15),AC(15)
      DIMENSION         B(6),BV(3),BMAX(3),BMIN(3)
C
C       CONSTANTS
C
      OS=1.D0/6.D0
      OH=1.D0/2.D0
      TT=2.D0/3.D0
C
      XI=2.1735D6*TC(JC)**OS / AMW(JC)**OH * PC(JC)**TT
C
C       SET UP RANGE FOR LEETSOU-STEIL
C
      TRL=0.76D0
      TRH=0.98D0
      TRD=(TRH-TRL)/50.D0
      TR=TRL-TRD
C
C         MARQUARDT SET DEFAULTS
C
C         NUMBER OF UNKNOWNS
      K=3
C         NUMBER OF DATA POINTS
      N=50
C
      IF(LDBUG.GE.5)THEN
       DEGFR=FLOAT(N-K)
      ENDIF
C
      ITER = 0
      IF(MAXIT.LE.0)MAXIT=10000
C
C       SET EQUAL TO 1 FOR INITAL CALL
      NDATA(1)=1
C
```

```
C        SET INPUT PARAMETER DATA
C                    DATA(1) - FNU, FACTOR USED TO CHANGE FLA.  SET INTER-
C                              NALLY TO 10.0  IF ZERO ON INITIAL CALL.
C                    DATA(2) - FLA, FACTOR USED TO COMBINE GRADIENT AND
C                              NEWTON-RAPHSON METHODS.  SET INTERNALLY TO
C                              .01 IF ZERO ON INITIAL CALL.
C                    DATA(3) - TAU, USED IN CONVERGENCE TEST.  SET INTER-
C                              NALLY TO 0.001 IF ZERO ON INITIAL CALL.
C                    DATA(4) - EPS, USED IN CONVERGENCE TEST.  SET INTER-
C                              NALLY TO 0.00002 IF ZERO ON INITIAL CALL.
C                    DATA(5) - PHMIN, WHEN PH .LT. PHMIN, PARTIAL DERIV-
C                              ITIVES FROM THE PREVIOUS ITERATION ARE USED
C                              INSTEAD OF COMPUTING THEM AGAIN.
C                    DATA(6) THRU DATA(16) - VARIABLES USED INTERNALLY
C
      DO 10 I=1,5
       DATA(I)=0.0D0
10    CONTINUE
C
C      BV = VARY VECTOR (0=HOLD PARAMETER CONST,1=ALLOW TO VARY)
C
      DO 20 I=1,K
       BV(I)=1.D0
20    CONTINUE
C
C      INITAL VALUES OF PARMS
C
      B(1)=1.D0
      B(2)=1.D0
      B(3)=0.D0
C
C      MIN AND MAX VALUES
C
      BMAX(1)=2000.D0
      BMIN(1)=-2000.D0
      BMAX(2)=200000.D0
      BMIN(2)=-900000.D0
      BMAX(3)=20000.D0
      BMIN(3)=-20000.D0
C
      IF(LDBUG.GE.7)THEN
       WRITE(NHSTRY,1008)K,N
       DO 30 I=1,K
        WRITE(NHSTRY,1009)B(I),BMIN(I),BMAX(I),BV(I)
30     CONTINUE
       WRITE(NHSTRY,1010)
       WRITE(NHSTRY,1100)
       XSUM=0.0D0
       XSUM2=0.0D0
       YSUM=0.0D0
       YSUM2=0.0D0
      ENDIF
C
C      BEGIN CALC (CALC 50 POINTS TO BE FIT)
C       LOG(ETA)=A+B/TEMP(F) + C*LOG(TEMP(K))
C
C      UNIVERAL FUNCTIONS FOR LETSOU-STIEL MODEL
C                L    (0)                L    (1)
C      UF0 = (N XI)           UF1 = (N XI)
C
      DO 40 I=1,50
       TR=TR+TRD
       UF0=0.015174D0-0.02145D0*TR+0.0075D0*TR*TR
       UF1=0.042552D0-0.07674D0*TR+0.0340D0*TR*TR
       Y(I)=LOG((UF0+UF1*OMEGA(JC))/XI)
       X(I)=TR*TC(JC)
C
       IF(LDBUG.GE.7)THEN
```

```
          WRITE(NHSTRY,1020)X(I),Y(I)
          XSUM=XSUM+X(I)
          XSUM2=XSUM2+X(I)**2
          YSUM=YSUM+Y(I)
          YSUM2=YSUM2+Y(I)**2
         ENDIF
40      CONTINUE
C
C        MEANS, VARIANCES AND STANDARD DEV.
C
        IF(LDBUG.GE.7)THEN
         XMEAN=XSUM/FLOAT(N)
         XVAR=(FLOAT(N)*XSUM2-XSUM*XSUM)/FLOAT(N)/FLOAT(N-1)
         XSD=SQRT(XVAR)
         YMEAN=YSUM/FLOAT(N)
         YVAR=(FLOAT(N)*YSUM2-YSUM*YSUM)/FLOAT(N)/FLOAT(N-1)
         YSD=SQRT(YVAR)
         WRITE(NHSTRY,1120)XMEAN,YMEAN,XVAR,YVAR,XSD,YSD
        ENDIF
C
C        BEGIN REGRESSION
C
50      ITER=ITER+1
        IF(ITER.GT.MAXIT)THEN
         IERR=-11
         WRITE(NHSTRY,1045)MAXIT,ITER
         GOTO 9000
        ENDIF
C
C          EVALUATE Z VECTOR (FUNCTION VALUE)
C
C       REGRESS TO MODIFIED ANDRADE MODEL
C        VIS=MULAND(1)+MULAND(2)/T+MULAND(3)*LN(T)
C
        DO 60 I=1,N
         Z(I)=B(1)+B(2)/X(I)+B(3)*LOG(X(I))
60      CONTINUE
C
C       CALC ANALYTICAL DERIVATIVES (PJ VECTOR)
C
70      CONTINUE
C
C          CALC DERIVATIVE
C
        IF(NDATA(2).GT.0)THEN
         IERR=-10
         WRITE(NHSTRY,1090)IERR
         GOTO 9000
        ENDIF
C
C
        IF(LDBUG.GE.7)THEN
         WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
         YMYC =0.0D0
         SS   =0.0D0
         SSSAS=0.0D0
         DO 90 I=1,N
          YMYC=YMYC+(Y(I)-Z(I))**2
          SS=SS+(Z(I)-YMEAN)**2
          SSSAS=SSSAS+(Y(I)**2 - YMEAN**2)
90       CONTINUE
C
C        CALC R-SQUARE(SAS VERSION) AND ADJ R-SQUARE
C             1-VARIANCE OF FULL MODEL/VARIANCE OF MEAN MODEL
C
         RSQU=SS/(SS+YMYC)
         IF(SSSAS.NE.0.D0)THEN
          RSQUSAS=1.D0-YMYC/(SSSAS)
```

```
        ELSE
         RSQUSAS=0.D0
        ENDIF
        IF(DEGFR.EQ.0.D0)THEN
         ADJRSQU=0.0D0
        ELSE
         ADJRSQU=1.D0-(1.D0-RSQU)*(FLOAT(N)-1.D0)/DEGFR
        ENDIF
        IF(ABS(RSQU-RSQUSAS).GT.1.D8)THEN
         WRITE(NHSTRY,1112)RSQU,ADJRSQU,RSQUSAS,ADJRSQUSAS
        ELSE
         WRITE(NHSTRY,1110)RSQU,ADJRSQU
        ENDIF
C
        DO 100 J=1,K
         WRITE(NHSTRY,1030)J,B(J)
100     CONTINUE
C
        IF(LDBUG.EQ.8)THEN
         WRITE(NHSTRY,1040)
         DO 110 I=1,N
          YMYC=YMYC+(Y(I)-Z(I))**2
          SS=SS+(Z(I)-YMEAN)**2
          PERERR=ABS(Z(I)-Y(I))/ABS(Y(I))*100.D0
          WRITE(NHSTRY,1095)I,Z(I),Y(I),Z(I)-Y(I),PERERR
110      CONTINUE
        ENDIF
       ENDIF
C
120    CALL YSOLVE (K, N, NDATA, DATA, B, BV, BMAX, BMIN, Y, Z, PJ,
     1              OUTPUT, P, A, AC)
C
C                     NDATA(2) - NFCTDR, USED FOR CONTROL IN CALLING PROG
C                        IF = 0, CALCULATE FUNCTION
C                        IF = 1, CALCULATE DERIVATIVE
C                        IF =-1, EXAMINE IERR FOR WHAT TO DO NEXT
C
       IF(NDATA(2))130,50,70
C
C                     NDATA(3) - IERR, MAY TAKE ON VARIOUS VALUES
C                        IF POSITIVE, CONTAINS THE NUMBER OF VARIABLES NO
C                                     SATISFYING CONVERGENCE CRITERION
C                        IF =  0, CONVERGENCE SATISFIED AND SOLUTION RETU
C                        IF = -1, NO IMPROVEMENT POSSIBLE IN THE VALUE OF
C                                 PH EVEN THOUGH CONVERGENCE HAS NOT BEEN
C                                 REACHED.
C                        IF = -2, MORE UNKNOWNS THAN FUNCTIONS AND UNIQUE
C                                 SOLUTION GENERALLY IS IMPOSSIBLE.
C                        IF = -3, TOTAL NUMBER OF VARIABLES TO BE VARIED
C                                 IS ZERO
C                        IF = -4, CONVERGENCE CRITERION MET BUT FLA STILL
C                                 LARGE
C                        IF = -5, IC NOT A VALID NUMBER ON ENTRY
C                        IF = -6, B(I) IS NOT WITHIN BMIN(I) TO BMAX(I)
C                        IF = -7, ZERO DIAGONAL ELEMENT IN EQUATION SOLVE
C
130    IF(NDATA(3))140,140,120
C
C       FINAL STATISTICAL RESULTS
C
140    CONTINUE
       IF(LDBUG.GE.6)THEN
        WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
        YMYC  =0.0D0
        SS    =0.0D0
        SSSAS =0.0D0
        DO 150 I=1,N
         YMYC=YMYC+(Y(I)-Z(I))**2
```

```
          SS=SS+(Z(I)-YMEAN)**2
          SSSAS=SSSAS+(Y(I)**2-YMEAN**2)
150       CONTINUE
C
C         CALC R-SQUARE(SAS VERSION) AND ADJ R-SQUARE
C
C          RSQUSAS=1-VARIANCE (FULL MODEL)/VARIANCE (MEAN MODEL)
C
          RSQU=SS/(SS+YMYC)
          RSQUSAS=1.D0-YMYC/(SSSAS)
          IF(DEGFR.EQ.0.0D0)THEN
           ADJRSQU=0.0D0
           ADJRSQUSAS=0.0D0
          ELSE
           ADJRSQU=1.D0-(1.D0-RSQU)*(FLOAT(N)-1.D0)/DEGFR
           ADJRSQUSAS=1.D0-(1.D0-RSQUSAS)*(FLOAT(N)-1.D0)/DEGFR
          ENDIF
          IF(ABS(RSQU-RSQUSAS).GT.1.D8)THEN
           WRITE(NHSTRY,1112)RSQU,ADJRSQU,RSQUSAS,ADJRSQUSAS
          ELSE
           WRITE(NHSTRY,1110)RSQU,ADJRSQU
          ENDIF
C
C         FINAL PARAMETERS
C
         DO 160 J=1,K
          WRITE(NHSTRY,1030)J,B(J)
160      CONTINUE
C
C         FINAL SUMMARY
C
         WRITE(NHSTRY,1040)
         DO 170 I=1,N
          PERERR=ABS(Z(I)-Y(I))/ABS(Y(I))*100.D0
          WRITE(NHSTRY,1095)I,Z(I),Y(I),Z(I)-Y(I),PERERR
170      CONTINUE
        ENDIF
C
C        LOAD DATA INTO MULAND ARRAY
C
        IERR=NDATA(3)
        DO 900 JJ=1,5
          MULAND(JJ,JC)=0.0D0
900     CONTINUE
C
        IF(IERR.EQ.0)THEN
C
C         CONVERGED
C
          MULAND(1,JC)=B(1)
          MULAND(2,JC)=B(2)
          MULAND(3,JC)=B(3)
          MULAND(4,JC)=TRL*TC(JC)
          MULAND(5,JC)=TRH*TC(JC)
C
          IF(LDBUG.GE.1)WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
        ELSE IF(IERR.EQ.-1)THEN
          MULAND(1,JC)=B(1)
          MULAND(2,JC)=B(2)
          MULAND(3,JC)=B(3)
          MULAND(4,JC)=TRL*TC(JC)
          MULAND(5,JC)=TRH*TC(JC)
          WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
          WRITE(NHSTRY,1001)
        ELSE IF(IERR.EQ.-2)THEN
          MULAND(1,JC)=B(1)
          MULAND(2,JC)=B(2)
          MULAND(3,JC)=B(3)
```

```
        MULAND(4,JC)=TRL*TC(JC)
        MULAND(5,JC)=TRH*TC(JC)
        WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
        WRITE(NHSTRY,1002)
       ELSE IF(IERR.EQ.-3)THEN
        WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
        WRITE(NHSTRY,1003)
       ELSE IF(IERR.EQ.-4)THEN
        MULAND(1,JC)=B(1)
        MULAND(2,JC)=B(2)
        MULAND(3,JC)=B(3)
        MULAND(4,JC)=TRL*TC(JC)
        MULAND(5,JC)=TRH*TC(JC)
        WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
        WRITE(NHSTRY,1004)
       ELSE IF(IERR.EQ.-5)THEN
        WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
        WRITE(NHSTRY,1005)
       ELSE IF(IERR.EQ.-6)THEN
        WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
        WRITE(NHSTRY,1006)
       ELSE IF(IERR.EQ.-7)THEN
        WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
        WRITE(NHSTRY,1007)
       ENDIF
       MULREG(1,JC)=FLOAT(ITER)
       MULREG(2,JC)=FLOAT(NDATA(3))
       MULREG(3,JC)=OUTPUT(1)
C
C        FORMATS
C
1000   FORMAT(/,1X,'IN MODULE ANDRA',/,
      1     1X,'ITERATION: ',I9,/,
      2     1X,'IERR                                          = ',I15,/,
      3     1X,'SUM OF SQUARES                                = ',G15.8,/,
      4     1X,'ANGLE (DEGREES)                               = ',F15.2,/,
      5     1X,'NUMBER OF TIMES YSOLVE CALLED                 = ',F15.1,/,
      6     1X,'NUMBER OF FUNCTIONAL EVALUATIONS              = ',F15.1,/,
      7     1X,'NUMBER OF ANALYTICAL DERIVATIVE EVALUATIONS   = ',F15.1,/)
1001   FORMAT(1X,'NO IMPROVEMENT POSSIBLE IN THE VALUE OF',/,
      1       1X,'PH EVEN THOUGH CONVERGENCE HAS NOT BEEN REACHED.',/)
1002   FORMAT(1X,'MORE UNKNOWNS THAN FUNCTIONS AND UNIQUE',/)
1003   FORMAT(1X,'TOTAL NUMBER OF VARIABLES TO BE VARIED = 0',/)
1004   FORMAT(1X,'CONVERGENCE CRITERION MET BUT FLA STILL LARGE',/)
1005   FORMAT(1X,'IC NOT A VALID NUMBER ON ENTRY',/)
1006   FORMAT(1X,'X(I) IS NOT WITHIN XMIN(I) TO XMAX(I)',/)
1007   FORMAT(1X,'ZERO DIAGONAL ELEMENT IN EQUATION SOLVE',/)
1008   FORMAT(//,5X,'*****MARQUARDT METHOD REGRESSION*****',//,
      1 5X,'K (NUMBER OF PARAMETERS TO BE VARIED) = ',I4,/,
      2 5X,'N (NUMBER OF DATA POINTS)             = ',I4,//,
      3 5X,'INITAL B            B-MIN            B-MAX',
      4'VARY FLAG',/)
1009   FORMAT(2X,4(G15.5,1X))
1010   FORMAT(5X,'VARY FLAG:',/,
      1 10X,'0 = HOLD PARAMETER CONSTANT',/,
      2 10X,'1 = VARY PARAMETER USING NUMERICAL DERIVATIVE',/,
      3 9X,'-1 = VARY PARAMETER USING ANALYTICAL DERIVATIVE')
1020   FORMAT(1X,3G15.6)
1030   FORMAT(1X,'B(',I2,') = ',G13.5)
1040   FORMAT(/,1X,'OBS.  Y-CALC         Y-ACTUAL        DIFF.          ',
      1 '% ERROR',/)
1095   FORMAT(  1X,I4,  4(1X,G13.5))
1100   FORMAT(/,10X,'INPUT DATA',//,
      1 5X,'X-VALUE         Y-VALUE ',/,
      2 5X,'-------         ------- ',/)
1110   FORMAT(
      1 1X,'R-SQUARE                                      = ',F15.8,/,
      2 1X,'ADJ R-SQUARE                                  = ',F15.8,/)
```

```
1112  FORMAT(
     1 1X,'R-SQUARE                                          = ',F15.8,/,
     2 1X,'ADJ R-SQUARE                                      = ',F15.8,/,
     3 1X,'R-SQUARE(1-VAR.FM/VAR.MM)                         = ',F15.8,/,
     4 1X,'ADJ R-SQUARE(FOR 2ND R-SQUARE)                    = ',F15.8,/)
1120  FORMAT(//,10X,'STATISTICS',//,
     1 5X,'X-VALUES ',26X,'Y-VALUES',/,
     2 5X,'----------',26X,'--------',/,
     3 5X,'MEAN       = ',G15.5,8X,'MEAN       = ',G15.5,/
     4 5X,'VARIANCE   = ',G15.5,8X,'VARIANCE   = ',G15.5,/
     5 5X,'STD. DEV. = ',G15.5,8X,'STD. DEV. = ',G15.5,/)
1045  FORMAT(/,1X,'IN ANDRA',/,
     1 1X,'******RUN EXCEEDED MAXIT OF ',I5,' ITER = ',I5,'******'//)
1090  FORMAT(1X,'IN MODULE ANDRA IERR = ',I5,' TRY TO CALC.',
     1       ' DERIVATIVE ANALYTICALY, CALC. ABORTED')
9000  CONTINUE
      RETURN
      END
C*****************************************************************
C
      SUBROUTINE ASTMCF(VABP,SASTM,CABP,MABP,IERR)
C
C*****************************************************************
C
C       NAME OF MODULE - ASTMCF
C       MODULE TITLE - PROCEDURE 2B1.1 API DATA BOOK P2-11,12 (1980)
C       PURPOSE - METHOD FOR CHARACTERIZE PETROLEUM FRACTION BOILING
C                 POINTS OF ASTM D86
C       MODIFIED - 1-6-88
C
C       LIMITATIONS:
C          ASTM SLOPE       0-9.0
C          CABP           200-800
C
C       VARIABLES USED-
C
C VARIABLE I/O TYPE-SPEC DIMENSION      DESCRIPTION AND RANGE
C   VABP     I       R          -       VOLUME AVERAGE BOILING POINT (DEG F)
C  SASTM     I       R          -       ATSTM D86 10% TO 90% SLOPE
C                                       (DEG F/%OFF)
C   CABP     O       R          -       CUBIC AVERAGE BOILING POINT (DEG F)
C   MABP     O       R          -       MOLAL AVERAGE BOILING POINT (DEG F)
C   IERR     O       I          -       ERROR CODE
C                                        0 = OK
C                                       -1 = ASTM NOT IN RANGE ABOVE
C                                       -2 = CABP NOT IN RANGE ABOVE
C
      IMPLICIT REAL*8 (A-H,O-Z)
      IMPLICIT INTEGER(I-N)
C
      REAL*8           MABP,MABPC
C
      COMMON /IO     / NIN,NOUT,NHSTRY,NRCPT
      COMMON /DEBUG  / LDBUG,LDBUGR
C
      DIMENSION CC(8),CW(8),CM(8)
C
      IERR=0
C
      IF(LDBUG.GT.7)WRITE(NHSTRY,900)
C
C       CHECK IF IN RANGE
C
      IF(SASTM.LT.0.D0.OR.SASTM.GT.9.0)THEN
        IERR=-1
        CALL MESS(1)
        WRITE(NHSTRY,900)
        WRITE(NHSTRY,1000)SASTM
```

```
     1       READONLY,ERR=100)
C
C         .HIS FILE
C
      ELSE IF(ITYP.EQ.2.OR.ITYP.EQ.0)THEN
C
C         HISTORY FILE FILE.HIS
C
        FILHIS=FILE
        IOPHIS=0
200     IOPHIS=IOPHIS+1
        IF(IOPHIS.GT.MAXOPE)THEN
         WRITE(*,5000)
         WRITE(*,900)
         IERR=3
         WRITE(*,2000)FILHIS
         WRITE(*,2000)FILHIS
         GOTO 9999
        ENDIF
C
        OPEN(UNIT=NHISTRY,FILE=FILHIS,STATUS='NEW',DEFAULTFILE='.HIS',
     1      ERR=200)
C
C       .REP FILE
C
      ELSE IF(ITYP.EQ.3.OR.ITYP.EQ.0)THEN
C
C       REPORT FILE FILE.REP
C
        FILREP=FILE
        IOPREP=0
300     IOPREP=IOPREP+1
        IF(IOPREP.GT.MAXOPE)THEN
         WRITE(*,5000)
         WRITE(*,900)
         IERR=4
         WRITE(*,2000)FILREP
         GOTO 9999
        ENDIF
C
        OPEN(UNIT=NREPT,FILE=FILREP,STATUS='NEW',DEFAULTFILE='.REP',
     1      CARRIAGECONTROL='LIST',ERR=300)
C
      ELSE
        WRITE(*,5000)
        WRITE(*,900)
        WRITE(*,4000)
        STOP
      ENDIF
C
C       FORMATS
C
900   FORMAT(1X,'IN MODULE OPENF')
1000  FORMAT(5X,'PROBLEM ON OPEN OF INPUT FILE ',A32)
2000  FORMAT(5X,'PROBLEM ON OPEN OF HISTORY FILE ',A32)
3000  FORMAT(5X,'PROBLEM ON OPEN OF REPORT FILE ',A32)
4000  FORMAT(5X,'PROBLEM ON OPEN FILE TYPE')
5000  FORMAT(5X,'***SEVERE ERROR***')
C
9999  CONTINUE
C
      RETURN
      END
C*****************************************************************************
C
      SUBROUTINE OUTP(JC,IERR)
C
C*****************************************************************************
```

```
C
C       NAME OF MODULE - OUTP
C       MODULE TITLE - OUTPUT OF RESULTS OF PROPS
C       PURPOSE - TO OUTPUT RESULTS TO FILE IN ASPEN INPUT FORMAT
C                 OR DFMS INPUT FORMAT
C       MODIFIED - 12-19-88
C
C       VARIABLES USED-
C
C VARIABLE I/O TYPE-SPEC DIMENSION      DESCRIPTION AND RANGE
C  JC        1       I          -       COMPONENT ARRAY ID
C  IERR      O       I          -       ERROR CODE
C                                        0 = OK
C
      IMPLICIT REAL*8 (A-H,O-Z)
      IMPLICIT INTEGER(I-N)
C
      REAL*8            MABP,MEABP,MULAND,MUP,MULREG
C
      PARAMETER         (MNC=25)
C
      CHARACTER*62      TITLE
      CHARACTER*80      DESC(MNC),REC
      CHARACTER*32      CNAME
C
      COMMON /IO     / NIN,NOUT,NHSTRY,NREPT
      COMMON /DEBUG  / LDBUG,LDBUGR
      COMMON /INFO   / TITLE,DESC,IDESC
      COMMON /PRINT  / IPTYPE
      COMMON /SYS1   / RMISS
      COMMON /SYS2   / NSYSOP,NPCVEC(22)
C
      COMMON /NPROP1/ NCOMP,CNAME(MNC),ICF
      COMMON /NPROP2/ VABP(MNC),SLOP(MNC),CABP(MNC),MABP(MNC),MEABP(MNC)
      COMMON /NPROP3/ UOPK(MNC),API(MNC),SG(MNC),AMW(MNC)
      COMMON /NPROP4/ PA(MNC),PN(MNC),PP(MNC),IPF
C
      COMMON /CPRP01/ TC(MNC)
      COMMON /CPRP02/ PC(MNC)
      COMMON /CPRP03/ VC(MNC)
      COMMON /CPRP04/ ZC(MNC)
      COMMON /CPRP05/ OMEGA(MNC)
      COMMON /CPRP06/ PLXANT(9,MNC),PLXREG(3,MNC)
      COMMON /CPRP07/ CPIG(11,MNC),CPREG(3,MNC)
      COMMON /CPRP08/ DHVLWT(5,MNC)
      COMMON /CPRP09/ MULAND(5,MNC),MULREG(3,MNC)
      COMMON /CPRP10/ DHFORM(MNC)
      COMMON /CPRP11/ DGFORM(MNC)
      COMMON /CPRP12/ RKTZRA(MNC),RKTREG(3,MNC)
      COMMON /CPRP13/ DHLCVT(MNC)
      COMMON /CPRP14/ TB(MNC)
      COMMON /CPRP15/ VB(MNC)
      COMMON /CPRP16/ DHVLB(MNC)
      COMMON /CPRP17/ TFP(MNC)
      COMMON /CPRP18/ DELTA(MNC)
      COMMON /CPRP19/ MUP(MNC)
      COMMON /CPRP20/ RGYR(MNC)
      COMMON /CPRP21/ PLCAVT(4,MNC),PLCREG(3,MNC)
      COMMON /CPRP22/ VLCVTI(MNC)
C
      IERR=0
C
C      MAIN LOOP
C
C       CALC ORDER
C
C           1         2         3         4         5
C        TC      , PC     ,VC       , ZC      , OMEGA   ,
```

```
C             6          7          8          9         10
C          PLXANT  , CPIG   , DHFORM , DGFORM , DHLCVT ,
C            11         12         13         14         15
C          TB      , VB     , DHVLWT , RKTZRA , DHVLB  ,
C            16         17         18         19         20
C          TFP     , DELTA  , MUP    , MULAND , RGYR   ,
C            21         22
C          PLCAVT  , VLCVT1
C
C
C          TITLE AND DESCRIPTIONS
C
        IF(JC.EQ.1)THEN
         IF(IPTYPE.EQ.1)THEN
          WRITE(NREPT,1000)TITLE
         ELSE
          WRITE(NREPT,3000)TITLE
         ENDIF
C
         DO 10 JJ=1,IDESC
          CALL FEND(DESC(JJ),IEND,IERF)
          WRITE(NREPT,3100)DESC(JJ)(1:IEND)
10       CONTINUE
         IF(IPTYPE.EQ.1)THEN
          WRITE(NREPT,1100)
          DO 20 JJ=1,NCOMP-1
           REC=CNAME(JJ)
           CALL FEND(REC,IEND,IERF)
           WRITE(NREPT,1200)CNAME(JJ)(1:IEND),CNAME(JJ)(1:IEND)
20        CONTINUE
          WRITE(NREPT,1300)CNAME(NCOMP),CNAME(NCOMP)
         ENDIF
        ENDIF
C
C          FOR INPUT TO 'DFMS'
C
        IF(IPTYPE.EQ.1)THEN
         WRITE(NREPT,1400)CNAME(JC),
     1                    AMW(JC),TFP(JC),TB(JC),TC(JC),PC(JC),VC(JC),
     2                    ZC(JC),OMEGA(JC),RKTZRA(JC),VB(JC),
     3                    (CPIG(IV,JC),IV=1,11),
     4                    DELTA(JC),MUP(JC),
     5                    (PLXANT(IV,JC),IV=1,9),
     6                    (MULAND(IV,JC),IV=1,5),
     7                    DHFORM(JC),DGFORM(JC),DHVLB(JC),
     8                    (DHVLWT(IV,JC),IV=1,5),
     9                    (PLCAVT(IV,JC),IV=1,4),
     T                    DHLCVT(JC),VLCVT1(JC),RGYR(JC)
C
        ELSE
C
C          FOR INPUT DIRECTLY INTO ASPEN .INP FILE
C
C           INPUT AND CALCULATED VALUES FOR COMPONENT
C
          IF(LDBUGR.GT.0)THEN
           WRITE(NREPT,3110)CNAME(JC),VARP(JC),AMW(JC)
           IF(ICF.EQ.1)THEN
            WRITE(NREPT,3114)SLOP(JC)
           ELSE
            WRITE(NREPT,3112)SLOP(JC)
           ENDIF
           WRITE(NREPT,3120)CABP(JC),MABP(JC),MEABP(JC)
           WRITE(NREPT,3130)UOPK(JC),API(JC),SG(JC)
           WRITE(NREPT,3140)PA(JC),PN(JC),PP(JC)
           IF(NSYSOP.GE.0)THEN
            WRITE(NREPT,3150)FLOAT(NSYSOP)
           ELSE
```

```
          WRITE(NREPT,3152)
         ENDIF
        ENDIF
C
C         COMPONENT NAME
C
        WRITE(NREPT,3200)CNAME(JC)
C
        WRITE(NREPT,3300)AMW(JC),TC(JC),PC(JC),VC(JC),ZC(JC),OMEGA(JC)
C
        WRITE(NREPT,2000)(PLXREG(IV,JC),IV=1,3)
        WRITE(NREPT,3400)(PLXANT(IV,JC),IV=1,9)
C
        WRITE(NREPT,2000)(CPREG(IV,JC),IV=1,3)
        WRITE(NREPT,3500)(CPIG(IV,JC),IV=1,11)
C
        WRITE(NREPT,3800)DHFORM(JC),DGFORM(JC)
C
        IF(NPCVEC(10).EQ.1)THEN
         WRITE(NREPT,3810)DHLCVT(JC)
        ENDIF
C
        WRITE(NREPT,3820)TB(JC),VB(JC)
C
        WRITE(NREPT,3830)(DHVLWT(IV,JC),IV=1,5)
C
        IF(RKTREG(1,JC).NE.RMISS)THEN
         WRITE(NREPT,2000)(RKTREG(IV,JC),IV=1,3)
        ENDIF
        WRITE(NREPT,3840)RKTZRA(JC)
C
        IF(NPCVEC(15).EQ.1)THEN
         WRITE(NREPT,3850)DHVLB(JC)
        ENDIF
C
        IF(NPCVEC(16).EQ.1)THEN
         WRITE(NREPT,3860)TFP(JC)
        ENDIF
C
        IF(NPCVEC(17).EQ.1)THEN
         WRITE(NREPT,3870)DELTA(JC)
        ENDIF
C
        WRITE(NREPT,3880)MUP(JC)
C
        WRITE(NREPT,2000)(MULREG(IV,JC),IV=1,3)
        WRITE(NREPT,3890)(MULAND(IV,JC),IV=1,5)
C
        IF(NPCVEC(20).EQ.1)THEN
         WRITE(NREPT,3900)RGVR(JC)
        ENDIF
C
        IF(NPCVEC(21).EQ.1)THEN
         WRITE(NREPT,2000)(ELCREG(IV,JC),IV=1,3)
         IF(LDBUGR.GT.4)WRITE(NREPT,4020)OMEGA(JC)/0.1412357D0
         WRITE(NREPT,4100)(PLCAVT(IV,JC),IV=1,4)
        ENDIF
        IF(NPCVEC(22).EQ.1)THEN
         WRITE(NREPT,4200)VLCVTI(JC)
        ENDIF
C
       ENDIF
C
C       FORMATS
C
1000   FORMAT('TITLE ',1H',A62,1H')
1100   FORMAT(';NO-ECHO',/,';FILE   ASPENPCD ASPENPCD NEW',/,
     1         ';FILE   USRPPIA CCC NEW',/,';WRFILE ASPENPCD SESAME',/,
```

```
     2        'NEW-COMP')
1200  FORMAT(5X,A,5X,A,'/')
1300  FORMAT(5X,A,5X,A,/,
     1 'NEW-PROP MW      1/ TFP     1/ TB      1/ TC      1/ PC      ',
     2 '1/ VC      1/',/,9X,
     3 'ZC      1/ OMEGA  1/ RKTZRA 1/ VB      1/ CPIG  11/ DELTA  1/',/,
     4 9X,
     5 'MUP     1/ PLXANT 9/ MULAND 5/ DHFORM 1/ DGFORM 1/ DHVLB  1/',/,
     6 9X,'DHVLWT 5/ PLCAVT 4/ DHLCVT 1/ VLCVT1 1/ RGYR   1',/,
     6 'PROP-DATA',/,
     7 4X,'PROP-LIST MW      1 0/ TFP     1 0/ TB      1 0/ TC      1 0/',
     8 ' PC      1 0/',/,14X,
     9 'VC      1 0/ ZC      1 0/ OMEGA  1 0/ RKTZRA 1 0/ VB      1 0/',/,
     T 14X,'CPIG    1 0/ DELTA  1 0/ MUP    1 0/ PLXANT 1 0/ MULAND 1 0/'
     1 ,/,14X,'DHFORM 1 0/ DGFORM 1 0/ DHVLB  1 0/ DHVLWT 1 0/',
     2 ' PLCAVT 1 0/',/,14X,'DHLCVT 1 0/ VLCVT1 1 0/ RGYR   1 0')
1400  FORMAT(4X,'PVAL ',A32,/,
C       MW,TFP,TB,TC,PC,VC,ZC,OMEGA,RKTZRA,VB
     1 5(5X,G20.10,1X,'/',1X,G20.10,1X,'/',/)
C       CPIG(11)
     2 5(5X,G20.10,2X,G20.10,1X,/)5X,G20.10,1X,'/',/,
C  DELTA,MUP
     3    5X,G20.10,1X,'/',1X,G20.10,1X,'/',/,
C  PLXANT(9)
     4 4(5X,G20.10,2X,G20.10,1X,/)5X,G20.10,1X,'/',/,
C  MULAND(5)
     5 2(5X,G20.10,2X,G20.10,1X,/)5X,G20.10,1X,'/',/,
C  DHFORM,DGFORM,DHVLB
     6    5X,G20.10,1X,'/',1X,G20.10,1X,'/',/,5X,G20.10,1X,'/',/,
C  DHVLWT(5)
     7 2(5X,G20.10,2X,G20.10,1X,/)5X,G20.10,1X,'/',/,
C  PLCAVT(4)
     8 5X,G20.10,2X,G20.10,1X,/,5X,G20.10,2X,G20.10,1X,'/',/,
C  DHLCVT,VLCVT1,RGYR
     9    5X,G20.10,1X,'/',1X,G20.10,1X,'/',/,5X,G20.10,1X
     T )
3000  FORMAT('; TITLE ',A62)
3100  FORMAT(';',A)
3110  FORMAT(';',/,
     1        ';  SUMMARY FOR COMPONENT ',A32,/,
     2        ';',5X,'VOLUME AVERAGE BOILING POINT (DEG K) = ',G12.6,/,
     4        ';',5X,'AVERAGE MOLE WEIGHT                  = ',G12.6)
3112  FORMAT(';',5X,'SLOPE OF THE TBP CURVE                = ',G12.6)
3114  FORMAT(';',5X,'SLOPE OF THE ASTMD86 CURVE            = ',G12.6)
3120  FORMAT(';',5X,'CUBIC AVERAGE BOILING POINT (DEG K)   = ',G12.6,/,
     1        ';',5X,'MOLAL AVERAGE BOILING POINT (DEG K)  = ',G12.6,/,
     2        ';',5X,'MEAN  AVERAGE BOILING POINT (DEG K)  = ',G12.6)
3130  FORMAT(';',5X,'HOP (WATSON) K CHAR. FACTOR           = ',G12.6,/,
     1        ';',5X,'API GRAVITY                          = ',G12.6,/,
     2        ';',5X,'SG GRAVITY  (60/60 F)                = ',G12.6)
3140  FORMAT(';',5X,'PERCENT AROMATICS                     = ',G12.6,/,
     1        ';',5X,'PERCENT NAPTHENES                    = ',G12.6,/,
     2        ';',5X,'PERCENT PARAFINS                     = ',G12.6)
3150  FORMAT(';',5X,'SYSOP SELECTED                        = ',G12.6)
3152  FORMAT(';',5X,'SYSOP SELECTED                        = ',5X,'ALL')
3200  FORMAT(';',/,'PROP-DATA',/,2X,'COMP-LIST ',A32)
3300  FORMAT(5X,'CVAL MW      1    1 ',G20.10,/,
     1        5X,'CVAL TC      1    1 ',G20.10,/,
     2        5X,'CVAL PC      1    1 ',G20.10,/,
     3        5X,'CVAL VC      1    1 ',G20.10,/,
     4        5X,'CVAL ZC      1    1 ',G20.10,/,
     5        5X,'CVAL OMEGA   1    1 ',G20.10)
2000  FORMAT(';',/,
     1        ';   REGRESSION SUMMARY',/,
     2        ';     ITERATION               = ',G15.8,/,
     3        ';     NUMBER OF PARMS UNFIT:  = ',F15.0,/,
     4        ';     SUM OF SQUARES          = ',G15.8,/,
     5        ';')
```

```
3400  FORMAT(
     1        5X,'CVAL PLXANT 1    1 ',G20.10,'/2',2X,G20.10,'/',/,
     2        5X,          12X,'3      ',G20.10,'/4',2X,G20.10,'/',/,
     3        5X,          12X,'5      ',G20.10,'/6',2X,G20.10,'/',/,
     4        5X,          12X,'7      ',G20.10,'/8',2X,G20.10,'/',/,
     5        5X,          12X,'9      ',G20.10,/,';')
3500   FORMAT(
     1        5X,'CVAL CPIG   1    1 ',G20.10,'/2 ',2X,G20.10,'/',/,
     2        5X,          12X,'3      ',G20.10,'/4 ',2X,G20.10,'/',/,
     3        5X,          12X,'5      ',G20.10,'/6 ',2X,G20.10,'/',/,
     4        5X,          12X,'7      ',G20.10,'/8 ',2X,G20.10,'/',/,
     5        5X,          12X,'9      ',G20.10,'/10',2X,G20.10,'/',/,
     6        5X,          12X,'11     ',G20.10,/,';')
3800  FORMAT(5X,'CVAL DHFORM 1    1 ',G20.10,/,
     1        5X,'CVAL DGFORM 1    1 ',G20.10)
3810  FORMAT(5X,'CVAL DHLCVT 1    1 ',G20.10)
3820  FORMAT(5X,'CVAL TB      1    1 ',G20.10,/,
     1        5X,'CVAL VB      1    1 ',G20.10)
3830  FORMAT(
     1        5X,'CVAL DHVLWT 1    1 ',G20.10,'/2',2X,G20.10,'/',/,
     2        5X,          12X,'3      ',G20.10,'/4',2X,G20.10,'/',/,
     3        5X,          12X,'5      ',G20.10,/,';')
3840  FORMAT(5X,'CVAL RKTZRA 1    1 ',G20.10)
3850  FORMAT(5X,'CVAL DHVLB  1    1 ',G20.10)
3860  FORMAT(5X,'CVAL TFP    1    1 ',G20.10)
3870  FORMAT(5X,'CVAL DELTA  1    1 ',G20.10)
3880  FORMAT(5X,'CVAL MUP    1    1 ',G20.10)
3890  FORMAT(
     1        5X,'CVAL MULAND 1    1 ',G20.10,'/2',2X,G20.10,'/',/,
     2        5X,          12X,'3      ',G20.10,'/4',2X,G20.10,'/',/,
     3        5X,          12X,'5      ',G20.10,/,';')
3900  FORMAT(5X,'CVAL RGYR   1    1 ',G20.10)
4040  FORMAT(';     1ST CAVETT VAPOR PRES. CONST. OMEGA/0.14123357 = ',
     1        G15.8,/,
     2        ';     2ND CAVETT VAPOR PRES. CONST. RANGE (-0.2 TO 0.2)')
4100  FORMAT(5X,'CVAL PLCAVT 1    1 ',G20.10,'/2',2X,G20.10,'/',/,
     2        5X,          12X,'3      ',G20.10,'/4',2X,G20.10)
4200  FORMAT(5X,'CVAL VLCVT1 1    1 ',G20.10)
C
      RETURN
      END
C*******************************************************************************
C
      SUBROUTINE FEND(REC,IEND,IERR)
C
C*******************************************************************************
C
C       NAME OF MODULE - FEND
C       MODULE TITLE - FIND END OF RECORD
C       PURPOSE - TO FIND LAST NON BLANK CHARACTER
C       MODIFIED - 12-16-88
C
C
C       VARIABLES USED-
C
C VARIABLE I/O TYPE-SPEC DIMENSION      DESCRIPTION AND RANGE
C     REC    I/O      C         80      RECORD TO BE WRITTEN
C    IEND     I       I          -      LAST NON BLANK CHARACTER
C    IERR     O       I          -      ERROR FLAG
C                                       0 = OK
C                                       1 = NO CHARACTERS IN RECORD
      IMPLICIT INTEGER(I-N)
      CHARACTER*80     REC
C
      IERR=0
C
      DO 10 IEND=80,1,-1
       IF(REC(IEND:IEND).NE.' ')GOTO 20
```

```
10     CONTINUE
       IEND=1
C
       IERR=1
       GOTO 9990
20     RETURN
C
9990   RETURN
       END
C*******************************************************************************
C
       SUBROUTINE PROPS(IERR)
C
C*******************************************************************************
C
C        NAME OF MODULE - PROPS
C        MODULE TITLE - CALC PROPERTIES OF PETROLEUM FRACTIONS
C        PURPOSE - TO CALC PROPETIES OF PETROLEUM FRACTIONS
C        MODIFIED - 12-22-88
C
C        VARIABLES USED-
C
C VARIABLE I/O TYPE-SPEC DIMENSION      DESCRIPTION AND RANGE
C   IERR    O      I          -         ERROR CODE
C                                       0 = OK
C                                       .GT.0 NUMBER OF CALLS TO PROERTIES
C                                       IN WHICH AN ERROR OR WARNING OCCURED
C
       IMPLICIT REAL*8 (A-H,O-Z)
       IMPLICIT INTEGER(I-N)
C
       REAL*8           MABP,MEABP,MABPF,MULAND,MULREG,MUP
C
       CHARACTER*32     CNAME
       CHARACTER*80     REC
C
       PARAMETER        (MNC=25)
C
       COMMON /IO     / NIN,NOUT,NHSTRY,NREPT
       COMMON /DEBUG  / LDBUG,LDBUGR
       COMMON /SYS2   / NSYSOP,NPCVEC(22)
       COMMON /SYS3   / IERCAL(22)
C
       COMMON /NPROP1/ NCOMP,CNAME(MNC),ICF
       COMMON /NPROP2/ VABP(MNC),SLOP(MNC),CABP(MNC),MABP(MNC),MEABP(MNC)
       COMMON /NPROP3/ UOPK(MNC),API(MNC),SG(MNC),AMW(MNC)
       COMMON /NPROP4/ PA(MNC),PN(MNC),PP(MNC),IPF
       COMMON /CALCV / NCALC(MNC)
C
       COMMON /EPROP1/ XPAR(MNC),XNAP(MNC),XARO(MNC)
       COMMON /EPROP2/ NDAT(MNC),ST(MNC),BT(MNC)
C
       COMMON /CPRP01/ TC(MNC)
       COMMON /CPRP02/ PC(MNC)
       COMMON /CPRP03/ VC(MNC)
       COMMON /CPRP04/ ZC(MNC)
       COMMON /CPRP05/ OMEGA(MNC)
       COMMON /CPRP06/ PLXANT(9,MNC),PLXREG(3,MNC)
       COMMON /CPRP07/ CPIG(11,MNC),CPREG(3,MNC)
       COMMON /CPRP08/ DHVLWP(5,MNC)
       COMMON /CPRP09/ MULAND(5,MNC),MULREG(3,MNC)
       COMMON /CPRP10/ DHFORM(MNC)
       COMMON /CPRP11/ DGFORM(MNC)
       COMMON /CPRP12/ RKTZRA(MNC),RKTREG(3,MNC)
       COMMON /CPRP13/ DHLCVT(MNC)
       COMMON /CPRP14/ TB(MNC)
       COMMON /CPRP15/ VB(MNC)
       COMMON /CPRP16/ DHVLB(MNC)
```

```
      COMMON /CPRP17/ TFP(MNC)
      COMMON /CPRP18/ DELTA(MNC)
      COMMON /CPRP19/ MUP(MNC)
      COMMON /CPRP20/ RGYR(MNC)
      COMMON /CPRP21/ PLCAVT(4,MNC),PLCREG(3,MNC)
      COMMON /CPRP22/ VLCVT1(MNC)
C
C
      IF(LDBUG.GT.7)WRITE(NHSTRY,900)
      IERR=0
C
C NPCVEC IS 1 CALC PROP IF NPCVEC IS 0 NO CALC
C
C       CALC ORDER
C
C            1          2          3          4          5
C         TC      , PC      ,VC        , ZC       , OMEGA   ,
C            6          7          8          9         10
C         PLXANT  , CPIG    , DHFORM   , DGFORM   , DHLCVT  ,
C           11         12         13         14         15
C         TB      , VB      , DHVLWT   , RKTZRA   , DHVLB   ,
C           16         17         18         19         20
C         TFP     , DELTA   , MUP      , MULAND   , RGYR    ,
C           21         22
C         PLCAVT  , VLCVT1
C
      DO 200 JC=1,NCOMP
C
C       NOT ENOUGH DATA FOR CALCUATION
C
       IF(NCALC(JC).EQ.0)GOTO 100
C
C         CALC TC (CRITICAL TEMP)
C
C        CONVERT TO CALLED SUBROUTINE UNITS
C
       IF(NPCVEC(1).EQ.1)THEN
        CALL TCON(MEABP(JC),TEMPR,42,IERRT1)
         CALL RDTC(AMW(JC),TEMPR,API(JC),SG(JC),TEMPRO,IERCAL(1))
        CALL TCON(TEMPRO,TC(JC),24,IERRT2)
       ENDIF
C
C         CALC PC (CRITICAL PRES)
C
       IF(NPCVEC(2).EQ.1)THEN
        CALL RDPC(AMW(JC),TEMPR,API(JC),SG(JC),PRES,IERCAL(2))
        CALL PCON(PRES,PC(JC),15,IERRP1)
       ENDIF
C
C        CALC VC (CRITICAL VOL)
C
       IF(NPCVEC(3).EQ.1)THEN
        CALL RDVC(AMW(JC),TEMPR,SG(JC),VOL,IERCAL(3))
        VC(JC)=VOL
       ENDIF
C
C        CALC ZC (CRITICAL COMPRES. FACTOR)
C
       IF(NPCVEC(4).EQ.1)THEN
        CALL ZCCAL(TC(JC),PC(JC),VC(JC),ZC(JC),IERCAL(4))
       ENDIF
C
C        CALC OMEGA (ACENTRIC FACTOR)
C
       IF(NPCVEC(5).EQ.1)THEN
        CALL TCON(MEABP(JC),TEMPR,42,IERRT2)
        CALL TCON(TC(JC),TCR,42,IERRT3)
        CALL PCON(PC(JC),PRPSIA,51,IERRP1)
```

```
          CALL GYKL(TEMPR,TCR,PRPSIA,UOPK(JC),API(JC),OMEGA(JC),IERCAL(5))
         ENDIF
C
C         CALC PLXANT (VAPOR PRESSURE) AND REGRESS INTO FORM LN(PA)=A+B/(C+T)
C
         IF(NPCVEC(6).EQ.1)THEN
          CALL TCON(MABP(JC),MABPF,41,IERRT4)
C
          CALL MAXBN1(MABPF,UOPK(JC),SG(JC),MAXIT,NDAT,ST(JC),BT(JC),JC,
     1                IERCAL(6))
         ENDIF
C
C         CALC CPIG (IDEAL GAS HEAT CAPACITY) AND REGRESS INTO FORM
C
         IF(NPCVEC(7).EQ.1)THEN
          CALL RDCPIG(VABP(JC),SG(JC),MAXIT,JC,IERCAL(7))
         ENDIF
C
C         CALC DHFORM (STANDARD HEAT OF FORMATION)
C
         IF(NPCVEC(8).EQ.1)THEN
          CALL DHFRM(MEABP(JC),XPAR(JC),XNAP(JC),XARO(JC),DHFORM(JC),
     1              IERCAL(8))
         ENDIF
C
C         CALC DGFORM (STANDARD FREE ENERGY OF FORMATION)
C
         IF(NPCVEC(9).EQ.1)THEN
          CALL DGFRM(MEABP(JC),XPAR(JC),XNAP(JC),XARO(JC),DGFORM(JC),
     1              IERCAL(9))
         ENDIF
C
C         CALC DHLCVT (CAVETT EQUATION FOR ENTHALPY)
C
         IF(NPCVEC(10).EQ.1)THEN
          CALL CAVENT(JC,IERCAL(10))
         ENDIF
C
C         CALC TB (BOILING POINT)
C
         IF(NPCVEC(11).EQ.1)THEN
          CALL TBCALC(JC,IERCAL(11))
         ENDIF
C
C         CALC VB (LIQUID MOLAR VOLUME AT THE BOILING POINT)
C
         IF(NPCVEC(12).EQ.1)THEN
          CALL LMVABP(JC,IERCAL(12))
         ENDIF
C
C         CALC DHVLWT (WATSON HEAT OF VAPORIZATION)
C
         IF(NPCVEC(13).EQ.1)THEN
          CALL WATHOV(JC,IERCAL(13))
         ENDIF
C
C         CALC RKTZRA (RACKET EQUATION FOR LIQ. VOLUME)
C
         IF(NPCVEC(14).EQ.1)THEN
          IRKTZ=1
          CALL REFLV(JC,IRKTZ,IERCAL(14))
         ENDIF
C
C         CALC DHVLB (HEAT OF VAPORIZATION AT BP)
C
         IF(NPCVEC(15).EQ.1)THEN
          CALL HVABP(JC,IERCAL(15))
         ENDIF
```

```
C
C        CALC TFP (NORMAL FREEZING/MELTING POINT)
C
         IF(NPCVEC(16).EQ.1)THEN
          CALL NFMP(MEABP(JC),SG(JC),XPAR(JC),XNAP(JC),XARO(JC),
     1              TFP(JC),IERCAL(16))
         ENDIF
C
C        CALC DELTA (SOLUBILITY PARAMETER)
C
         IF(NPCVEC(17).EQ.1)THEN
          CALL SOLPAR(JC,IERCAL(17))
         ENDIF
C
C        CALC MUP (DIPOLE MOMENT)
C
         IF(NPCVEC(18).EQ.1)THEN
          CALL DIPOLE(JC,IERCAL(18))
         ENDIF
C
C        CALC MULAND (MODIFIED ANDRADE MODEL FOR LIQ VISCOSITY)
C                     AND REGRESS TO FORM A+B/T+C*LOG(T)
C
         IF(NPCVEC(19).EQ.1)THEN
          CALL ANDRA(JC,IERCAL(19))
         ENDIF
C
C        CALC RGYR (RADIUS OF GYRATION)
C
         IF(NPCVEC(20).EQ.1)THEN
          CALL RADGYR(AMW(JC),UOPK(JC),XPAR(JC),XNAP(JC),XARO(JC),
     1                RGYR(JC),IERCAL(20))
         ENDIF
C
C        CALC PLCAVT (CAVETT EQUATION VAPOR PRESSURE CONST)
C
         IF(NPCVEC(21).EQ.1)THEN
          ICPLC=0
          CALL CAVVP(JC,ICPLC,IERCAL(21))
         ENDIF
C
C        CALC VLCVT1 (EXTENDED SCHATCHARD-HILDEBRAND
C                     CHARACTERISTIC VOLUME PARAMETER)
C
         IF(NPCVEC(22).EQ.1)THEN
          CALL VFSH(TEMPR,SG(JC),JC,IERCAL(22))
         ENDIF
C
         CALL OUTP(JC,IERR)
         CALL SECOND(TIME)
C
         REC=CNAME(JC)
         CALL FEND(REC,IE,IERR)
         PRINT 1000,JC,CNAME(JC)(1:IE),TIME
         WRITE(NHSTRY,2000)JC,CNAME(JC)(1:IE),TIME
C
         IERR=0
         DO 100 IEE=1,22
          IF(IERCAL(IEE).NE.0)IERR=IERR+1
100      CONTINUE
200     CONTINUE
        CALL SECOND(TIME)
C
C         FORMATS
C
900     FORMAT(1X,'IN MODULE PROPS')
1000    FORMAT(1X,'FINISHED COMPONENT ',I2,1X,'(',A,') C-TIME = ',G12.6)
2000    FORMAT(//,1X,'FINISHED COMPONENT ',I2,1X,'(',A,')',/,
```

```
     1           1X,'CUMULATIVE-CPU-TIME = ',G12.6,//)
C
      RETURN
      END
C*****************************************************************************
C
      SUBROUTINE RADGYR(AMW,UOPK,XP,XN,XA,RGY,IERR)
C
C*****************************************************************************
C
C        NAME OF MODULE - RADGYR
C        MODULE TITLE - CALC
C        PURPOSE - TO CALC RADIUS OF GYRATION
C        MODIFIED - 12-19-88
C        METHOD - REGRESSION OF ASPEN DATA BANK FOR PARAFFINS,NAPTHENES,
C                 AND AROMATICS TO FORM: RADGYR=A*MW**B
C
C        VARIABLES USED-
C
C VARIABLE I/O TYPE-SPEC DIMENSION      DESCRIPTION AND RANGE
C      AMW   I       R          -       AVERAGE MOLE WT.
C     UOPK   I       R          -       UOP CHARACTERIZATION FACTOR
C       XP   I       R          -       MOLE FRACTION PARAFFINS
C       XN   I       R          -       MOLE FRACTION NAPTHENES
C       XA   I       R          -       MOLE FRACTION AROMATICS
C      RGY   O       R          -       RADIUS OF GYRATION
C
      IMPLICIT REAL*8 (A-H,O-Z)
      IMPLICIT INTEGER(I-N)
C
      COMMON /DEBUG / LDBUG,LDBUGR
      COMMON /IO    / NIN,NOUT,NHSTRY,NREPT
C
      IERR=0
      IF(LDBUG.GT.7)WRITE(NHSTRY,900)
C
C       DATA REGRESSED FOR PARAFFINS
C
      AP=EXP(-26.129D0)
      BP=0.30375D0
      CP=0.80725D0
C
      RGP=AP*UOPK**BP*AMW**CP
C
      IF(RGP.LT.0.3182D-9.AND.XP.GT.0.D0)THEN
       CALL MESS(1)
       WRITE(NHSTRY,900)
       WRITE(NHSTRY,1000)RGP
       RGP=0.3182D-9
      ENDIF
      IF(RGP.GT.0.8318D-9.AND.XP.GT.0.D0)THEN
       CALL MESS(1)
       WRITE(NHSTRY,900)
       WRITE(NHSTRY,1100)RGP
       RGP=0.8318D-9
      ENDIF
C
C       DATA REGRESSED FOR NAPTHENES
C
      AN=EXP(-25.879D0)
      BN=0.26866D0
      CN=0.76607D0
C
      RGN=AN*UOPK**BN*AMW**CN
C
      IF(RGN.LT.0.285D-9.AND.XN.GT.0.D0)THEN
       CALL MESS(1)
       WRITE(NHSTRY,900)
```

```
        WRITE(NHSTRY,2000)RGN
        RGN=0.285D-9
       ENDIF
       IF(RGN.GT.0.4367D-9.AND.XN.GT.0.D0)THEN
        CALL MESS(1)
        WRITE(NHSTRY,900)
        WRITE(NHSTRY,2100)RGN
        RGN=0.4367D-9
       ENDIF
C
C       DATA REGRESSED FOR AROMATICS
C
       AA=EXP(-28.663D0)
       BA=2.2211D0
       CA=0.38475D0
C
       RGA=AA*UOPK**BA*AMW**CA
C
       IF(RGA.LT.0.30037D-9.AND.XA.GT.0.D0)THEN
        CALL MESS(1)
        WRITE(NHSTRY,900)
        WRITE(NHSTRY,3000)RGA
        RGA=0.30037D-9
       ENDIF
       IF(RGA.GT.0.4849D-9.AND.XA.GT.0.D0)THEN
        CALL MESS(1)
        WRITE(NHSTRY,900)
        WRITE(NHSTRY,3100)RGA
        RGA=0.4849D-9
       ENDIF
C
C       EST. FOR FRACTION
C
       RGY=XP*RGP + XN*RGN + XA*RGA
C
C       FORMATS
C
900    FORMAT(1X,'IN MODULE RADGYR')
1000   FORMAT(1X,'RGY VALUE FOR PARAFFINS IS LESS THAN 0.3182D-9 ',/,
     1   1X,'RGY-VALUE OF ',G15.6,' SET TO 0.3182D-9 CALC. CONTINUES')
1100   FORMAT(1X,'RGY VALUE FOR PARAFFINS IS GREATER THAN 0.8318D-9',/,
     1   1X,'RGY-VALUE OF ',G15.6,' SET TO 0.8318D-9 CALC. CONTINUES')
2000   FORMAT(1X,'RGY VALUE FOR NAPTHENES IS LESS THAN 0.285D-9',/,
     1   1X,'RGY-VALUE OF ',G15.6,' SET TO 0.285D-9CALC. CONTINUES')
2100   FORMAT(1X,'RGY VALUE FOR NAPTHENES IS GREATER THAN 0.4367D-9',/,
     1   1X,'RGY-VALUE OF ',G15.6,' SET TO 0.4367D-9 CALC. CONTINUES')
3000   FORMAT(1X,'RGY VALUE FOR AROMATICS IS LESS THAN 0.30037D-9',/,
     1   1X,'RGY-VALUE OF ',G15.6,' SET TO 0.30037D-9 CALC. CONTINUES')
3100   FORMAT(1X,'RGY VALUE FOR AROMATICS IS GREATER THAN 0.4849D-9',/,
     1   1X,'RGY-VALUE OF ',G15.6,' SET TO 0.4849D-9 CALC. CONTINUES')
C
       RETURN
       END
C*************************************************************************
C
       SUBROUTINE RDCHECK(AMW,TBR,SG,ITYP)
C
C*************************************************************************
C
C        NAME OF MODULE - RDCHECK
C        MODULE TITLE - CHECK LIMITS ON RIAZI DAUBERT CORR.
C        PURPOSE - TO CHECK LIMITS ON RIAZI DAUBERT CORR.
C        MODIFED - 10-3-88
C
C        LIMITATIONS:
C           MW           77.2-294.5
C           TB(DEG R)    569.67-1309.67
C           SG           0.6247-1.0244
```

```
C
C        VARIABLES USED-
C
C VARIABLE I/O TYPE-SPEC DIMENSION      DESCRIPTION AND RANGE
C    AMW      I       R          -      MOLE WEIGHT
C    TBR      I       R          -      BOILING POINT TEMPERATURE (DEG R)
C     SG      I       R          -      SPECIFIC GRAVITY (60/60F)
C   ITYP      I       I          -      TYPE OF CORRELATION
C                                        1 = MW
C                                        2 = TC
C                                        3 = PC
C                                        4 = VC
C                                        5 = LAMBDA
C                                        6 = CP
C                                        7 = VB
C
      IMPLICIT REAL*8 (A-H,O-Z)
      IMPLICIT INTEGER(I-N)
C
      CHARACTER*6      NAMES(7)
C
C
      COMMON /IO     / NIN,NOUT,NHSTRY,NREPT
      COMMON /DEBUG / LDBUG,LDBUGR
C
      DATA NAMES     /'MW     ','TC     ','PC     ','VC
     1                 'LAMBDA','CPIG   ','VB     '/
C
       IF(AMW.LT.77.2D0.OR.AMW.GT.694.D0)THEN
        CALL MESS(1)
        WRITE(NHSTRY,900)NAMES(ITYP)
        WRITE(NHSTRY,1000)AMW
       ENDIF
C
       IF(TBR.LT.569.67D0.OR.TBR.GT.1309.67)THEN
        CALL MESS(1)
        WRITE(NHSTRY,900)NAMES(ITYP)
        WRITE(NHSTRY,2000)TBR
       ENDIF
C
       IF(SG.LT.0.6247D0.OR.SG.GT.1.0244D0)THEN
        CALL MESS(1)
        WRITE(NHSTRY,900)NAMES(ITYP)
        WRITE(NHSTRY,3000)SG
       ENDIF
C
C       FORMATS
C
900    FORMAT(5X,'USING PROCEDURE RD',A6)
1000   FORMAT(1X,'MW VALUE IS NOT IN RANGE 77.2-294.5',/,
     1        1X,'MW-VALUE = ',G12.6,' CALC. CONTINUES')
2000   FORMAT(1X,'TB(DEG R) VALUE IS NOT IN RANGE 569.67-1309.67',/,
     1        1X,'TB-VALUE = ',G12.6,' CALC. CONTINUES')
3000   FORMAT(1X,'SG VALUE IS NOT IN RANGE 0.6247-1.0244',/,
     1        1X,'SG VALUE = ',G12.6,' CALC. CONTINUES')
C
       RETURN
       END
C*****************************************************************************
C
       SUBROUTINE RDCPIG(TBK,SG,MAXIT,JC,IERR)
C
C*****************************************************************************
C
C        NAME OF MODULE - RDCPIG
C        MODULE TITLE - TO ESTIMATE IDEAL GAS HEAT CAPACITY
C        PURPOSE - TO ESTIMATE IDEAL GAS HEAT CAPACITY USING RIAZI AND DAUBERT
C                  METHOD
```

```
C                  REF: HYDROCARBON PROCESSING MARCH 1980 P115-116
C                       RIAZI AND DAUBERT
C        MODIFIED - 11-8-86
C
C        VARIABLES USED-
C
C VARIABLE I/O TYPE-SPEC DIMENSION      DESCRIPTION AND RANGE
C    TBK      I       R          -      TEMP BOILING DEG K
C     SG      I       R          -      SPECIFIC GRAVITY (60/60F)
C MAXIT      I       I          -      MAXIMUM ITER. ON REGRESSION OF CP VALUES
C     JC     I       I          -      COMPONENT ARRAY ID
C  IERR      O       I          -      ERROR CODE ON MARQUARDT
C                                       0 = CONVERGED CP
C                                      -1 = NO IMPROVEMENT POSSIBLE IN THE
C                                           VALUE OF PH EVEN THOUGH CONV. HAS
C                                           NOT BEEN REACHED.
C                                      -2 = MORE UNKNOWNS THAN FUNCTIONS
C                                      -3 = TOTAL NUMBER OF VARIABLES TO BE
C                                           VARIED IS ZERO
C                                      -4 = CONV. CRITERION MET BUT FLA STILL
C                                           LARGE
C                                      -5 = IC NOT A VALID NUMBER ON ENTRY
C                                      -6 = X(I) IS NOT WITHIN XMIN(I)-XMAX(I)
C                                      -7 = ZERO DIAGONAL ELEMENT IN EQUATION
C                                           SOLVE
C                                     -10 = ASKED FOR ANALYTICAL DERIVATIVE
C                                     -11 = ITERATIONS EXCEEDED MAXIT
C
C
      IMPLICIT REAL*8 (A-H,O-Z)
      IMPLICIT INTEGER(I-N)
C
C
      PARAMETER        (MNC=25)
C
      COMMON /IO     / NIN,NOUT,NHSTRY,NREPT
      COMMON /DEBUG  / LDBUG,LDBUGR
C
      COMMON /CPRP07/ CPIG(11,MNC),CPREG(3,MNC)
C
      DIMENSION        NDATA(26),DATA(16),OUTPUT(6)
C
      DIMENSION        X(6),XV(3),XMAX(3),XMIN(3),Y(3),
     1                 Z(6),PJ(3),P(18),A(15),AC(15),XO(3)
C
      DIMENSION        CP(11)
C
      IF(LDBUG.GT.7)WRITE(NHSTRY,900)
C
C       CONVERT
C
      CALL TCON(TBK,TB,42,IERR)
C
C       MAX ITERATIONS
C
      IF(MAXIT.EQ.0)MAXIT=1000
C
C        CPIG 1 2 AND 3
C        IDEAL GAS HEAT CAPACITY (BTU/LB MOLE DEG F) AT 0 F
C
      CP00=4.0394D-7 * TB**(2.6724D0) * SG**(-2.363D0)
C
C        IDEAL GAS HEAT CAPACITY (BTU/LB-MOLE DEG F) AT 600 F
C
      CP0600=4.935D-6 * TB**(2.4219D0) * SG**(-1.9436D0)
C
C        IDEAL GAS HEAT CAPACITY (BTU/LB-MOLE DEG F) AT 1200 F
C
```

```
      CP01200=8.352D-6 * TB**(2.3853D0) * SG**(-1.9320D0)
C
C       IDEAL GAS HEAT CAPACITY (J/KMOLE DEG K) AT 0 F
C
      CP00=CP00/9.486D-4/0.453593D0*1.8D0
C
C       IDEAL GAS HEAT CAPACITY (J/KMOLE DEG K) AT 600 F
C
      CP0600=CP0600/9.486D-4/0.453593D0*1.8D0
C
C       IDEAL GAS HEAT CAPACITY (J/KMOLE DEG K) AT 1200 F
C
      CP01200=CP01200/9.486D-4/0.453593D0*1.8D0
C
C       REGRESS CP VALUES USING MARQUARDT (ASPEN YSOLVE)
C
C       NUMBER OF UNKNOWNS
      K=3
C       NUMBER OF EQUATIONS
      N=3
C       INITIAL GUESS
      X(1)=CP00
      X(2)=0.D0
      X(3)=0.D0
      NDATA(1)=1
C
      DO 10 I=1,5
       DATA(I)=0.0D0
10    CONTINUE
      DO 20 I=1,K
       XV(I)=1.D0
       Y(I)=0.D0
       XMAX(I)= 500000.D0
       XMIN(I)=-500000.D0
20    CONTINUE
C
50    ITER=ITER+1
      IF(ITER.GT.MAXIT)THEN
       CALL MESS(3)
       WRITE(NHSTRY,900)
       IERR=-11
       WRITE(NHSTRY,1080)MAXIT,ITER
       GOTO 9000
      ENDIF
C
C       EQUATION OF FORM A+BT+CT*T
C
       TEMP1=(0.D0+459.67D0)/1.8D0
      Z(1)=X(1)+X(2)*TEMP1+X(3)*TEMP1*TEMP1 - CP00
       TEMP2=(600.D0+459.67D0)/1.8D0
      Z(2)=X(1)+X(2)*TEMP2+X(3)*TEMP2*TEMP2 - CP0600
       TEMP3=(1200.D0+459.67D0)/1.8D0
      Z(3)=X(1)+X(2)*TEMP3+X(3)*TEMP3*TEMP3 - CP01200
C
80    CALL YSOLVE (K, N, NDATA, DATA, X, XV, XMAX, XMIN, Y, Z, PJ,
     1               OUTPUT, P, A, AC)
C
C       CALC FUNCTION
C
      IF(NDATA(2).EQ.0)THEN
       GOTO 50
C
C       CALC DERIVATIVE
C
      ELSE IF(NDATA(2).GT.0)THEN
       IERR=-10
       CALL MESS(3)
       WRITE(NHSTRY,900)
```

```
      WRITE(NHSTRY,1090)IERR
      GOTO 9000
     ENDIF
C
C       NDATA(3) = NUMBER OF VARIABLES NOT SATISFYING CONV. CRITERION
C
     IF(NDATA(3).GT.0)GOTO 80
C
     IERR=NDATA(3)
C     CONVERGED
     IF(IERR.EQ.0)THEN
      CP(1)=X(1)
      CP(2)=X(2)
      CP(3)=X(3)
     ELSE IF(IERR.EQ.-1)THEN
      CP(1)=X(1)
      CP(2)=X(2)
      CP(3)=X(3)
      CALL MESS(1)
      WRITE(NHSTRY,900)
      WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
      WRITE(NHSTRY,1001)
     ELSE IF(IERR.EQ.-2)THEN
      CP(1)=X(1)
      CP(2)=X(2)
      CP(3)=X(3)
      CALL MESS(1)
      WRITE(NHSTRY,900)
      WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
      WRITE(NHSTRY,1002)
     ELSE IF(IERR.EQ.-3)THEN
      CALL MESS(2)
      WRITE(NHSTRY,900)
      WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
      WRITE(NHSTRY,1003)
     ELSE IF(IERR.EQ.-4)THEN
      CP(1)=X(1)
      CP(2)=X(2)
      CP(3)=X(3)
      CALL MESS(1)
      WRITE(NHSTRY,900)
      WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
      WRITE(NHSTRY,1004)
     ELSE IF(IERR.EQ.-5)THEN
      CALL MESS(2)
      WRITE(NHSTRY,900)
      WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
      WRITE(NHSTRY,1005)
     ELSE IF(IERR.EQ.-6)THEN
      CALL MESS(2)
      WRITE(NHSTRY,900)
      WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
      WRITE(NHSTRY,1006)
     ELSE IF(IERR.EQ.-7)THEN
      CALL MESS(2)
      WRITE(NHSTRY,900)
      WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
      WRITE(NHSTRY,1007)
     ENDIF
C
C       ASPEN
C
     CPIG(1,JC)=CP(1)
     CPIG(2,JC)=CP(2)
     CPIG(3,JC)=CP(3)
     CPIG(4,JC)=0.D0
     CPIG(5,JC)=0.D0
     CPIG(6,JC)=0.D0
```

```
      CPIG(7,JC)=TEMP1
      CPIG(8,JC)=TEMP3
      CPIG1=CP(1)+CP(2)*TEMP1+CP(3)*TEMP1**2
      CPIG2=CP(1)+CP(2)*TEMP2+CP(3)*TEMP2**2
      CPIG(10,JC)=(CPIG2-CPIG1)/(TEMP2-TEMP1)
      CPIG(9,JC)=-1.D0*CPIG(10,JC)*TEMP1+CPIG1
      CPIG(11,JC)=1.0D0
C
      CPREG(1,JC)=FLOAT(ITER)
      CPREG(2,JC)=FLOAT(NDATA(3))
      CPREG(3,JC)=OUTPUT(1)
C
C       FORMATS
C
900   FORMAT(1X,'IN MODULE RDCPIG')
1000  FORMAT(//,
     1     1X,'ITERATION: ',I9,/,
     2     1X,'IERR                                          = ',I15,/,
     3     1X,'SUM OF SQUARES                                = ',G15.8,/,
     4     1X,'ANGLE (DEGREES)                               = ',F15.2,/,
     5     1X,'NUMBER OF TIMES YSOLVE CALLED                 = ',F15.1,/,
     6     1X,'NUMBER OF FUNCTIONAL EVALUATIONS              = ',F15.1,/,
     7     1X,'NUMBER OF ANALYTICAL DERIVATIVE EVALUATIONS   = ',F15.1,/)
1001  FORMAT(1X,'NO IMPROVEMENT POSSIBLE IN THE VALUE OF',/,
     1       1X,'PH EVEN THOUGH CONVERGENCE HAS NOT BEEN REACHED.',/)
1002  FORMAT(1X,'MORE UNKNOWNS THAN FUNCTIONS AND UNIQUE',/)
1003  FORMAT(1X,'TOTAL NUMBER OF VARIABLES TO BE VARIED = 0',/)
1004  FORMAT(1X,'CONVERGENCE CRITERION MET BUT PLA STILL LARGE',/)
1005  FORMAT(1X,'IC NOT A VALID NUMBER ON ENTRY',/)
1006  FORMAT(1X,'X(I) IS NOT WITHIN XMIN(I) TO XMAX(I)',/)
1007  FORMAT(1X,'ZERO DIAGONAL ELEMENT IN EQUATION SOLVE',/)
1080  FORMAT(//,1X,'*****RUN EXCEEDED MAXIT OF ',I5,' ITER = ',I5,
     1           '*****',//)
1090  FORMAT(1X,'IERR = ',I5,' TRY TO CALC.',
     1       1X,'DERIVATIVE ANALYTICALY, CALC. ABORTED')
9000  CONTINUE
      RETURN
      END
C*******************************************************************************
C
      SUBROUTINE RDMW(MEABP,API,SG,AMW,IERR)
C
C*******************************************************************************
C
C       NAME OF MODULE - RDMW
C       MODULE TITLE - PROCEDURE 2B2.1 API DATA BOOK P2-13 (1980)
C       PURPOSE - METHOD FOR THE MOLECULAR WEIGHT OF PETROLEUM
C                 FRACTIONS
C       MODIFIED - 10-3-88
C
C       LIMITATIONS:
C          MEABP(DEG F)    97-1036
C          API             14.4-93.1
C          AMW             70-724
C
C       VARIABLES USED-
C
C VARIABLE I/O TYPE-SPEC DIMENSION      DESCRIPTION AND RANGE
C  MEABP    I       R          -        MEAN BOILING
C                                       POINT (DEG R)
C    API    I       R          -        API GRAVITY
C     SG    I       R          -        SPEC. GRAVITY
C    AMW    O       R          -        PSEUDOCRITICAL AVE MOLE WT OF PET.
C                                       FRAC.
C   IERR    O       I          -        ERROR CODE
C                                        0 = OK
C                                       -1 = MEABP NOT IN RANGE ABOVE
C                                       -2 = API NOT IN RANGE ABOVE
```

```
C                                          -3 = AMW NOT IN RANGE ABOVE
C
C
      IMPLICIT REAL*8 (A-H,O-Z)
      IMPLICIT INTEGER(I-N)
C
      REAL*8           MEABP
C
      PARAMETER        (MNC=25)
C
      COMMON /IO     / NIN,NOUT,NHSTRY,NREPT
      COMMON /DEBUG  / LDBUG,LDBUGR
C
      IF(LDBUG.GT.7)WRITE(NHSTRY,900)
C
      IERR=0
C
C       CHECK IF IN RANGE
C
      IF(MEABP.LE.556.67D0.OR.MEABP.GT.1495.67D0)THEN
        IERR=-1
        WRITE(NHSTRY,900)
        CALL MESS(1)
        WRITE(NHSTRY,1000)MEABP
      ENDIF
C
      IF(API.LE.14.4D0.OR.API.GT.93.1D0)THEN
        IERR=-2
        WRITE(NHSTRY,900)
        CALL MESS(1)
        WRITE(NHSTRY,2000)API
      ENDIF
C
C       CALC AVE MW
C
      AMW=2.0436D2 * EXP(0.00218D0*MEABP) * EXP(-3.07D0*SG)
     1          * (MEABP**0.118D0) * (SG**1.88D0)
C
C
      IF(AMW.LE.70.D0.OR.AMW.GT.724.D0)THEN
        IERR=-3
        WRITE(NHSTRY,900)
        CALL MESS(1)
        WRITE(NHSTRY,3000)AMW
      ENDIF
C
C         FORMATS
C
900   FORMAT(1X,'IN MODULE RDMW')
1000  FORMAT(
     1      1X,'MEABP(DEG R) VALUE IS NOT IN RANGE 556.67-1495.67',/,
     2      1X,'MEABP-VALUE = ',G12.6,' CALC. CONTINUES')
2000  FORMAT(
     1      1X,'API VALUE IS NOT IN RANGE 14.4-93.1',/,
     2      1X,'API-VALUE = ',G12.6,' CALC. CONTINUES')
3000  FORMAT(
     1      1X,'MW VALUE IS NOT IN RANGE 70-724',/,
     2      1X,'MW-VALUE = ',G12.6,' CALC. CONTINUES')
C
      RETURN
C
      END
C*****************************************************************************
C
      SUBROUTINE RDPC(AMW,TBR,API,SG,PC,IERR)
C
C*****************************************************************************
C
```

```
C
C       NAME OF MODULE - API4D4P1
C       MODULE TITLE - PROCEDURE 4D4.1 API DATA BOOK P4-57 (1980)
C       PURPOSE - METHOD FOR THE PSEUDOCRITICAL PRESSURE OF PETROLEUM
C                 FRACTIONS
C       MODIFIED - 10-3-88
C
C       LIMITATIONS:
C          MW           82-694
C          TB(DEG F)    100-850
C          API          6.6-95.0
C
C       VARIABLES USED-
C
C VARIABLE I/O TYPE-SPEC DIMENSION      DESCRIPTION AND RANGE
C   AMW      I       R          -       MOLE WEIGHT
C   TBR      I       R          -       MEAN AVERAGE BOILING POINT
C                                       (DEG R)
C    SG      I       R          -       SPECIFIC GRAVITY (60/60F)
C    PC      O       R          -       PSEUDOCRITICAL PRES. OF PET.
C                                       FRAC.,PSIA
C  IERR      O       I          -       ERROR CODE
C                                        0 = OK
C                                       -1 = MW NOT IN RANGE ABOVE
C                                       -2 = TB NOT IN RANGE ABOVE
C                                       -3 = API NOT IN RANGE ABOVE
C
      IMPLICIT REAL*8 (A-H,O-Z)
      IMPLICIT INTEGER(I-N)
C
      PARAMETER        (MNC=25)
C
      COMMON /IO     / NIN,NOUT,NHSTRY,NREPT
      COMMON /DEBUG  / LDBUG,LDBUGR
C
      IERR=0
C
C      CHECK IF IN RANGE
C
      IF(AMW.LT.82.D0.OR.AMW.GT.694.D0)THEN
       WRITE(NHSTRY,900)
       CALL MESS(1)
       IERR=-1
       WRITE(NHSTRY,1000)AMW
      ENDIF
C
      CALL TCON(TBR,TBF,21,IERR1)
C
      IF(TBF.LT.100.D0.OR.TBF.GT.850.D0)THEN
       WRITE(NHSTRY,900)
       CALL MESS(1)
       IERR=-2
       WRITE(NHSTRY,2000)TBF
      ENDIF
C
      IF(API.LT.6.6D0.OR.API.GT.95.D0)THEN
       WRITE(NHSTRY,900)
       CALL MESS(1)
       IERR=-3
       WRITE(NHSTRY,3000)API
      ENDIF
C
C      PSEUDOCRITICAL PRES. OF FRACTION, PA
C
      PC=3.12281D9 * TBR**(-2.3125D0) * SG**(2.3201D0)
C
C      FORMATS
C
```

```
900    FORMAT(1X,'IN MODULE RDPC')
1000   FORMAT(
      1     1X,'MW VALUE IS NOT IN RANGE 82-694',/,
      2     1X,'MW-VALUE = ',G12.6,' CALC. CONTINUES')
2000   FORMAT(
      1     1X,'TB(DEG F) VALUE IS NOT IN RANGE 70-295',/,
      2     1X,'TB-VALUE = ',G12.6,' CALC. CONTINUES')
3000   FORMAT(
      1     1X,'API VALUE IS NOT IN RANGE 6.6-95',/,
      2     1X,'API VALUE = ',G12.6,' CALC. CONTINUES')
C
       RETURN
C
       END
C*****************************************************************************
C
       SUBROUTINE RDTC(AMW,TBR,API,SG,TC,IERR)
C
C*****************************************************************************
C
C
C         NAME OF MODULE - RDTC
C         MODULE TITLE - PROCEDURE 4D3.1 API DATA BOOK P4-51 (1980)
C         PURPOSE - METHOD FOR THE PSEUDOCRITICAL TEMP. OF PETROLEUM
C                   FRACTIONS
C         MODIFIED - 10-3-88
C
C         LIMITATIONS:
C            MW           82-694
C            TB(DEG F)    100-850
C            API          6.6-95.0
C
C         VARIABLES USED-
C
C VARIABLE I/O TYPE-SPEC DIMENSION      DESCRIPTION AND RANGE
C    AMW      I       R          -      MOLECULAR WT
C    TBR      I       R          -      MEAN AVERAGE BOILING POINT
C                                       (DEG R)
C    API      I       R          -      API GRAVITY
C     SG      I       R          -      SPECIFIC GRAVITY (60/60F)
C     TC      O       R          -      PSEUDOCRITICAL TEMP. OF PET.
C                                       FRAC., (DEG R)
C   IERR      O       I          -      ERROR CODE
C                                        0 = OK
C                                       -1 = MW NOT IN RANGE ABOVE
C                                       -2 = TB NOT IN RANGE ABOVE
C                                       -3 = API NOT IN RANGE ABOVE
C
       IMPLICIT REAL*8 (A-H,O-Z)
       IMPLICIT INTEGER(I-N)
C
       PARAMETER        (MNC=25)
C
       COMMON /IO     / NIN,NOUT,NHSTRY,NRPT
       COMMON /DEBUG  / LDBUG,LDBUGR
C
       IF(LDBUG.GT.7)WRITE(NHSTRY,900)
       IERR=0
C
C       CHECK IF IN RANGE
C
       IF(AMW.LT.100.D0.OR.AMW.GT.850.D0)THEN
        WRITE(NHSTRY,900)
        CALL MESS(1)
        IERR=-1
        WRITE(NHSTRY,1000)AMW
       ENDIF
C
```

```
      CALL TCON(TBR,TBF,21,IERR1)
      IF(TBF.LT.100.D0.OR.TBF.GT.850.D0)THEN
       IERR=-2
       WRITE(NHSTRY,900)
       CALL MESS(1)
       WRITE(NHSTRY,2000)TBF
      ENDIF
C
      IF(API.LT.6.6D0.OR.API.GT.95.D0)THEN
       IERR=-3
       WRITE(NHSTRY,900)
       CALL MESS(1)
       WRITE(NHSTRY,3000)API
      ENDIF
C
C      PSEUDOCRITICAL TEMP. OF FRACTION, IN DEGREES R
C
      TC=24.2787D0 * TBR**(0.58848D0) * SG**(0.3596D0)
C
C        FORMATS
C
900   FORMAT(1X,'IN MODULE RDTC')
1000  FORMAT(1X,'MW VALUE IS NOT IN RANGE 82-694',/,
     1       1X,'MW-VALUE = ',G12.6,' CALC. CONTINUES')
2000  FORMAT(1X,'TB(DEG F) VALUE IS NOT IN RANGE 100-850',/,
     1       1X,'TB-VALUE = ',G12.6,' CALC. CONTINUES')
3000  FORMAT(1X,'API VALUE IS NOT IN RANGE 6.6-95',/,
     1       1X,'API VALUE = ',G12.6,' CALC. CONTINUES')
C
      RETURN
C
      END
C*****************************************************************************
C
      SUBROUTINE RDVC(AMW,TBR,SG,VC,IERR)
C
C*****************************************************************************
C
C        NAME OF MODULE - RDVC
C        MODULE TITLE - TO ESTIMATE PHYSICAL PROPS BY RIAZI DAUBERT METH
C        PURPOSE - TO ESTIMATE PHYSICAL PROPERTIES USING RIAZI AND DAUBERT
C                  METHOD
C                  REF: HYDROCARBON PROCESSING MARCH 1980 P115-116
C                       RIAZI AND DAUBERT
C        MODIFIED - 10-3-88
C
C        LIMITATIONS:
C           MW            77.2-294.5
C           TB(DEG F)     100-850
C           SG            0.6247-1.0244
C
C        VARIABLES USED-
C
C VARIABLE I/O TYPE-SPEC DIMENSION      DESCRIPTION AND RANGE
C     AMW     I       R          -      MOLE WEIGHT
C     TBR     I       R          -      MEAN AVERAGE BOILING POINT
C                                       (DEG R)
C     SG      I       R          -      SPECIFIC GRAVITY (60/60F)
C     VC      I       R          -      MOLAR CRITICAL VOLUME (M**3/KG-MOLE)
C   IERR      O       I          -      ERROR CODE
C                                        0 = OK
C                                       -1 = TR NOT IN RANGE ABOVE
C
      IMPLICIT REAL*8 (A-H,O-Z)
      IMPLICIT INTEGER(I-N)
C
      PARAMETER        (MNC=25)
C
```

```
      COMMON /IO     / NIN,NOUT,NHSTRY,NREPT
      COMMON /DEBUG  / LDBUG,LDBUGR
C
      IF(LDBUG.GT.7)WRITE(NHSTRY,900)
      IERR=0
      ITYP=4
C
      CALL RDCHECK(AMW,TBR,SG,ITYP)
C
C       MOLAR CRITICAL VOLUME (FT**3/LB-MOLE)
C
      VCM=7.0434D-7 * TBR**(2.3829D0) * SG**(-1.683D0)
C
C       CONVERT CRITICAL VOLUME TO CORRECT UNITS (M**3/KG-MOLE)
C
      VC=VCM/35.3145D0/0.453593D0
C
C       FORMATS
C
900   FORMAT(1X,'IN MODULE RDVC')
      RETURN
      END
C*****************************************************************
C
      SUBROUTINE REFLV(JC,ICT,IERR)
C
C*****************************************************************
C
C       NAME OF MODULE - REFLV
C       MODULE TITLE - RACKETT EQUATION FOR LIQUID VOLUME
C       PURPOSE - TO ESTIMATE THE RACKETT EQUATION LIQUID VOLUME
C                 PARAMETER RKTZRA
C       MODIFIED - 10-5-88
C       METHOD - GENERATE VALUES FOR MODIFIED RACKETT EQUATION
C                BY DEFAULT=ZC OR FITTING GUNN YAMADA METHOD.
C
C
C       VARIABLES USED-
C
C VARIABLE I/O TYPE-SPEC DIMENSION     DESCRIPTION AND RANGE
C      JC    I       I         -       COMPONENT ARRAY ID
C     ICT    I       I         -       ICALC TYPE
C                                      0 = USE ZC
C                                      1 = FIT DATA
C    IERR    O       I         -       ERROR CODE
C                                       0 = OK
C                                      -1 = NO IMPROVEMENT POSSIBLE IN
C                                      THE VALUE OF PH EVEN THOUGH
C                                      CONVERGENCE HAS NOT BEEN REACHED.
C                                      -2 = MORE UNKNOWNS THAN FUNCTIONS AND
C                                      UNIQUE SOLUTION GENERALLY IS IMPOSSIBLE.
C                                      -3 = TOTAL NUMBER OF VARIABLES TO BE
C                                      VARIED IS ZERO
C                                      -4 = CONVERGENCE CRITERION MET BUT FLA
C                                      STILL LARGE
C                                      -5 = IC NOT A VALID NUMBER ON ENTRY
C                                      -6 = X(I) IS NOT WITHIN XMIN(I) TO
C                                       XMAX(I)
C                                      -7 = ZERO DIAGONAL ELEMENT IN EQUATION
C                                      SOLVE
C                                      -10 = TRY TO CALC. DERIVATIVE
C                                      ANALYTICALY
C                                      -11 = RUN EXCEEDED MAXIT SPECIFIED
C
      IMPLICIT REAL*8 (A-H,O-Z)
      IMPLICIT INTEGER(I-N)
C
      PARAMETER       (MNC=25)
```

```
C
      COMMON /IO     / NIN,NOUT,NHSTRY,NREPT
      COMMON /DEBUG  / LDBUG,LDBUGR
      COMMON /REFS   / TREF,PREF,RGAS
C
      COMMON /CPRP01/ TC(MNC)
      COMMON /CPRP02/ PC(MNC)
      COMMON /CPRP04/ ZC(MNC)
      COMMON /CPRP05/ OMEGA(MNC)
      COMMON /CPRP12/ RKTZRA(MNC),RKTREG(3,MNC)
      COMMON /CPRP14/ TB(MNC)
      COMMON /CPRP15/ VB(MNC)
C
      DIMENSION       NDATA(26),DATA(16),OUTPUT(6)
C
C      DIMENSION B(2*K),BV(K),BMAX(K),BMIN(K),Y(N),Z(2*N),PJ(N)
C      DIMENSION P(K*(N+2)+N),A(K*K+2*K),AC(K*K+2*K),XO(K)
C
C
      DIMENSION       X(50),Y(50),
     1                Z(100),PJ(50),P(102),A(5),AC(5)
      DIMENSION       B(2),BV(1),BMAX(1),BMIN(1)
C
      IF(LDBUG.GT.7)WRITE(NHSTRY,900)
C
      IF(ICT.EQ.0)THEN
       RKTZRA(JC)=ZC(JC)
      ELSE
C
C        FIT GUNN YAMADA IN RANGE 0.2<TR<0.99
C         SET DEFAULTS
C
       MAXIT=1000
C
C        NUMBER OF UNKNOWNS
       K=1
C
C        NUMBER OF DATA POINTS
       N=50
C
       ITER = 0
C
C        INITIAL GUESS
C
       B(1) = ZC(JC)
C
       NDATA(1)=1
C
       DO 10 I=1,5
        DATA(I)=0.0D0
10     CONTINUE
       DO 20 I=1,K
        BV(I)=1.D0
        BMAX(I)= 0.99D0
        BMIN(I)= 0.01D0
20     CONTINUE
       IF(B(I).LT.BMIN(I))B(I)=BMIN(I)
       IF(B(I).GT.BMAX(I))B(I)=BMAX(I)
C
       IF(LDBUG.GE.7)THEN
        WRITE(NHSTRY,1008)K,N
        DO 30 I=1,K
         WRITE(NHSTRY,1009)B(I),BMIN(I),BMAX(I),BV(I)
30      CONTINUE
        WRITE(NHSTRY,1010)
        WRITE(NHSTRY,1100)
        XSUM=0.0D0
        XSUM2=0.0D0
```

```
         YSUM=0.0D0
         YSUM2=0.0D0
        ENDIF
C
C       BEGIN CALC (CALC 50 POINTS TO BE FIT)
C
        ICALC=0
C
        DEL=(0.99D0-0.20D0)/FLOAT(N)
        TRD=0.20D0-DEL
        OMEGAI=OMEGA(JC)
        VR=VB(JC)
        TR=TB(JC)/TC(JC)
C
        DO 40 I=1,N
         TRD=TRD+DEL
C
         CALL GUNYAM(VR,TR,OMEGAI,TRD,ICALC,VD,IERR)
         X(I)=TRD*TC(JC)
         Y(I)=VD
C
        IF(LDBUG.GE.7)THEN
         WRITE(NHSTRY,1020)X(I),Y(I)
         XSUM=XSUM+X(I)
         XSUM2=XSUM2+X(I)**2
         YSUM=YSUM+Y(I)
         YSUM2=YSUM2+Y(I)**2
        ENDIF
C
C       MEANS, VARIANCES AND STANDARD DEV.
C
         IF(LDBUG.GE.7)THEN
          XMEAN=XSUM/FLOAT(N)
          XVAR=(FLOAT(N)*XSUM2-XSUM*XSUM)/FLOAT(N)/FLOAT(N-1)
          XSD=SQRT(XVAR)
          YMEAN=YSUM/FLOAT(N)
          YVAR=(FLOAT(N)*YSUM2-YSUM*YSUM)/FLOAT(N)/FLOAT(N-1)
          YSD=SQRT(YVAR)
          WRITE(NHSTRY,1120)XMEAN,YMEAN,XVAR,YVAR,XSD,YSD
         ENDIF
40      CONTINUE
C
C         MARQUARDT LOOP BEGINS TO FIT RKZRA
C
50      ITER=ITER+1
        IF(ITER.GT.MAXIT)THEN
         IERR=-11
         CALL MESS(2)
         WRITE(NHSTRY,900)
         WRITE(NHSTRY,1045)MAXIT,ITER
         GOTO 9000
        ENDIF
C
C         EVALUATE Z VECTOR (FUNCTION VALUE)
C          VOL=R*TC/PC*ZRKZRA**(1+(1-TR)**2/7)
C
        TS=2.D0/7.D0
        DO 60 I=1,N
         TR=X(I)/TC(JC)
         Z(I)=RGAS*TC(JC)/PC(JC) * B(I)**(1.D0+(1.D0-TR)**TS)
60      CONTINUE
C
C       CALC ANALYTICAL DERIVATIVES (PJ VECTOR)
C
70      CONTINUE
C
C         CALC DERIVATIVE
C
```

```
      IF(NDATA(2).GT.0)THEN
       IERR=-10
       CALL MESS(3)
       WRITE(NHSTRY,900)
       WRITE(NHSTRY,1090)IERR
       WRITE(NHSTRY,1022)
       RKTZRA(JC)=ZC(JC)
       GOTO 9000
      ENDIF
C
C
      IF(LDBUG.GE.7)THEN
       WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
       YMYC =0.0D0
       SS   =0.0D0
       SSSAS=0.0D0
       DO 90 I=1,N
        YMYC=YMYC+(Y(I)-Z(I))**2
        SS=SS+(Z(I)-YMEAN)**2
        SSSAS=SSSAS+(Y(I)**2 - YMEAN**2)
90     CONTINUE
C
C      CALC R-SQUARE(SAS VERSION) AND ADJ R-SQUARE
C           1-VARIANCE OF FULL MODEL/VARIANCE OF MEAN MODEL
C
       RSQU=SS/(SS+YMYC)
       IF(SSSAS.NE.0.D0)THEN
        RSQUSAS=1.D0-YMYC/(SSSAS)
       ELSE
        RSQUSAS=0.D0
       ENDIF
       IF(DEGFR.EQ.0.D0)THEN
        ADJRSQU=0.0D0
       ELSE
        ADJRSQU=1.D0-(1.D0-RSQU)*(FLOAT(N)-1.D0)/DEGFR
       ENDIF
       IF(ABS(RSQU-RSQUSAS).GT.1.D0)THEN
        WRITE(NHSTRY,1112)RSQU,ADJRSQU,RSQUSAS,ADJRSQUSAS
       ELSE
        WRITE(NHSTRY,1110)RSQU,ADJRSQU
       ENDIF
C
       DO 100 J=1,K
        WRITE(NHSTRY,1030)J,B(J)
100    CONTINUE
C
       IF(LDBUG.EQ.8)THEN
        WRITE(NHSTRY,1040)
        DO 110 I=1,N
         YMYC=YMYC+(Y(I)-Z(I))**2
        SS=SS+(Z(I)-YMEAN)**2
         PERERR=ABS(Z(I)-Y(I))/ABS(Y(I))*100.D0
         WRITE(NHSTRY,1095)I,Z(I),Y(I),Z(I)-Y(I),PERERR
110     CONTINUE
       ENDIF
      ENDIF
C
120   CALL VSOLVE (K, N, NDATA, DATA, B, BV, BMAX, BMIN, Y, Z, PJ,
     1              OUTPUT, P, A, AC)
C
C                    NDATA(2) - NFCTDR, USED FOR CONTROL IN CALLING PROG
C                        IF = 0, CALCULATE FUNCTION
C                        IF = 1, CALCULATE DERIVATIVE
C                        IF =-1, EXAMINE IERR FOR WHAT TO DO NEXT
C
      IF(NDATA(2))130,50,70
C
C                    NDATA(3) - IERR, MAY TAKE ON VARIOUS VALUES
```

```
C                          IF POSITIVE, CONTAINS THE NUMBER OF VARIABLES NO
C                                    SATISFYING CONVERGENCE CRITERION
C                          IF =  0, CONVERGENCE SATISFIED AND SOLUTION RETU
C                          IF = -1, NO IMPROVEMENT POSSIBLE IN THE VALUE OF
C                                   PR EVEN THOUGH CONVERGENCE HAS NOT BEEN
C                                   REACHED.
C                          IF = -2, MORE UNKNOWNS THAN FUNCTIONS AND UNIQUE
C                                   SOLUTION GENERALLY IS IMPOSSIBLE.
C                          IF = -3, TOTAL NUMBER OF VARIABLES TO BE VARIED
C                                   IS ZERO
C                          IF = -4, CONVERGENCE CRITERION MET BUT FLA STILL
C                                   LARGE
C                          IF = -5, IC NOT A VALID NUMBER ON ENTRY
C                          IF = -6, B(I) IS NOT WITHIN BMIN(I) TO BMAX(I)
C                          IF = -7, ZERO DIAGONAL ELEMENT IN EQUATION SOLVE
C
130      IF(NDATA(3))140,140,120
C
C        FINAL STATISTICAL RESULTS
C
140      CONTINUE
         IF(LDBUG.GE.6)THEN
          WRITE(NHSTRY,900)
          WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
          YMYC  =0.0D0
          SS    =0.0D0
          SSSAS =0.0D0
          DO 150 I=1,N
           YMYC=YMYC+(Y(I)-Z(I))**2
           SS=SS+(Z(I)-YMEAN)**2
           SSSAS=SSSAS+(Y(I)**2-YMEAN**2)
150       CONTINUE
C
C         CALC R-SQUARE(SAS VERSION) AND ADJ R-SQUARE
C
C         RSQUSAS=1-VARIANCE (FULL MODEL)/VARIANCE (MEAN MODEL)
C
          RSQU=SS/(SS+YMYC)
          RSQUSAS=1.D0-YMYC/(SSSAS)
          IF(DEGFR.EQ.0.0D0)THEN
           ADJRSQU=0.0D0
           ADJRSQUSAS=0.0D0
          ELSE
           ADJRSQU=1.D0-(1.D0-RSQU)*(FLOAT(N)-1.D0)/DEGFR
           ADJRSQUSAS=1.D0-(1.D0-RSQUSAS)*(FLOAT(N)-1.D0)/DEGFR
          ENDIF
          IF(ABS(RSQU-RSQUSAS).GT.1.D0)THEN
           WRITE(NHSTRY,1112)RSQU,ADJRSQU,RSQUSAS,ADJRSQUSAS
          ELSE
           WRITE(NHSTRY,1110)RSQU,ADJRSQU
          ENDIF
C
C         FINAL PARAMETERS
C
          DO 160 J=1,K
           WRITE(NHSTRY,1030)J,B(J)
160       CONTINUE
C
C         FINAL SUMMARY
C
          WRITE(NHSTRY,1040)
          DO 170 I=1,N
           PERERR=ABS(Z(I)-Y(I))/ABS(Y(I))*100.D0
           WRITE(NHSTRY,1095)I,Z(I),Y(I),Z(I)-Y(I),PERERR
170       CONTINUE
         ENDIF
C
C        LOAD DATA INTO RKTZRA ARRAY
```

```
C
      IERR=NDATA(3)
C
      IF(IERR.EQ.0)THEN
C
C     CONVERGED
C
       RKTZRA(JC)=B(1)
C
       IF(LDBUG.GE.1)THEN
        WRITE(NHSTRY,900)
        WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
       ENDIF
      ELSE IF(IERR.EQ.-1)THEN
       RKTZRA(JC)=ZC(JC)
       CALL MESS(1)
       WRITE(NHSTRY,900)
       WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
       WRITE(NHSTRY,1001)
       WRITE(NHSTRY,1022)
      ELSE IF(IERR.EQ.-2)THEN
       RKTZRA(JC)=ZC(1)
       CALL MESS(1)
       WRITE(NHSTRY,900)
       WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
       WRITE(NHSTRY,1002)
       WRITE(NHSTRY,1022)
      ELSE IF(IERR.EQ.-3)THEN
       CALL MESS(2)
       WRITE(NHSTRY,900)
       WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
       WRITE(NHSTRY,1003)
       WRITE(NHSTRY,1022)
       RKTZRA(JC)=ZC(JC)
      ELSE IF(IERR.EQ.-4)THEN
       CALL MESS(2)
       WRITE(NHSTRY,900)
       WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
       WRITE(NHSTRY,1004)
       WRITE(NHSTRY,1022)
       RKTZRA(JC)=ZC(JC)
      ELSE IF(IERR.EQ.-5)THEN
       CALL MESS(2)
       WRITE(NHSTRY,900)
       WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
       WRITE(NHSTRY,1005)
       WRITE(NHSTRY,1022)
       RKTZRA(JC)=ZC(JC)
      ELSE IF(IERR.EQ.-6)THEN
       CALL MESS(2)
       WRITE(NHSTRY,900)
       WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
       WRITE(NHSTRY,1006)
       WRITE(NHSTRY,1022)
       RKTZRA(JC)=ZC(JC)
      ELSE IF(IERR.EQ.-7)THEN
       CALL MESS(2)
       WRITE(NHSTRY,900)
       WRITE(NHSTRY,1000)ITER,NDATA(3),(OUTPUT(J),J=1,5)
       WRITE(NHSTRY,1007)
       WRITE(NHSTRY,1022)
       RKTZRA(JC)=ZC(JC)
      ENDIF
      RKTREG(1,JC)=FLOAT(ITER)
      RKTREG(2,JC)=FLOAT(NDATA(3))
      RKTREG(3,JC)=OUTPUT(1)
     ENDIF
C
```

```
C        FORMATS
C
900    FORMAT(1X,'IN MODULE REFLV')
1000   FORMAT(/,
     1     1X,'ITERATION: ',I9,/,
     2     1X,'IERR                                          = ',I15,/,
     3     1X,'SUM OF SQUARES                                = ',G15.8,/,
     4     1X,'ANGLE (DEGREES)                               = ',F15.2,/,
     5     1X,'NUMBER OF TIMES YSOLVE CALLED                 = ',F15.1,/,
     6     1X,'NUMBER OF FUNCTIONAL EVALUATIONS              = ',F15.1,/,
     7     1X,'NUMBER OF ANALYTICAL DERIVATIVE EVALUATIONS   = ',F15.1,/)
1001   FORMAT(1X,'NO IMPROVEMENT POSSIBLE IN THE VALUE OF',/,
     1        1X,'PH EVEN THOUGH CONVERGENCE HAS NOT BEEN REACHED.',/)
1002   FORMAT(1X,'MORE UNKNOWNS THAN FUNCTIONS AND UNIQUE',/)
1003   FORMAT(1X,'TOTAL NUMBER OF VARIABLES TO BE VARIED = 0',/)
1004   FORMAT(1X,'CONVERGENCE CRITERION MET BUT FLA STILL LARGE',/)
1005   FORMAT(1X,'IC NOT A VALID NUMBER ON ENTRY',/)
1006   FORMAT(1X,'X(I) IS NOT WITHIN XMIN(I) TO XMAX(I)',/)
1007   FORMAT(1X,'ZERO DIAGONAL ELEMENT IN EQUATION SOLVE',/)
1008   FORMAT(/,5X,'*****MARQUARDT METHOD REGRESSION*****',//,
     1 5X,'K (NUMBER OF PARAMETERS TO BE VARIED) = ',I4,/,
     2 5X,'N (NUMBER OF DATA POINTS)             = ',I4,//,
     3 5X,'INITAL B            B-MIN            B-MAX',
     4'VARY FLAG',/)
1009   FORMAT(2X,4(G15.5,1X))
1010   FORMAT(5X,'VARY FLAG:',/,
     1 10X,'0 = HOLD PARAMETER CONSTANT',/,
     2 10X,'1 = VARY PARAMETER USING NUMERICAL DERIVATIVE',/,
     3 9X,'-1 = VARY PARAMETER USING ANALYTICAL DERIVATIVE')
1020   FORMAT(1X,3G15.6)
1022   FORMAT(1X,'*** VALUE IS DEFAULTED TO ZC ***')
1030   FORMAT(1X,'B(',I2,') = ',G13.5)
1040   FORMAT(/,1X,'OBS.   Y-CALC         Y-ACTUAL        DIFF.          ',
     1 '% ERROR',/)
1095   FORMAT(1X,I4,4(1X,G13.5))
1100   FORMAT(/,10X,'INPUT DATA',//,
     1 5X,'X-VALUE          Y-VALUE ',/,
     2 5X,'-------          ------- ',/)
1110   FORMAT(
     1 1X,'R-SQUARE                                        = ',F15.8,/,
     2 1X,'ADJ R-SQUARE                                    = ',F15.8,/)
1112   FORMAT(
     1 1X,'R-SQUARE                                        = ',F15.8,/,
     2 1X,'ADJ R-SQUARE                                    = ',F15.8,/,
     3 1X,'R-SQUARE(1-VAR.FM/VAR.MI)                       = ',F15.8,/,
     4 1X,'ADJ R-SQUARE(FOR 2ND R-SQUARE)                  = ',F15.8,/)
1120   FORMAT(//,10X,'STATISTICS',//,
     1 5X,'X-VALUES ',26X,'Y-VALUES',/,
     2 5X,'---------',26X,'---------',/,
     3 5X,'MEAN       = ',G15.5,8X,'MEAN       = ',G15.5,/
     4 5X,'VARIANCE   = ',G15.5,8X,'VARIANCE   = ',G15.5,/
     5 5X,'STD. DEV.  = ',G15.5,8X,'STD. DEV.  = ',G15.5,/)
1045   FORMAT(/,1X,'*****RUN EXCEEDED MAXIT OF ',I5,' ITER = ',I5,
     2          '*******',//)
1090   FORMAT(1X,'IERR = ',I5,' TRY TO CALC.',
     1        ' DERIVATIVE ANALYTICALY, CALC. ABORTED')
9000   CONTINUE
       RETURN
       END
C*************************************************************************
C
       SUBROUTINE SOLPAR(JC,IERR)
C
C*************************************************************************
C
C        NAME OF MODULE - SOLPAR
C        MODULE TITLE - CALCULATION OF SOLUBILITY PARAMETER AT 25 DEG C
C        PURPOSE - TO CALC SOLUBILITY PARAMETER AT 25 DEG C
```

```
C        MODIFIED - 11-12-88
C        METHOD - ESTIMATE SOLUBILITY PARAMETER PER API REPORT API-1-77.
C                 USING HEAT OF VAPORIZATION AT 25 C BY WATSON METHOD AND
C                 VOLUME AT 20 C AND 1 ATM BY RAIZI DAUBERT METHOD
C                 AND CORRECT TO 25 C BY GUNN & YAMADA METHOD
C
C
C        VARIABLES USED-
C
C VARIABLE I/O TYPE-SPEC DIMENSION      DESCRIPTION AND RANGE
C      JC    I       I         -        COMPONENT ARRAY ID
C    IERR    O       I         -        ERROR CODE
C                                       0 = OK
C                                       -1 = GUNYAM REDUCED TEMP > 0.99
C                                       -2 = GUNYAM REDUCED TEMP < 0.2
C                                       -3 = TB OUT OF RANGE
C                                       -4 = SG OUT OF RANGE
C                                       -5 = WATSON CALC OUT OF RANGE
C
      IMPLICIT REAL*8 (A-H,O-Z)
      IMPLICIT INTEGER(I-N)
C
C
      PARAMETER        (MNC=25)
C
      COMMON /IO     / NIN,NOUT,NHSTRY,NREPT
      COMMON /DEBUG  / LDBUG,LDBUGR
      COMMON /REFS   / TREF,PREF,RGAS
C
      COMMON /NPROP3/ UOPK(MNC),API(MNC),SG(MNC),AMW(MNC)
C
      COMMON /CPRP01/ TC(MNC)
      COMMON /CPRP05/ OMEGA(MNC)
      COMMON /CPRP08/ DHVLWT(5,MNC)
      COMMON /CPRP14/ TB(MNC)
      COMMON /CPRP18/ DELTA(MNC)
C
      IERR=0
      IF(LDBUG.GT.7)WRITE(NHSTRY,900)
C
C       CALC HEAT OF VAPORIZATION (J/KMOLE) AT 25 C USING ASPEN'S
C       WATSON EQUATION
C
      T25CK=TREF
C
      IF(T25CK.LT.0.D0.OR.T25CK.GT.TC(JC))THEN
       IERR=-5
       CALL MESS(1)
       WRITE(NHSTRY,3000)T25CK
      ENDIF
C
      HVA25=DHVLWT(1,JC) *
     1       ((1.D0-T25CK/TC(JC))/(1.D0-DHVLWT(2,JC)/TC(JC)))**
     2       (DHVLWT(3,JC)+DHVLWT(4,JC)*(1.D0-T25CK/TC(JC)))
C
C       CONVERT TO CAL/GM
C
      HVA25=HVA25*0.23901D0/1000.D0/AMW(JC)
C
C        CALC ENERGY OF VAPORIZATION AT 25 C
C
C       CALL TCON(T25CK,T25CR,42,IERR1)
      EVA25=HVA25 - 1.98719D0*T25CK/AMW(JC)
C
C        LIQUID MOLAR VOLUME AT 20 DEG C AND 1 ATM (CM**3/G-MOLE)
C        AT (BTU/LB-MOLE) AT TB AND SG
C
      CALL TCON(TB(JC),TBR,42,IERR2)
```

```
      CALL TCON(TBR,TBF,21,IERR1)
C
      IF(TBF.LT.100.D0.OR.TBF.GT.850.D0)THEN
       IERR=-3
       CALL MESS(1)
       WRITE(NHSTRY,900)
       WRITE(NHSTRY,2000)TBF
      ENDIF
C
      SM=SG(JC)
      IF(SM.LT.0.6247D0.OR.SM.GT.1.0244D0)THEN
       IERR=-4
       CALL MESS(1)
       WRITE(NHSTRY,900)
       WRITE(NHSTRY,1000)SM
      ENDIF
C
      V=7.6211D-5 *TBR**(2.1262D0) * SM**(-1.8688D0)
C
C       CORRECT TO 25 C BY GUNYAM
C
      VR=V
      TR=293.15D0/TC(JC)
      OMEGAI=OMEGA(JC)
      TRD=TREF/TC(JC)
      ICALC=0
      CALL GUNYAM(VR,TR,OMEGAI,TRD,ICALC,VD,IERR)
C
C         DENSITY AT 25 C (GM/CM**3)
C
      RHO=1.D0/VD*AMW(JC)
C
C         CALC SOLUBILITY PARAMETER (CAL/CM**3)
C
      SOLP=EVA25*RHO
C
C         SOLUBILITY PARAMETER (CAL/CM**3)**1/2
C
      SOLP=SQRT(SOLP)
C
C         SOLUBILITY PARAMETER (J/M**3)**1/2
C
      CFACT=SQRT(1.D6/.23901D0)
      DELTA(JC)=SOLP * CFACT
C
C        FORMATS
C
900   FORMAT(1X,'IN MODULE SOLPAR')
1000  FORMAT(1X,'SG VALUE IS NOT IN RANGE 0.6247-1.0244',/,
     1        1X,'SG VALUE = ',G12.6,' CALC. CONTINUES')
2000  FORMAT(1X,'TB(DEG F) VALUE IS NOT IN RANGE 100-850',/,
     1        1X,'TB-VALUE = ',G12.6,' CALC. CONTINUES')
3000  FORMAT(1X,'WATSON VALUE IS NOT IN RANGE 0-TC',/,
     1        1X,'WATSON VALUE = ',G12.6,' CALC. CONTINUES')
      RETURN
      END
C*****************************************************************************
C
      SUBROUTINE TBCALC(JC,IERR)
C
C*****************************************************************************
C
C         NAME OF MODULE - TBCALC
C         MODULE TITLE - LOAD NORMAL BOILING POINT ARRAY
C         PURPOSE - TO LOAD NORMAL BOILING POINT ARRAY
C         MODIFIED - 10-28-88
C         METHOD - SET EQUAL TO INPUT VOLUME AVERAGE BOILING POINT
C
```

```
C        VARIABLES USED-
C
C VARIABLE I/O TYPE-SPEC DIMENSION      DESCRIPTION AND RANGE
C      JC     I       I         -       COMPONENT ARRAY ID
C    IERR     O       I         -       ERROR CODE
C                                       0 = OK
C
       IMPLICIT REAL*8 (A-H,O-Z)
       IMPLICIT INTEGER(I-N)
C
       REAL*8           MABP,MEABP
C
       PARAMETER        (MNC=25)
C
       COMMON /IO     / NIN,NOUT,NHSTRY,NREPT
       COMMON /DEBUG  / LDBUG,LDBUGR
C
       COMMON /NPROP2/ VABP(MNC),SLOP(MNC),CABP(MNC),MABP(MNC),MEABP(MNC)
C
       COMMON /CPRP14/ TB(MNC)
C
       IF(LDBUG.GT.7)WRITE(NHSTRY,900)
       IERR=0
C
       TB(JC)=VABP(JC)
C
C       FORMATS
C
900    FORMAT(1X,'IN MODULE TBCALC')
C
       RETURN
       END
C*******************************************************************************
C
       SUBROUTINE TBPCF(VABPI,STBP,CABP,MABP,IERR)
C
C*******************************************************************************
C
C        NAME OF MODULE - TBPCF
C        MODULE TITLE - CHARACTERIZE PETROLEUM FRACTION BOILING PTS
C        PURPOSE - METHOD FOR CHARACTERIZE PETROLEUM FRACTION BOILING
C                  POINTS
C        MODIFIED - 1-6-89
C
C        LIMITATIONS:
C           SLOPE           0-10.0
C           CABP          200-600
C
C        VARIABLES USED-
C
C VARIABLE I/O TYPE-SPEC DIMENSION      DESCRIPTION AND RANGE
C  VABPI     I       R          -       VOLUME AVERAGE BOILING POINT (DEG F)
C   STBP     I       R          -       SLOPE OF TBP CURVE
C                                       (T70-T10)/60 (DEG F/DEG F)
C   CABP     O       R          -       CUBIC AVERAGE BOILING POINT (DEG F)
C   MABP     O       R          -       MOLAL AVERAGE BOILING POINT (DEG F)
C   IERR     O       I          -       ERROR CODE
C                                        0 = OK
C                                       -1 = SLOPE NOT IN RANGE ABOVE
C                                       -2 = CABP NOT IN RANGE ABOVE
C
       IMPLICIT REAL*8 (A-H,O-Z)
       IMPLICIT INTEGER(I-N)
C
       REAL*8           MABP,MABPC,INEX
C
       COMMON /IO     / NIN,NOUT,NHSTRY,NREPT
       COMMON /DEBUG  / LDBUG,LDBUGR
```

```
C
      IERR=0
C
      IF(LDBUG.GT.7)WRITE(NHSTRY,900)
C
      CABPC=0.D0
      MABPC=0.D0
      VABP=VABPI
C
C       CHECK IF SLOPE IN RANGE (0-10)
C
      IF(STBP.LT.0.D0)THEN
        IERR=-1
        CALL MESS(1)
        WRITE(NHSTRY,900)
        WRITE(NHSTRY,1000)STBP
        STBP=0.0D0
      ENDIF
      IF(STBP.GT.10.0)THEN
        IERR=-1
        CALL MESS(1)
        WRITE(NHSTRY,900)
        WRITE(NHSTRY,2000)STBP
        STBP=10.0D0
      ENDIF
C
C       CHECK APPLICATION RANGE FOR MABP
C
      IF(VABP.LT.200.D0)THEN
        IERR=-2
        CALL MESS(1)
        WRITE(NHSTRY,900)
        WRITE(NHSTRY,3000)VABP
        MABPC=INEX(200.0D0,VM(STBP,1),400.D0,VM(STBP,2),VABP)
      ELSE IF(VABP.GE.200.D0.AND.VABP.LT.400.D0)THEN
        MABPC=INEX(200.0D0,VM(STBP,1),400.D0,VM(STBP,2),VABP)
      ELSE IF(VABP.GE.400.D0.AND.VABP.LT.500.D0)THEN
        MABPC=INEX(400.0D0,VM(STBP,2),500.D0,VM(STBP,3),VABP)
      ELSE IF(VABP.GE.500.D0.AND.VABP.LE.600.D0)THEN
        MABPC=INEX(500.0D0,VM(STBP,3),600.D0,VM(STBP,4),VABP)
      ELSE IF(VABP.GT.600.D0)THEN
        IERR=-2
        CALL MESS(1)
        WRITE(NHSTRY,900)
        WRITE(NHSTRY,3000)VABP
        MABPC=VM(STBP,4)
      ENDIF
C
C       CORRECT MABP
C
      IF(MABPC.LE.0.D0)THEN
       MABP=VABP+MABPC
      ELSE
       MABP=VABP
      ENDIF
C
C       CHECK APPLICATION RANGE FOR CABP
C
      IF(VABP.LT.200.D0)THEN
        IERR=-2
        CALL MESS(1)
        WRITE(NHSTRY,900)
        WRITE(NHSTRY,4000)VABP
        CABPC=INEX(200.0D0,VC(STBP,1),300.D0,VC(STBP,2),VABP)
      ELSE IF(VABP.GE.200.D0.AND.VABP.LT.300.D0)THEN
        CABPC=INEX(200.0D0,VC(STBP,1),300.D0,VC(STBP,2),VABP)
      ELSE IF(VABP.GE.300.D0.AND.VABP.LT.400.D0)THEN
        CABPC=INEX(300.0D0,VC(STBP,2),400.D0,VC(STBP,3),VABP)
```

```
      ELSE IF(VABP.GE.400.D0.AND.VABP.LE.500.D0)THEN
        CABPC=INEX(400.0D0,VC(STBP,3),500.D0,VC(STBP,4),VABP)
      ELSE IF(VABP.GT.500.D0)THEN
        IERR=-2
        CALL MESS(1)
        WRITE(NHSTRY,900)
        WRITE(NHSTRY,4000)VABP
        CABPC=VC(STBP,4)
      ENDIF
C
C       CORRECT CABP
C
      IF(CABPC.LE.0.D0)THEN
       CABP=VABP+CABPC
      ELSE
       CABP=VABP
      ENDIF
C
C         FORMATS
C
900   FORMAT(1X,'IN MODULE TBPCF')
1000  FORMAT(1X,'SLOPE VALUE IS NOT IN RANGE 0-10.0',/,
     1        1X,'SLOPE-VALUE = ',G12.6,/,
     2        1X,'SLOPE-VALUE SET TO 0.0 AND CALC. CONTINUES')
2000  FORMAT(1X,'SLOPE VALUE IS NOT IN RANGE 0-10.0',/,
     1        1X,'SLOPE-VALUE = ',G12.6,/,
     2        1X,'SLOPE-VALUE SET TO 10.0 AND CALC. CONTINUES')
3000  FORMAT(1X,'VABP VALUE IS NOT IN RANGE 200-600',/,
     1        1X,'VABP-VALUE = ',G12.6,/,
     2        1X,'CALC IS EXTRAPOLATION. MABP CALC CONTINUES')
4000  FORMAT(1X,'VABP VALUE IS NOT IN RANGE 200-500',/,
     1        1X,'VABP-VALUE = ',G12.6,/,
     2        1X,'CALC IS EXTRAPOLATION. CABP CALC CONTINUES')
C
      RETURN
C
      END
C*************************************************************************
C
      FUNCTION INEX(XL,YL,XH,YH,XW)
C
C*************************************************************************
C
C         NAME OF MODULE - INEX
C         MODULE TITLE - INTERPOLATION/EXTRAPOLATION
C         PURPOSE - TO CALC LINEAR INTERPOLATION/EXTRAPOLATION
C         MODIFIED - 1-6-89
C
C         LIMITATIONS:
C
C         VARIABLES USED-
C
C VARIABLE I/O TYPE-SPEC DIMENSION      DESCRIPTION AND RANGE
C      XL     I       R                 LOW VALUE DEPENDENT VARIABLE
C      YL     I       R                 LOW VALUE INDEPENDENT VARIABLE
C      XH     I       R                 HIGH VALUE DEPENDENT VARIABLE
C      YH     I       R                 HIGH VALUE INDEPENDENT VARIABLE
C      XW     I       R                 DESIRED VALUE INDEPENDENT VARIABLE
C
      IMPLICIT REAL*8 (A-H,O-Z)
      IMPLICIT INTEGER(I-N)
      REAL*8            INEX
C
      IF((XH-XL).NE.0.D0)THEN
       INEX=YL+((XW-XL)/(XH-XL))*(YH-YL)
      ELSE
       INEX=(YL-YH)/2.D0
      ENDIF
```

```
C
      RETURN
      END
C***********************************************************************
C
      FUNCTION VM(STBP,ITEMP)
C
C***********************************************************************
C
C        NAME OF MODULE - VM
C        MODULE TITLE - CORRECTION TO VABP VALUE FOR MABP
C        PURPOSE - CORRECTION OF VABP TO GIVE MABP FROM SLOPE OF TBP
C                  CURVE
C        MODIFIED - 1-6-83
C
C        LIMITATIONS:
C
C        VARIABLES USED-
C
C VARIABLE I/O TYPE-SPEC DIMENSION      DESCRIPTION AND RANGE
C   STBP     I        R          -      SLOPE OF TBP CURVE
C                                       (T70-T10)/60 (DEG F/DEG F)
C  ITEMP     I        I          -      CALC TYPE
C                                        1 = 200
C                                        2 = 400
C                                        3 = 500
C                                        4 = 600+
C
      IMPLICIT REAL*8 (A-H,O-Z)
      IMPLICIT INTEGER(I-N)
      REAL*8            LLIM
C
      DIMENSION         EQVAL(5,4)
      DIMENSION         LLIM(4)
C
C      5 EACH 200 400 500 600
      DATA EQVAL/7.1975451D0,-3.8525766D0,-2.4902721D0,
     1           0.36406431 2D0,-0.36525545 6D-1,
     2           17.319323 4D0,-11.301312 4D0,2.2420161 1D0,
     3           -0.45036614 1D0,0.11276055 5D-1,
     4           12.7936883D0,-6.3549039 1D0,-0.47907065 6D0,
     5           -0.55528274 3D-1,-0.33358966 7D-2,
     6           11.3691513D0,-4.2650333 0D0,-0.70128443 9D0,
     7           -0.33216067 8D-1,0.0D0/
C
      DATA LLIM/1.123496D0,1.146043D0,1.733813D0,1.935252D0/
C
      IF(STBP.GT.LLIM(ITEMP))THEN
       VM=EQVAL(1,ITEMP)+EQVAL(2,ITEMP)*STBP+EQVAL(3,ITEMP)*STBP*STBP
     1    +EQVAL(4,ITEMP)*STBP**3+EQVAL(5,ITEMP)*STBP**4
      ELSE
       VM=0.D0
      ENDIF
C
      IF(VM.GT.0.D0)VM=0.0D0
C
      RETURN
      END
C***********************************************************************
C
      FUNCTION VC(STBP,ITEMP)
C
C***********************************************************************
C
C        NAME OF MODULE - VC
C        MODULE TITLE - CORRECTION TO VABP VALUE FOR CABP
C        PURPOSE - CORRECTION OF VABP TO GIVE CABP FROM SLOPE OF TBP
C                  CURVE
```

```
C        MODIFIED - 1-6-89
C
C        LIMITATIONS:
C
C        VARIABLES USED-
C
C VARIABLE I/O TYPE-SPEC DIMENSION      DESCRIPTION AND RANGE
C   STBP     I       R          -       SLOPE OF TBP CURVE
C                                       (T70-T10)/60 (DEG F/DEG F)
C  ITEMP     I       I          -       CALC TYPE
C                                        1 = 200
C                                        2 = 300
C                                        3 = 400
C                                        4 = 500+
C
      IMPLICIT REAL*8 (A-H,O-Z)
      IMPLICIT INTEGER(I-N)
      REAL*8            LLIM
C
      DIMENSION         EQVAL(2,4)
      DIMENSION         LLIM(4)
C
      DATA EQVAL/8.026836676D0,-7.47320554D0,
     1           5.40190649D0,-4.40487232D0,
     2           2.53096753D0,-1.61026247D0,
     3           0.837906014D0,-0.415556279D0/
C
      DATA LLIM /1.067821D0,1.298701D0,1.500722D0,1.998557D0/
C
      IF(STBP.GT.LLIM(ITEMP))THEN
       VC=EQVAL(1,ITEMP)+EQVAL(2,ITEMP)*STBP
      ELSE
       VC=0.D0
      ENDIF
C
      IF(VC.GT.0.0D0)VC=0.0D0
C
      RETURN
      END
C*************************************************************************
C
      SUBROUTINE PCON(PRESI,PRESO,ICALC,IERR)
C
C*************************************************************************
C
C        NAME OF MODULE - PCON
C        MODULE TITLE - CONVERSION OF PRESSURES
C        PURPOSE - TO CONVERT PRESSURES
C        MODIFIED 9-14-88 (COMPLETED)
C
C        VARIABLES USED-
C
C VARIABLE I/O TYPE-SPEC DIMENSION      DESCRIPTION AND RANGE
C  PRESI     I       R          -       INPUT PRESSURE
C  PRESO     O       R          -       OUTPUT PRESSURE
C  ICALC     I       I          -       INPUT CODE(1=PSIA,2=PSIG,3=ATM,
C                                                 4=MMHG,5=PA)
C                                       12 FOR PSIA TO PSIG
C                                       13 FOR PSIA TO ATM
C                                         ETC.
C                                       21 FOR PSIG TO PSIA
C                                         ETC.
C  IERR      O       I          -       ERROR CODE
C                                        0 = OK
C                                       -1 = NOT VALID ICALC NUMBER
C
      IMPLICIT REAL*8 (A-H,O-Z)
      IMPLICIT INTEGER(I-N)
```

```
C
      COMMON /IO     / NIN,NOUT,NHSTRY,NREPT
      COMMON /DEBUG  / LDBUG,LDBUGR
C
      IERR=0
C
      PRES=PRESI
C
      IF(ICALC.EQ.12)THEN
C       PSIA TO PSIG
        PRES=PRES-14.696D0
      ELSE IF(ICALC.EQ.13)THEN
C       PSIA TO ATM
        PRES=PRES/14.696D0
      ELSE IF(ICALC.EQ.14)THEN
C       PSIA TO MMHG
        PRES=PRES/14.696D0*760.D0
      ELSE IF(ICALC.EQ.15)THEN
C       PSIA TO PA
        PRES=PRES/14.696D0*1.01325D5
      ELSE IF(ICALC.EQ.21)THEN
C       PSIG TO PSIA
        PRES=PRES+14.696
      ELSE IF(ICALC.EQ.23)THEN
C       PSIG TO ATM
        PRES=(PRES+14.696D0)/14.696D0
      ELSE IF(ICALC.EQ.24)THEN
C       PSIG TO MMHG
        PRES=(PRES+14.696D0)/14.696D0*760.D0
      ELSE IF(ICALC.EQ.25)THEN
C       PSIG TO PA
        PRES=(PRES+14.696D0)/14.696D0*1.01325D5
      ELSE IF(ICALC.EQ.31)THEN
C       ATM TO PSIA
        PRES=PRES*14.696D0
      ELSE IF(ICALC.EQ.32)THEN
C       ATM TO PSIG
        PRES=PRES*14.696D0-14.696D0
      ELSE IF(ICALC.EQ.34)THEN
C       ATM TO MMHG
        PRES=PRES*760.D0
      ELSE IF(ICALC.EQ.35)THEN
C       ATM TO PA
        PRES=PRES*1.01325D5
      ELSE IF(ICALC.EQ.41)THEN
C       MMHG TO PSIA
        PRES=PRES/760.D0*14.696D0
      ELSE IF(ICALC.EQ.42)THEN
C       MMHG TO PSIG
        PRES=PRES/760.D0*14.696D0-14.696D0
      ELSE IF(ICALC.EQ.43)THEN
C       MMHG TO ATM
        PRES=PRES/760.D0
      ELSE IF(ICALC.EQ.45)THEN
C       MMHG TO PA
        PRES=PRES/760.D0*1.01325D5
      ELSE IF(ICALC.EQ.51)THEN
C       PA TO PSIA
        PRES=PRES/1.01325D5*14.696D0
      ELSE IF(ICALC.EQ.52)THEN
C       PA TO PSIG
        PRES=PRES/1.01325D5*14.696D0-14.696D0
      ELSE IF(ICALC.EQ.53)THEN
C       PA TO ATM
        PRES=PRES/1.01325D5
      ELSE IF(ICALC.EQ.54)THEN
C       PA TO MMHG
        PRES=PRES/1.01325D5*760.D0
```

```
      ELSE
C       ERROR MESSAGE
       CALL MESS(2)
       WRITE(NHSTRY,900)
       WRITE(NHSTRY,1000)ICALC
       IERR=-1
      ENDIF
C
      PRESO=PRES
C
C      FORMATS
C
900   FORMAT(1X,'IN MODULE PCON')
1000  FORMAT(1X,'INVALID VALUE OF ICALC OF ',I10,/,
     1       1X,'NO PRES CONVERSION & CALC. CONTINUES')
      RETURN
      END
C*****************************************************************************
C
      SUBROUTINE TCON(TEMPI,TEMPO,ICALC,IERR)
C
C*****************************************************************************
C
C       NAME OF MODULE - TCON
C       MODULE TITLE - CONVERSION OF TEMPERATURE
C       PURPOSE - TO CONVERT TEMPERATURES
C       MODIFIED - 9-14-88 (COMPLETED)
C
C       VARIABLES USED-
C
C VARIABLE I/O TYPE-SPEC DIMENSION      DESCRIPTION AND RANGE
C  TEMPI     I       R          -       INPUT TEMPERATURE
C  TEMPO     O       R          -       OUTPUT TEMPERATURE
C  ICALC     I       I          -       INPUT CODE (1=F,2=R,3=C,4=K)
C                                        12 FOR F TO R
C                                        13 FOR F TO C
C                                        14 FOR F TO K
C                                        21 FOR R TO F
C                                        23 FOR R TO C
C                                        24 FOR R TO K
C                                        31 FOR C TO F
C                                        32 FOR C TO R
C                                        34 FOR C TO K
C                                        41 FOR K TO F
C                                        42 FOR K TO R
C                                        43 FOR K TO C
C  IERR      O       I          -       ERROR CODE
C                                        0 = OK
C                                        -1 = NOT VALID ICALC NUMBER
C
      IMPLICIT REAL*8 (A-H,O-Z)
      IMPLICIT INTEGER(I-N)
C
      COMMON /IO     / NIN,NOUT,NHSTRY,NREPT
      COMMON /DEBUG / LDBUG,LDBUGR
C
      IERR=0
      TEMP=TEMPI
      IF(ICALC.EQ.12)THEN
C       F TO R
       TEMP=TEMP+459.67D0
      ELSE IF(ICALC.EQ.13)THEN
C       F TO C
       TEMP=(TEMP-32.D0)/1.8D0
      ELSE IF(ICALC.EQ.14)THEN
C       F TO K
       TEMP=(TEMP-32.D0)/1.8D0+273.15D0
      ELSE IF(ICALC.EQ.21)THEN
```

```
C         R TO F
          TEMP=TEMP-459.67D0
         ELSE IF(ICALC.EQ.23)THEN
C         R TO C
          TEMP=TEMP/1.8D0-273.15D0
         ELSE IF(ICALC.EQ.24)THEN
C         R TO K
          TEMP=TEMP/1.8D0
         ELSE IF(ICALC.EQ.31)THEN
C         C TO F
          TEMP=1.8D0*TEMP+32.D0
         ELSE IF(ICALC.EQ.32)THEN
C         C TO R
          TEMP=1.8D0*TEMP+32.D0+459.67D0
         ELSE IF(ICALC.EQ.34)THEN
C         C TO K
          TEMP=TEMP+273.15D0
         ELSE IF(ICALC.EQ.41)THEN
C         K TO F
          TEMP=1.8D0*TEMP-459.67D0
         ELSE IF(ICALC.EQ.42)THEN
C         K TO R
          TEMP=1.8D0*TEMP
         ELSE IF(ICALC.EQ.43)THEN
C         K TO C
          TEMP=TEMP-273.15D0
         ELSE
C         ERROR MESSAGE
          CALL MESS(2)
          WRITE(NHSTRY,900)
          WRITE(NHSTRY,1000)ICALC
          IERR=-3
         ENDIF
C
         TEMPO=TEMP
C
C         FORMATS
C
900      FORMAT(1X,'IN MODULE TCON')
1000     FORMAT(1X,'INVALID VALUE OF ICALC OF ',I10,/,
        1         1X,'NO TEMP CONVERSION & CALC. CONTINUES')
         RETURN
         END
C*************************************************************************
C
         SUBROUTINE VFSH(TBR,SG,JC,IERR)
C
C*************************************************************************
C
C         NAME OF MODULE - VFSH
C         MODULE TITLE - CALC OF CHARACTERISTIC VOLUME PARAMETER(VLCVT1)
C         PURPOSE - TO CALC OF CHARACTERISTIC VOLUME PARAM.
C                   FOR SCATCHARD-HILDEBRAND EQ.
C         MODIFIED - 12-20-88
C
C         VARIABLES USED-
C
C VARIABLE I/O TYPE-SPEC DIMENSION      DESCRIPTION AND RANGE
C      TBR    I       R         -       BOILING POINT (DEG R)
C       SG    I       R         -       SPECIFIC GRAVITY (60/60F)
C       JC    I       I         -       COMPONENT NUMBER ARRAY
C     IERR    O       I         -       ERROR CODE ID
C                                        0 = OK
C                                       -1 = REDUCED TEMP > 0.99
C                                       -2 = REDUCED TEMP < 0.2
C                                        1 = TBR OUT OF RANGE
C                                        2 = SG OUT OF RANGE
C
```

```
      IMPLICIT REAL*8 (A-H,O-Z)
      IMPLICIT INTEGER(I-N)
C
      PARAMETER        (MNC=25)
C
      COMMON /IO     / NIN,NOUT,NHSTRY,NREPT
      COMMON /REFS   / TREF,PREF,RGAS
C
      COMMON /CPRP01/ TC(MNC)
      COMMON /CPRP05/ OMEGA(MNC)
      COMMON /CPRP22/ VLCVT1(MNC)
C
      IERR=0
C
C       CHECK LIMITS OF TBR AND SG
C
      IF(TBR.LT.569.67D0.OR.TBR.GT.1309.67)THEN
       CALL MESS(1)
       WRITE(NHSTRY,900)
       WRITE(NHSTRY,1000)TBR
       IERR=1
      ENDIF
C
      IF(SG.LT.0.6247D0.OR.SG.GT.1.0244D0)THEN
       CALL MESS(1)
       WRITE(NHSTRY,900)
       WRITE(NHSTRY,2000)SG
       IERR=2
      ENDIF
C
C       LIQUID MOLAR VOLUME AT 20 DEG C ANT 1 ATM (CM**3/G-MOLE)
C
      V=7.6211D-5 * TBR**(2.1262D0) * SG**(-1.8688D0)
C
C       LIQUID MOLAR VOLUME AT 20 DEG C AND 1 ATM (M**3/KG-MOLE)
C
      VR=V/1.D6*1000.D0
C
      TR=293.15D0/TC(JC)
      OMEGAI=OMEGA(JC)
      TRD=TREF/TC(JC)
      ICALC=0
C
C       CORRECT TO 25 C BY RACKETT FOR GUNYAM
C
      CALL GUNYAM(VR,TR,OMEGAI,TRD,ICALC,VD,IERR)
C
      IF(IERR.LT.0)THEN
       CALL MESS(1)
       WRITE(NHSTRY,900)
       WRITE(NHSTRY,3000)IERR
      ENDIF
C
      VLCVT1(JC)=VD/(5.7D0+3.0D0*TREF/TC(JC))
C
C       FORMATS
C
900   FORMAT(1X,'IN MODULE VFSH')
1000  FORMAT(1X,'TB(DEG R) VALUE IS NOT IN RANGE 569.67-1309.67',/,
     1       1X,'TB-VALUE = ',G12.6,' CALC. CONTINUES')
2000  FORMAT(1X,'SG VALUE IS NOT IN RANGE 0.6247-1.0244',/,
     1       1X,'SG VALUE = ',G12.6,' CALC. CONTINUES')
3000  FORMAT(1X,'IN CALL TO GUNYAM IERR RETURNED = ',I5,' CALC CONT.')
C
      RETURN
      END
C*****************************************************************************
C
```

```
      SUBROUTINE WATHOV(JC,IERR)
C
C*****************************************************************************
C
C       NAME OF MODULE - WATHOV
C       MODULE TITLE - WATSON HEAT OF VAPORIZATION
C       PURPOSE - EST OF WATSON HEAT OF VAPORIZATION PARAMETERS
C       MODIFIED - 12-20-88
C       METHOD - WATSON HEAT OF VAPORIZATION EQUATION
C                REF: REID,R.C. ET AL.,"THE PROPERTIES OF GASES AND LIQUIDS"
C                     MCGRAW HILL,NY,1977
C
C
C       VARIABLES USED-
C
C VARIABLE I/O TYPE-SPEC DIMENSION      DESCRIPTION AND RANGE
C     JC     I       I         -        COMPONENT ARRAY ID
C   IERR     O       I         -        ERROR CODE
C                                       0 = OK
C                                       1 = TB(R) NOT IN OPT. RANGE
C                                       2 = SG NOT IN OPT. RANGE
C
      IMPLICIT REAL*8 (A-H,O-Z)
      IMPLICIT INTEGER(I-N)
C
C
      PARAMETER        (MNC=25)
C
      COMMON /IO     / NIN,NOUT,NHSTRY,NREPT
      COMMON /DEBUG  / LDBUG,LDBUGR
C
      COMMON /NPROP3/ UOPK(MNC),API(MNC),SG(MNC),AMW(MNC)
C
      COMMON /CPRP08/ DHVLWT(5,MNC)
      COMMON /CPRP14/ TB(MNC)
C
      IERR=0
      IF(LDBUG.GT.7)WRITE(NHSTRY,900)
C
C       HEAT OF VAP (BTU/LB-MOLE) AT TB AND SG FOR COMPOUND
C
      CALL TCON(TB(JC),T1,42,IERRT)
C
      S1=SG(JC)
C
      IF(T1.LT.569.67D0.OR.T1.GT.1309.67)THEN
       CALL MESS(1)
       WRITE(NHSTRY,900)
       WRITE(NHSTRY,2000)T1
       IERR=1
      ENDIF
C
      IF(S1.LT.0.6247D0.OR.S1.GT.1.0244D0)THEN
       CALL MESS(1)
       WRITE(NHSTRY,900)
       WRITE(NHSTRY,2000)S1
       IERR=2
      ENDIF
C
      HVAP1=8.48585D0 * T1**(1.1347D0) * S1**(0.0214D0)
C
C       HEAT OF VAP (J/KMOL)
C
      HVAP1=HVAP1/9.486D-4/0.453593D0
C
      DHVLWT(1,JC)=HVAP1
      DHVLWT(2,JC)=TB(JC)
      DHVLWT(3,JC)=0.38D0
```

```
      DHVLWT(4,JC)=0.0D0
      DHVLWT(5,JC)=0.0D0
C
C
C       FORMATS
C
900   FORMAT(1X,'IN MODULE WATHOV')
1000  FORMAT(1X,'TB(DEG R) VALUE IS NOT IN RANGE 569.67-1309.67',/,
     1       1X,'TB-VALUE = ',G12.6,' CALC. CONTINUES')
2000  FORMAT(1X,'SG VALUE IS NOT IN RANGE 0.6247-1.0244',/,
     1       1X,'SG VALUE = ',G12.6,' CALC. CONTINUES')
C
      RETURN
      END

C*****************************************************************************
C
      SUBROUTINE ZCCAL(TC,PC,VC,ZC,IERR)
C
C*****************************************************************************
C
C       NAME OF MODULE - ZCCAL
C       MODULE TITLE - CALC CRITICAL COMPRESS. FACTOR
C       PURPOSE - TO CALC CRITICAL COMPRES. FACTOR
C       MODIFIED - 10-3-88
C
C       LIMITATIONS:
C          ZC           0.26-0.28
C
C       VARIABLES USED-
C
C VARIABLE I/O TYPE-SPEC DIMENSION     DESCRIPTION AND RANGE
C    TC      I       R          -      CRITICAL TEMPERATURE (K)
C    PC      I       R          -      CRITICAL PRESSURE (PA)
C    VC      I       R          -      CRITICAL VOLUME (M**3/KG-MOLE)
C    ZC      O       R          -      CRITICAL COMPRES. FACTOR
C  IERR      O       I          -      ERROR CODE
C                                       0 = OK
C                                      -1 = VALUE NOT IN OPTIMAL RANGE
C                                           0.26-0.28
C
      IMPLICIT REAL*8 (A-H,O-Z)
      IMPLICIT INTEGER(I-N)
C
      PARAMETER        (MNC=25)
C
      COMMON /IO    / NIN,NOUT,NHSTRY,NREPT
      COMMON /DEBUG / LDBUG,LDBUGR
      COMMON /REFS  / TREF,PREF,RGAS
C
      IERR=0
      IF(LDBUG.GT.0)WRITE(NHSTRY,900)
C
C        CRITICAL COMPRESS FACTOR
C
      ZC=(PC*VC)/(TC*RGAS)
C
      IF(ZC.LT.0.26D0.OR.ZC.GT.0.28D0)THEN
       CALL MESS(1)
       WRITE(NHSTRY,900)
       WRITE(NHSTRY,1000)ZC
      ENDIF
C
C       FORMATS
C
900   FORMAT(1X,'IN MODULE ZCCAL')
1000  FORMAT(1X,'ZC VALUE IS NOT IN OPTIMAL RANGE 0.26-0.28',/,
     1       1X,'ZC-VALUE = ',G12.6,' CALC. CONTINUES')
```

```
C
      RETURN
      END
C*************************************************************************
C
      SUBROUTINE SECOND(USED)
C
C*************************************************************************
C
C       NAME OF MODULE - SECOND
C       MODULE TITLE - CALC ELAPSED CPU TIME
C       PURPOSE - CALCS CPU TIME IN SECONDS (VAX DEPENDENT)
C       MODIFIED - 3-23-89
C
C       VARIABLES USED-
C
C VARIABLE I/O TYPE-SPEC DIMENSION      DESCRIPTION AND RANGE
C  USED    I/O     R          -         CPU TIME USED
C
      INTEGER TIMESTATS,ELAPSED
      LOGICAL STATUS,LIB$INIT_TIMER,LIB$STAT_TIMER
      COMMON /TIMEDATA/ TIMESTATS
C
      DATA ISWT/1/
C
      SAVE TIMEDATA
C
      IF(ISWT.EQ.1)CALL TIME_INIT
      ISWT=2
      STATUS=LIB$STAT_TIMER(2,ELAPSED,TIMESTATS)
      USED=FLOAT(ELAPSED)/100.0
C
      RETURN
      END
C*************************************************************************
C
      SUBROUTINE TIME_INIT
C
C*************************************************************************
C
C       NAME OF MODULE - TIME_INIT
C       MODULE TITLE - INITIALIZE TIME ROUTINE
C       PURPOSE - TO INITIALIZE COUNTERS FOR FUTURE REFERENCE
C                 (VAX DEPENDENT)
C       MODIFIED - 3-23-89
C
      INTEGER TIMESTATS
      LOGICAL STATUS,LIB$INIT_TIMER,LIB$STAT_TIMER
C
      COMMON /TIMEDATA/ TIMESTATS
C
      SAVE TIMEDATA
      TIMESTATS=0
      STATUS=LIB$INIT_TIMER(TIMESTATS)
C
      RETURN
      END
C
C     BEGIN ASPEN USER SUBROUTINE YSOLVE
C
C$ #4 BY: SUND  DATE: 02/28/86 FIX DIVIDE BY ZERO AND DACOS
C$ #3 BY: BRITT DATE: 08/23/81 CHANGE REAL CONSTANT TO REAL*8
C$ #2 BY: VASANT DATE: 09/28/80 CODE REVIEW
C$ #1 BY: VASANT DATE: 03/01/79 CHANGES
C$ #1 BY: ESPEDAL DATE: 01/19/79 FIRST ABSORB
C-------------------------------------------------------------------------
C
C *-----------------------------------------------------------------------*
```

```
C *                          ****  NOTICE  ****                          *
C *----------------------------------------------------------------------*
C
C  %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
C
C           THIS CODE IS PART OF THE VAX SYSTEM DEVELOPED AT
C     MORGANTOWN ENERGY TECHNOLOGY CENTER, MORGANTOWN, WEST VIRGINIA
C
C  %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
C
C
C          COPYRIGHT (C) 1980
C           MASSACHUSETTS INSTITUTE OF TECHNOLOGY
C           CAMBRIDGE, MA
C----------------------------------------------------------------------
      SUBROUTINE YSOLVE (K, N, NDATA, DATA, X, XV, XMAX, XMIN, Y, Z, PJ,
     1       OUTPUT, P, A, AC)
C
C     TITLE         - NONLINEAR ESTIMATION AND EQUATION SOLVING
C
C     THE PURPOSE OF THIS SUBPROGRAM IS TO SOLVE SYSTEMS OF NONLINEAR
C     EQUATIONS.
C
C        A       - SCRATCH MATRIX OF LENGTH K*(K + 2)
C        AC      - SCRATCH MATRIX OF LENGTH K*(K + 2)
C        DATA    - ARRAY USED TO STORE VARIABLES USED IN SUBROUTINE
C                  DATA(1) - FNU, FACTOR USED TO CHANGE FLA.  SET INTER-
C                            NALLY TO 10.0  IF ZERO ON INITIAL CALL.
C                  DATA(2) - FLA, FACTOR USED TO COMBINE GRADIENT AND
C                            NEWTON-RAPHSON METHODS.  SET INTERNALLY TO
C                            .01 IF ZERO ON INITIAL CALL.
C                  DATA(3) - TAU, USED IN CONVERGENCE TEST.  SET INTER-
C                            NALLY TO 0.001 IF ZERO ON INITIAL CALL.
C                  DATA(4) - EPS, USED IN CONVERGENCE TEST.  SET INTER-
C                            NALLY TO 0.00002 IF ZERO ON INITIAL CALL.
C                  DATA(5) - PHMIN, WHEN PH .LT. PHMIN, PARTIAL DERIV-
C                            ITIVES FROM THE PREVIOUS ITERATION ARE USED
C                            INSTEAD OF COMPUTING THEM AGAIN.
C                  DATA(6) THRU DATA(16) - VARIABLES USED INTERNALLY
C        K       - NUMBER OF INDEPENDENT VARIABLES, UNKNOWNS
C        N       - NUMBER OF EQUATIONS TO BE SOLVED
C        NDATA   - ARRAY USED TO STORE INTEGER VARIABLES USED IN SUBROUTI
C                     NDATA(1) - IC, MUST BE SET EQUAL TO ONE ON INITIAL
C                                ENTRY TO YSOLVE.  USED TO CONTROL SEQUEN
C                                OF OPERATION.
C                     NDATA(2) - NFCTDR, USED FOR CONTROL IN CALLING PROG
C                        IF = 0, CALCULATE FUNCTION
C                        IF = 1, CALCULATE DERIVATIVE
C                        IF =-1, EXAMINE IERR FOR WHAT TO DO NEXT
C                     NDATA(3) - IERR, MAY TAKE ON VARIOUS VALUES
C                        IF POSITIVE, CONTAINS THE NUMBER OF VARIABLES NO
C                                     SATISFYING CONVERGENCE CRITERION
C                        IF =  0, CONVERGENCE SATISFIED AND SOLUTION RETU
C                        IF = -1, NO IMPROVEMENT POSSIBLE IN THE VALUE OF
C                                 PH EVEN THOUGH CONVERGENCE HAS NOT BEEN
C                                 REACHED.
C                        IF = -2, MORE UNKNOWNS THAN FUNCTIONS AND UNIQUE
C                                 SOLUTION GENERALLY IS IMPOSSIBLE.
C                        IF = -3, TOTAL NUMBER OF VARIABLES TO BE VARIED
C                                 IS ZERO
C                        IF = -4, CONVERGENCE CRITERION MET BUT FLA STILL
C                                 LARGE
C                        IF = -5, IC NOT A VALID NUMBER ON ENTRY
C                        IF = -6, X(I) IS NOT WITHIN XMIN(I) TO XMAX(I)
C                        IF = -7, ZERO DIAGONAL ELEMENT IN EQUATION SOLVE
C                     NDATA(4) - J, INDEX TO INDICATE WHICH PARTIAL DERIV
C                                ATIVE IS TO BE EVALUATED.
C                     NDATA(5) THRU NDATA(6) - NOT USED
```

```
C                   NDATA(7) THRU NDATA(26) - INTEGER VARIABLES USED
C                                             INTERNALLY
C       OUTPUT - VECTOR OF OUTPUT VALUES
C                   OUTPUT(1) - PH, VALUE OF THE SUM OF THE SQUARES OF
C                               Y(I) - Z(I) AS I=1,N.
C                   OUTPUT(2) - GAMM, ANGLE IN DEGREES BETWEEN THE STEP
C                               ACTUALLY TAKEN AND THE STEEPEST DESCENT
C                               DIRECTION.
C                   OUTPUT(3) - XITR, ITERATION COUNTER FOR YSOLVE.
C                               INITIALIZED TO ZERO BY YSOLVE.
C                   OUTPUT(4) - XFCT, ITERATION COUNTER TO COUNT NUMBER
C                               OF TIMES THE FUNCTION WAS EVALUATED.
C                               INITIALIZED TO ZERO BY YSOLVE.
C                   OUTPUT(5) - XDER, ITERATION COUNTER TO COUNT NUMBER
C                               OF TIMES THE DERIVATIVE WAS EVALUATED.
C                               INITIALIZED TO ZERO BY YSOLVE.
C                   OUTPUT(6) - VALUE OF FLA FOR CURRENT BASE POINT
C       P       - VECTOR OF LENGTH K*(N+2)+N  USED TO STORE PARTIAL DERI
C                 ATIVES AND AS A SCRATCH AREA.
C       PJ      - VECTOR OF PARTIAL DERIVATIVES OF LENGTH N. THIS IS ONE
C                 ROW OF THE P VECTOR CORRESPONDING WITH X(J).
C       X       - VECTOR OF LENGTH 2*K CONTAINING THE K BASE POINTS
C                 AND THE K UNKNOWNS
C       XMAX    - VECTOR OF LENGTH K CONTAINING UPPER BOUNDS OF X
C       XMIN    - VECTOR OF LENGTH K CONTAINING LOWER BOUNDS OF X
C       XV      - VECTOR OF LENGTH K INDICATING WHICH OF THE X VARIABLES
C                 ARE TO BE VARIED
C                   IF XV(I) = 0., HOLD X(I) CONSTANT
C                   IF XV(I) = 1., ALLOW X(I) TO VARY AND USE NUMERICAL
C                                  DERIVATIVES.
C                   IF XV(I) =-1., ALLOW X(I) TO VARY AND USE ANALYTIC
C                                  DERIVATIVES CALCULATED BY USER
C       Y       - VECTOR OF LENGTH K CONTAINING DESIRED FUNCTION VALUES
C       Z       - VECTOR OF LENGTH 2*N CONTAINING COMPUTED FUNCTION VALU
C                 AND BASE POINT FUNCTION VALUES
C
      IMPLICIT REAL*8 (A - H, O - Z)
      DIMENSION NDATA(26), DATA(16), X(1), XV(1), XMAX(1), XMIN(1),
     1       Y(1), Z(1), PJ(1), OUTPUT(6), P(1), A(K, 1), AC(K, 1)
C
C                               SET INTEGER VARIABLES USED IN SUBROUTINE
C                               EQUAL TO NDATA ARRAY
            IC      = NDATA(1)
            NFCTDR  = NDATA(2)
            IERR    = NDATA(3)
            J       = NDATA(4)
            KP1     = NDATA(7)
            KP2     = NDATA(8)
            KBI1    = NDATA(9)
            KBI2    = NDATA(10)
            KZI     = NDATA(11)
            J1      = NDATA(12)
            J2      = NDATA(13)
            J3      = NDATA(14)
            J4      = NDATA(15)
            JB      = NDATA(16)
            I1      = NDATA(17)
            L1      = NDATA(18)
            L2      = NDATA(19)
            L3      = NDATA(20)
            L4      = NDATA(21)
            N1      = NDATA(22)
            N2      = NDATA(23)
            N3      = NDATA(24)
            N4      = NDATA(25)
            JGAM    = NDATA(26)
C                               SET VARIABLES USED IN SUBROUTINE EQUAL TO
C                               DATA ARRAY
```

```
              FNU     = DATA(6)
              TAU     = DATA(7)
              EPS     = DATA(8)
              PHMIN   = DATA(9)
              GN      = DATA(10)
              FL      = DATA(11)
              DN      = DATA(12)
              DG      = DATA(13)
              COSG    = DATA(14)
              PHI     = DATA(15)
              DEN     = DATA(16)
C                                 SET OUTPUT VATIABLES EQUAL TO OUTPUT ARRAY
              PH      = OUTPUT(1)
              GAMM    = OUTPUT(2)
              XITR    = OUTPUT(3)
              XFCT    = OUTPUT(4)
              XDER    = OUTPUT(5)
              FLA     = OUTPUT(6)
C                                 DEFINE CONSTANTS USED IN PROGRAM
              C1      = 1.0D-02
              C2      = 1.0D-03
              C3      = 1.0D-20
              C4      = 1.0D0
              C5      = 1.8D+02
              C6      = 1.0D-10
              C7      = 9.0D+01
              C8      = 4.5D+01
              C9      = 1.0D+08
              PI      = 3.14159265D0
C
      IF      (IC .GT. 0 .AND. IC .LT. 6) GO TO 800
              IERR    = -5
      GO TO 805
  800 DO 801 I        = 1, K
      IF      (X(I) .LT. XMIN(I) .OR. X(I) .GT. XMAX(I)) GO TO 802
  801 CONTINUE
      GO TO 2
  802         IERR    = -6
      GO TO 805
  803         IERR    = -7
  805         NFCTDR  = -1
      GO TO 999
C
    2 GO TO (10, 20, 30, 40, 13), IC
   10         KP1     = K + 1
              KP2     = KP1 + 1
              KBI1    = K*N
              KBI2    = KBI1 + K
              KZI     = KBI2 + K
C
C                                 STORE INITIAL BASE POINT VALUES
      DO 82 KK        = 1, K
              KKK     = KK + K
   82         X(KKK)  = X(KK)
C                                 STORE FUNCTIONAL EVALUATIONS AT BASE POINT
      DO 80 LL        = 1, N
              LLL     = N + LL
   80         Z(LLL)  = Z(LL)
C                                 IF PARAMETERS ARE LESS THAN OR EQUAL TO
C                                 ZERO ON ENTRY, SUBPROGRAM DEFINES THEM
              FNU     = DATA(1)
              FLA     = DATA(2)
              TAU     = DATA(3)
              EPS     = DATA(4)
              PHMIN   = DATA(5)
      IF      (FNU .LE. 0D0) FNU = 10D0
      IF      (FLA .LE. 0D0) FLA = .01D0
      IF      (TAU .LE. 0D0) TAU = .001D0
```

```
      IF    (EPS .LE. 0D0) EPS = .00002D0
      IF    (PHMIN .LE. 0D0) PHMIN = 0D0
            PH      = 0D0
            GAMM    = 0D0
            XITR    = 0D0
            XFCT    = 1D0
            XDER    = 0D0
C
C                                 TEST TO SEE IF TOTAL NUMBER OF VARIABLES
C                                 TO BE VARIED IS ZERO
            KE      = 0
      DO 11 I1      = 1, K
      IF    (XV(I1) .NE. 0.D0) KE = KE + 1
   11 CONTINUE
      IF    (KE .GT. 0) GO TO 12
            IERR    = -3
            IC      = -1
            NFCTDR  = -1
      GO TO 999
C                                 TEST TO SEE IF THERE ARE MORE UNKNOWNS
C                                 PRESENT THAN FUNCTIONS, THUS MAKING A
C                                 UNIQUE SOLUTION GENERALLY IMPOSSIBLE
   12 IF    (N .GE. KE) GO TO 13
            IERR    = -2
            IC      = -1
            NFCTDR  = -1
      GO TO 999
   13       I1      = 1
   61 IF    (XITR .GT. 0D0) GO TO 47
      DO 14 J1      = 1, K
            J2      = KBI1 + J1
            P(J2)   = X(J1)
            J3      = KBI2 + J1
   14       P(J3)   = DABS(X(J1)) + C1
      GO TO 40
   15 IF    (PHMIN .GT. PH .AND. IC .GT. 1) GO TO 34
            J1      = 0
   16       J1      = J1 + 1
            N1      = (J1 - 1)*N
      IF    (XV(J1)) 17, 35, 22
C                                 CALCULATE ANALYTICAL DERIVATIVES IN CALLIN
C                                 PROGRAM
   17       NFCTDR  = 1
            J       = J1
            IC      = 2
      GO TO 999
C                                 RETURN FROM CALCULATING DERIVITIVE
   20 DO 21 KK      = 1, N
            KKK     = N1 + KK
   21       P(KKK)  = PJ(KK)
            XDER    = XDER + 1D0
      GO TO 35
C                                 CALCULATE NUMERICAL DERIVATIVES
   22 DO 23 J2      = 1, K
            J3      = KBI1 + J2
            LL      = K + J2
   23       P(J3)   = X(LL)
            J3      = KBI1 + J1
            J4      = KBI2 + J1
            DEN     = C2*DMAX1(P(J4), DABS(P(J3)))
      IF    (P(J3) + DEN .LE. XMAX(J1)) GO TO 55
            P(J3)   = P(J3) - DEN
            DEN     = -DEN
      GO TO 56
   55       P(J3)   = P(J3) + DEN
C
C                                 CALCULATE VALUE OF FUNCTION
   56       NFCTDR  = 0
```

```
      DO 24 LL      = 1, K
            LLL     = KBI1 + LL
   24       X(LL)   = P(LLL)
            IC      = 3
      GO TO 999
C                                   RETURN FROM CALCULATING VALUE OF FUNCTION
   30 DO 31 MM      = 1, N
            MMM     = N1 + MM
   31       P(MMM)  = Z(MM)
            XFCT    = XFCT + 1D0
      DO 32 J2      = 1, N
            JB      = J2 + N1
            J5      = J2 + N
   32       P(JB)   = (P(JB) - Z(J5))/DEN
   35 IF    (J1 .EQ. K) GO TO 34
      GO TO 16
C                                   SET UP CORRECTION EQUATIONS
   34 DO 38 J1      = 1, K
            N1      = (J1 - 1)*N
            A(J1, KP1) = 0.
      IF    (XV(J1)) 29, 28, 29
   29 DO 33 J2      = 1, N
            N2      = N1 + J2
            J3      = N + J2
   33       A(J1, KP1) = A(J1, KP1) + P(N2)*(Y(J2) - Z(J3))
      DO 36 J2      = 1, K
            A(J1, J2) = 0D0
            N2      = (J2 - 1)*N
      DO 36 J3      = 1, N
            N3      = N1 + J3
            N4      = N2 + J3
   36       A(J1, J2) = A(J1, J2) + P(N3)*P(N4)
      IF    (A(J1, J1) .GT. C3) GO TO 38
   28 DO 37 J2      = 1, KP1
   37       A(J1, J2) = 0D0
            A(J1, J1) = 1D0
   38 CONTINUE
            GN      = 0D0
      DO 25 J1      = 1, K
   25       GN      = GN + A(J1, KP1)**2
C
C                                   SCALE CORRECTION EQUATIONS
      DO 39 J1      = 1, K
   39       A(J1, KP2) = DSQRT(A(J1, J1))
      DO 27 J1      = 1, K
            A(J1, KP1) = A(J1, KP1)/A(J1, KP2)
      DO 27 J2      = 1, K
   27       A(J1, J2) = A(J1, J2)/(A(J1, KP2)*A(J2, KP2))
            FL      = FLA/FNU
      GO TO 3
   62       FL      = FNU*FL
    3 DO 5  J1      = 1, K
      DO 4  J2      = 1, KP1
    4       AC(J1, J2) = A(J1, J2)
    5       AC(J1, J1) = AC(J1, J1) + FL
C
C                                   SOLVE CORRECTION EQUATIONS
      DO 9  L1      = 1, K
      IF    (AC(L1, L1) .EQ. 0D0) GO TO 803
            L2      = L1 + 1
      DO 6  L3      = L2, KP1
    6       AC(L1, L3) = AC(L1, L3)/AC(L1, L1)
      DO 9  L3      = 1, K
      IF    (L1 - L3) 7, 9, 7
    7 DO 8  L4      = L2, KP1
    8       AC(L3, L4) = AC(L3, L4) - AC(L1, L4)*AC(L3, L1)
    9 CONTINUE
C
```

```
              DN      = 0D0
              DG      = 0D0
        DO 26 J1      = 1, K
              LL      = K + J1
              AC(J1, KP2) = AC(J1, KP1)/A(J1, KP2)
              J2      = KBI1 + J1
              P(J2)   = DMAX1(XMIN(J1), DMIN1(XMAX(J1), X(LL) + AC(J1,
     1                  KP2)))
              DG      = DG + AC(J1, KP2)*A(J1, KP1)*A(J1, KP2)
              DN      = DN + AC(J1, KP2)*AC(J1, KP2)
   26         AC(J1, KP2) = P(J2) - X(LL)
C
C SES MODIFICATION 2/89 TO AVOID DIV BY ZERO
C
        VALUE=SQRT(DN*GN)
        IF(VALUE.LE.0.D0)VALUE=VMIN
        COSG=DG/VALUE
C              COSG    = DG/DSQRT(DN*GN)
              JGAM    = 0
        IF    (COSG) 18, 19, 19
   18         JGAM    = 2
              COSG    = -COSG
   19         COSG    = DMIN1(COSG, C4)
C
C SES MODFICATION 2/89 DARCOS TO DACOS
C
              GAMM    = DACOS(COSG)*C5/PI
C              GAMM    = DARCOS(COSG)*C5/PI
        IF    (JGAM .GT. 0) GAMM = C5 - GAMM
C
C                                   CALCULATE VALUE OF FUNCTION
   48         NFCTDR = 0
        DO 41 LL      = 1, K
              LLL     = KBI1 + LL
   41         X(LL)   = P(LLL)
              IC      = 4
        GO TO 999
C                                   RETURN FROM CALCULATING VALUE OF FUNCTION
   40 DO 42 MM      = 1, N
              MMM     = KZI + MM
   42         P(MMM) = Z(MM)
              XFCT    = XFCT + 1D0
              PHI     = 0.
        DO 43 J1      = 1, N
              J2      = KZI + J1
   43         PHI     = PHI + (P(J2) - Y(J1))**2
        IF    (PHI .LT. C6) GO TO 90
        IF    (XITR .GT. 0D0) GO TO 44
              IERR    = K
              IC      = 5
              NFCTDR = -1
        GO TO 96
   44 IF    (PHI .GE. PH) GO TO 47
C
C                                   EPSILON TEST
              IERR    = 0
        DO 45 J1      = 1, K
              J2      = K + J1
        IF    (DABS(AC(J1, KP2))/(TAU + DABS(X(J2))) .GT. EPS) IERR=IERR +
     1                1
   45 CONTINUE
        IF    (IERR .EQ. 0) GO TO 46
C
C                                   GAMMA LAMBDA TEST
        IF    (FL .GT. C4 .AND. GAMM .GT. C7) IERR = -1
        IF    (IERR .EQ. (-1)) GO TO 51
              IC      = 5
        GO TO 52
```

```
   51         IC      = -1
   52         NFCTDR  = -1
      GO TO 92
C                                  GAMMA EPSILON TEST
   46 IF      (FL .GT. C4 .AND. GAMM .LE. C8) IERR = -4
              IC      = -1
              NFCTDR  = -1
      GO TO 92
   47 IF      (I1 - 2) 49, 49, 50
   49         I1      = I1 + 1
      GO TO (61, 15, 62), I1
   50 IF      (FL .LT. C9) GO TO 62
              IERR    = -1
              IC      = -1
              NFCTDR  = -1
      GO TO 92
   90         IERR    = 0
              IC      = -1
              NFCTDR  = -1
   92         FLA     = FL
      DO 93 J2        = 1, K
              J3      = KBI1 + J2
              LL      = K + J2
              X(LL)   = P(J3)
   93         X(J2)   = P(J3)
   96 DO 94 J2        = 1, N
              J3      = KZI + J2
              LL      = N + J2
              Z(LL)   = P(J3)
   94         Z(J2)   = P(J3)
              PH      = PHI
  999         XITR    = XITR + 1D0
C                                  SET NDATA ARRAY EQUAL TO INTEGER VARIABLES
C                                  FOR RETURN TO CALLING PROGRAM
              NDATA(1) = IC
              NDATA(2) = NFCTDR
              NDATA(3) = IERR
              NDATA(4) = J
              NDATA(7) = KP1
              NDATA(8) = KP2
              NDATA(9) = KBI1
              NDATA(10) = KBI2
              NDATA(11) = KZI
              NDATA(12) = J1
              NDATA(13) = J2
              NDATA(14) = J3
              NDATA(15) = J4
              NDATA(16) = JB
              NDATA(17) = I1
              NDATA(18) = L1
              NDATA(19) = L2
              NDATA(20) = L3
              NDATA(21) = L4
              NDATA(22) = N1
              NDATA(23) = N2
              NDATA(24) = N3
              NDATA(25) = N4
              NDATA(26) = JGAM
C                                  SET DATA ARRAY EQUAL TO VARIABLES FOR
C                                  RETURN TO CALLING PROGRAM
              DATA(6) = FNU
              DATA(7) = TAU
              DATA(8) = EPS
              DATA(9) = PHMIN
              DATA(10) = GN
              DATA(11) = FL
              DATA(12) = DN
              DATA(13) = DG
```

```
            DATA(14) = COSG
            DATA(15) = PHI
            DATA(16) = DEN
C                              SET OUTPUT ARRAY EQUAL TO OUTPUT VARIABLES
C                              FOR RETURN TO CALLING PROGRAM
            OUTPUT(1) = PH
            OUTPUT(2) = GAMM
            OUTPUT(3) = XITR
            OUTPUT(4) = XFCT
            OUTPUT(5) = XDER
            OUTPUT(6) = FLA
      RETURN
      END
```

APPENDIX C

ESTPRO/PROCESS™ Peng Robinson simulation summary

Figure C.1
ESTPRO input data file


```
TITLE  TEST RUN OF PROGRAM COMPEST
;
DESC   MASTERS OF SCIENCE
DESC   N.  J.  I.  T.   Chemical Engineering Department
DESC   Steven E. Sund
DESC   For partial fulfillment of a
DESC   Masters Of Science in CHe Eng.
DESC   Fall 1988 / Spring 1989
DESC   Advisor Dr. E. C. Roche
DESC    FOR SYSOP4 PENG ROBINSON
DESC
;
T-UNITS= F
P-UNITS= PSIA
;
PROP-DATA
 COMP-LIST BP225
  CVAL  VABP= 225.7
  CVAL STBP=0.0
  CVAL  API= 60.53
 COMP-LIST BP275
  CVAL  VABP= 275.4
  CVAL STBP=0.0
  CVAL  API= 55.32
 COMP-LIST BP324
  CVAL  VABP= 324.9
  CVAL STBP=0.0
  CVAL  API= 50.12
 COMP-LIST BP374
  CVAL  VABP= 374.9
  CVAL STBP=0.0
  CVAL  API= 46.07
 COMP-LIST BP424
  CVAL  VABP= 424.9
  CVAL STBP=0.0
  CVAL  API= 42.40
 COMP-LIST BP475
  CVAL  VABP= 475.0
  CVAL STBP=0.0
  CVAL  API= 39.44
 COMP-LIST BP525
  CVAL  VABP= 525.1
  CVAL STBP=0.0
  CVAL  API= 36.66
 COMP-LIST BP575
  CVAL VABP= 575.1
  CVAL STBP=0.0
  CVAL  API= 34.13
;
PRINT-OPT
 CAL-DBUG= 0
 REP-DBUG=8
 ASPENOUT=INPUT
; REP-FILE= MASTEST
 PROP-OPT= SYSOP4
;
END-INPUT
```

Figure C.2
ESTPRO history output file

```
     ESTPRO BEGINS EXECUTION
     RUN MADE ON  3/13/89

     INPUT ECHO FOR PROGRAM COMPEST
----  ------------------------------------------------------------------
   1 TITLE  TEST RUN OF PROGRAM COMPEST
   2 ;
   3 DESC   MASTERS OF SCIENCE
   4 DESC   N.  J.  I.  T.   CHEMICAL ENGINEERING DEPARTMENT
   5 DESC   STEVEN E. SUND
   6 DESC   FOR PARTIAL FULFILLMENT OF A
   7 DESC   MASTERS OF SCIENCE IN CHE ENG.
   8 DESC   FALL 1988   SPRING 1989
   9 DESC   ADVISOR DR. E. C. ROCHE
  10 DESC    FOR SYSOP4 PENG ROBINSON
  11 DESC
  12 ;
  13 T-UNITS= F
  14 P-UNITS= PSIA
  15 ;
  16 PROP-DATA
  17  COMP-LIST BP225
  18   CVAL  VABP= 225.7
  19   CVAL STBP=0.0
  20   CVAL  API= 60.53
  21  COMP-LIST BP275
  22   CVAL  VABP= 275.4
  23   CVAL STBP=0.0
  24   CVAL  API= 55.32
  25  COMP-LIST BP324
  26   CVAL  VABP= 324.9
  27   CVAL STBP=0.0
  28   CVAL  API= 50.12
  29  COMP-LIST BP374
  30   CVAL  VABP= 374.9
  31   CVAL STBP=0.0
  32   CVAL  API= 46.07
  33  COMP-LIST BP424
  34   CVAL  VABP= 424.9
  35   CVAL STBP=0.0
  36   CVAL  API= 42.40
  37  COMP-LIST BP475
  38   CVAL  VABP= 475.0
  39   CVAL STBP=0.0
  40   CVAL  API= 39.44
  41  COMP-LIST BP525
  42   CVAL  VABP= 525.1
  43   CVAL STBP=0.0
  44   CVAL  API= 36.66
  45  COMP-LIST BP575
  46   CVAL VABP= 575.1
  47   CVAL STBP=0.0
  48   CVAL  API= 34.13
  49 ;
  50 PRINT-OPT
  51 PRINT-OPT
  52  CAL-DBUG= 0
  53  REP-DBUG=8
```

```
 ASPENOUT=INPUT
; REP-FILE= MASTEST
 PROP-OPT= SYSOP4
;
END-INPUT
END-INPUT
```

```
**************************************************************
*                                                            *
*                    INPUT SUMMARY                           *
*                                                            *
*    NUMBER OF COMPOUNDS..................        8          *
*    NUMBER OF INPUT LINES................       59          *
*    SIMULATION DEBUG NUMBER..............        0          *
*    REPORT DEBUG NUMBER..................        8          *
*    NUMBER OF DESC. STORED...............        9          *
*    SYSOP NUMBER.........................        4          *
*    ASPEN PRINT TYPE.....................    INPUT          *
*    BOILING POINT CONV TYPE..............      TBP          *
*    REP FILE NAME: TJLASP3                                  *
*                                                            *
**************************************************************
```

```
   COMPONENT ESTIMATION SUMMARY

    *WARNING*
IN MODULE NEED
PERCENT PARAFFINS,NAPTHENES, AND AROMATICS ARE ALL
0.0  VALUES WILL BE ESTIMATED.
    *WARNING*
IN MODULE NEED
PERCENT PARAFFINS,NAPTHENES, AND AROMATICS ARE ALL
0.0  VALUES WILL BE ESTIMATED.
    *WARNING*
IN MODULE NEED
PERCENT PARAFFINS,NAPTHENES, AND AROMATICS ARE ALL
0.0  VALUES WILL BE ESTIMATED.
    *WARNING*
IN MODULE NEED
PERCENT PARAFFINS,NAPTHENES, AND AROMATICS ARE ALL
0.0  VALUES WILL BE ESTIMATED.
    *WARNING*
IN MODULE NEED
PERCENT PARAFFINS,NAPTHENES, AND AROMATICS ARE ALL
0.0  VALUES WILL BE ESTIMATED.
    *WARNING*
IN MODULE NEED
PERCENT PARAFFINS,NAPTHENES, AND AROMATICS ARE ALL
0.0  VALUES WILL BE ESTIMATED.
    *WARNING*
IN MODULE NEED
PERCENT PARAFFINS,NAPTHENES, AND AROMATICS ARE ALL
0.0  VALUES WILL BE ESTIMATED.
    *WARNING*
IN MODULE NEED
PERCENT PARAFFINS,NAPTHENES, AND AROMATICS ARE ALL
0.0  VALUES WILL BE ESTIMATED.
    *WARNING*
IN MODULE ESTFRA
TB(F) VALUE OF    575.100      IS NOT IN CORRELATION RANGE 113-549
CORRECTIVE ACTION TAKEN AND CALC. CONTINUES

FINISHED COMPONENT  1 (BP225)
CUMULATIVE-CPU-TIME =   6.71000
```

```
     *WARNING*
IN MODULE ZCCAL
ZC VALUE IS NOT IN OPTIMAL RANGE 0.26-0.28
ZC-VALUE = 0.255843      CALC. CONTINUES

FINISHED COMPONENT  2 (BP275)
CUMULATIVE-CPU-TIME =  13.2900

     *WARNING*
IN MODULE ZCCAL
ZC VALUE IS NOT IN OPTIMAL RANGE 0.26-0.28
ZC-VALUE = 0.249294      CALC. CONTINUES

FINISHED COMPONENT  3 (BP324)
CUMULATIVE-CPU-TIME =  20.4600

     *WARNING*
IN MODULE ZCCAL
ZC VALUE IS NOT IN OPTIMAL RANGE 0.26-0.28
ZC-VALUE = 0.242957      CALC. CONTINUES

FINISHED COMPONENT  4 (BP374)
CUMULATIVE-CPU-TIME =  28.2300

     *WARNING*
IN MODULE ZCCAL
ZC VALUE IS NOT IN OPTIMAL RANGE 0.26-0.28
ZC-VALUE = 0.237113      CALC. CONTINUES

FINISHED COMPONENT  5 (BP424)
CUMULATIVE-CPU-TIME =  36.8300

     *WARNING*
IN MODULE ZCCAL
ZC VALUE IS NOT IN OPTIMAL RANGE 0.26-0.28
ZC-VALUE = 0.231541      CALC. CONTINUES
     *WARNING*
IN MODULE DHFRM
TB(K) VALUE OF   519.261
 IS NOT IN AROMATIC CORRELATION RANGE 353.3-517.8
 CORRECTIVE ACTION TAKEN AND CALC. CONTINUES

FINISHED COMPONENT  6 (BP475)
CUMULATIVE-CPU-TIME =  46.1500

     *WARNING*
IN MODULE ZCCAL
ZC VALUE IS NOT IN OPTIMAL RANGE 0.26-0.28
ZC-VALUE = 0.226389      CALC. CONTINUES
     *WARNING*
IN MODULE DHFRM
TB(K) VALUE OF   547.094
 IS NOT IN AROMATIC CORRELATION RANGE 353.3-517.8
 CORRECTIVE ACTION TAKEN AND CALC. CONTINUES

FINISHED COMPONENT  7 (BP525)
CUMULATIVE-CPU-TIME =  56.1300

     *WARNING*
IN MODULE ZCCAL
ZC VALUE IS NOT IN OPTIMAL RANGE 0.26-0.28
ZC-VALUE = 0.221584      CALC. CONTINUES
     *WARNING*
IN MODULE DHFRM
TB(K) VALUE OF   574.872
 IS NOT IN AROMATIC CORRELATION RANGE 353.3-517.8
 CORRECTIVE ACTION TAKEN AND CALC. CONTINUES
```

```
FINISHED COMPONENT   8 (BP575)
CUMULATIVE-CPU-TIME =   66.8100


 ********************************************************************
 *                                                                  *
 *                    ESTPRO ENDS EXECUTION                         *
 *                                                                  *
 *   NUMBER OF COMPOUNDS.....................          8            *
 *   CPU TIME ...............................     66.8300           *
 *   NUMBER OF WARNINGS PRINTED..............         19            *
 *   NUMBER OF ERRORS PRINTED................          0            *
 *   NUMBER OF SEVERE ERRORS PRINTED.........          0            *
 *                                                                  *
 ********************************************************************
```

Figure C.3
ESTPRO report output file

```
; TITLE   TEST RUN OF PROGRAM COMPEST
;   MASTERS OF SCIENCE
;   N.  J.  I.  T.    CHEMICAL ENGINEERING DEPARTMENT
;   STEVEN E. SUND
;   FOR PARTIAL FULFILLMENT OF A
;   MASTERS OF SCIENCE IN CHE ENG.
;   FALL 1988   SPRING 1989
;   ADVISOR DR. E. C. ROCHE
;    FOR SYSOP4 PENG ROBINSON
;
;
;  SUMMARY FOR COMPONENT BP225
;     VOLUME AVERAGE BOILING POINT (DEG K) =   380.761
;     AVERAGE MOLE WEIGHT                  =   115.398
;     SLOPE OF THE TBP CURVE               = 0.000000E+00
;     CUBIC AVERAGE BOILING POINT (DEG K)  =   380.761
;     MOLAL AVERAGE BOILING POINT (DEG K)  =   380.761
;     MEAN  AVERAGE BOILING POINT (DEG K)  =   380.761
;     UOP (WATSON) K CHAR. FACTOR          =   11.9652
;     API GRAVITY                          =   60.5300
;     SG GRAVITY  (60/60 F)                = 0.736864
;     PERCENT AROMATICS                    =   8.84911
;     PERCENT NAPTHENES                    =   35.1108
;     PERCENT PARAFINS                     =   56.0400
;     SYSOP SELECTED                       =   4.00000
;
PROP-DATA
  COMP-LIST BP225
     CVAL MW      1    1       115.3981836
     CVAL TC      1    1       563.8331613
     CVAL PC      1    1       2932997.331
     CVAL VC      1    1      0.4208001854
     CVAL ZC      1    1      0.2632750582
     CVAL OMEGA   1    1      0.2971405428
;
;   REGRESSION SUMMARY
;    ITERATION                =    1238.0000
;    NUMBER OF PARMS UNFIT:   =                0.
;    SUM OF SQUARES           =  0.39046387E-03
;
     CVAL PLXANT  1    1       20.73581523     /2       -3010.526307     /
                  3           -53.90448885     /4       0.0000000000E+00/
                  5          0.0000000000E+00/6       0.0000000000E+00/
                  7          0.0000000000E+00/8        185.7000006
                  9            265.7000000
;
;
;   REGRESSION SUMMARY
;    ITERATION                =    21.000000
;    NUMBER OF PARMS UNFIT:   =                0.
;    SUM OF SQUARES           =  0.22482929E-15
;
     CVAL CPIG    1    1      -14969.63646     /2         636.4331858     /
                  3          -0.2415604390     /4        0.0000000000E+00/
                  5           0.0000000000E+00/6        0.0000000000E+00/
                  7            255.3722222     /8         922.0388889     /
                  9            21346.32947     /10        432.5373873     /
                  11           1.000000000
```

```
;
      CVAL DHFORM 1    1       -167093238.4
      CVAL DGFORM 1    1        33212999.57
      CVAL TB     1    1        380.7611111
      CVAL VB     1    1       0.1616009320
      CVAL DHVLWT 1    1        32361763.25     /2        380.7611111     /
                  3             0.3800000000     /4       0.0000000000E+00/
                  5            0.0000000000E+00
;
;
;    REGRESSION SUMMARY
;     ITERATION                 =    5.0000000
;     NUMBER OF PARMS UNFIT:    =                0.
;     SUM OF SQUARES            =  0.12979604E-04
;
      CVAL RKTZRA 1    1       0.2645251387
      CVAL MUP    1    1       0.0000000000E+00
;
;    REGRESSION SUMMARY
;     ITERATION                 =    37.000000
;     NUMBER OF PARMS UNFIT:    =                0.
;     SUM OF SQUARES            =  0.12078411E-02
;
      CVAL MULAND 1    1        102.8439674     /2       -7038.655849     /
                  3            -18.98690027     /4        428.5132026     /
                  5             552.5564981
;
;
;   SUMMARY FOR COMPONENT BP275
;      VOLUME AVERAGE BOILING POINT (DEG K) =   408.372
;      AVERAGE MOLE WEIGHT                  =   128.204
;      SLOPE OF THE TBP CURVE               = 0.000000E+00
;      CUBIC AVERAGE BOILING POINT (DEG K)  =   408.372
;      MOLAL AVERAGE BOILING POINT (DEG K)  =   408.372
;      MEAN  AVERAGE BOILING POINT (DEG K)  =   408.372
;      UOP (WATSON) K CHAR. FACTOR          =   11.9154
;      API GRAVITY                          =   55.3200
;      SG GRAVITY  (60/60 F)                = 0.757414
;      PERCENT AROMATICS                    =   15.3800
;      PERCENT NAPTHENES                    =   34.5340
;      PERCENT PARAFINS                     =   50.0859
;      SYSOP SELECTED                       =   1.00000
;
PROP-DATA
  COMP-LIST BP275
     CVAL MW     1    1        128.2036122
     CVAL TC     1    1        593.3872478
     CVAL PC     1    1        2659001.461
     CVAL VC     1    1       0.4747008866
     CVAL ZC     1    1       0.2558427720
     CVAL OMEGA  1    1       0.3392753513
;
;    REGRESSION SUMMARY
;     ITERATION                 =    1393.0000
;     NUMBER OF PARMS UNFIT:    =                0.
;     SUM OF SQUARES            =  0.38543110E-03
;
      CVAL PLXANT 1    1        20.85607706     /2       -3259.027149     /
                  3            -59.09760168     /4       0.0000000000E+00/
                  5           0.0000000000E+00/6       0.0000000000E+00/
                  7           0.0000000000E+00/8        235.4000000     /
                  9             315.4000000
;
;
;    REGRESSION SUMMARY
;     ITERATION                 =    42.000000
;     NUMBER OF PARMS UNFIT:    =                0.
;     SUM OF SQUARES            =  0.28200766E-15
```

```
;
     CVAL CPIG    1    1      -15259.99359     /2         712.2214912     /
                  3          -0.2714363679     /4        0.0000000000E+00/
                  5          0.0000000000E+00/6        0.0000000000E+00/
                  7           255.3722222      /8         922.0388889     /
                  9           25547.49099      /10        483.1080850     /
                  11          1.000000000
;
     CVAL DHFORM  1    1      -172921695.8
     CVAL DGFORM  1    1       47066760.39
     CVAL TB      1    1       408.3722222
     CVAL VB      1    1      0.1833769161
     CVAL DHVLWT  1    1       35057971.90     /2         408.3722222     /
                  3          0.3800000000     /4        0.0000000000E+00/
                  5          0.0000000000E+00
;
;
;    REGRESSION SUMMARY
;     ITERATION                =    7.0000000
;     NUMBER OF PARMS UNFIT:   =                0.
;     SUM OF SQUARES           =   0.34044353E-04
;
     CVAL RKTZRA  1    1      0.2593181988
     CVAL MUP     1    1      0.0000000000E+00
;
;    REGRESSION SUMMARY
;     ITERATION                =    37.000000
;     NUMBER OF PARMS UNFIT:   =                0.
;     SUM OF SQUARES           =   0.14154249E-02
;
     CVAL MULAND  1    1       110.5423513     /2        -7813.264935     /
                  3          -19.91686762     /4         450.9743084     /
                  5           581.5195029
;
;
;  SUMMARY FOR COMPONENT BP324
;     VOLUME AVERAGE BOILING POINT (DEG K) =   435.872
;     AVERAGE MOLE WEIGHT                  =   141.984
;     SLOPE OF THE TBP CURVE               = 0.000000E+00
;     CUBIC AVERAGE BOILING POINT (DEG K)  =   435.872
;     MOLAL AVERAGE BOILING POINT (DEG K)  =   435.872
;     MEAN  AVERAGE BOILING POINT (DEG K)  =   435.872
;     UOP (WATSON) K CHAR. FACTOR          =   11.8382
;     API GRAVITY                          =   50.1200
;     SG GRAVITY  (60/60 F)                = 0.779099
;     PERCENT AROMATICS                    =   19.2952
;     PERCENT NAPTHENES                    =   33.2572
;     PERCENT PARAFINS                     =   47.4476
;     SYSOP SELECTED                       =   4.00000
;
PROP-DATA
  COMP-LIST BP324
     CVAL MW      1    1       141.9841320
     CVAL TC      1    1       622.8773587
     CVAL PC      1    1       2411806.559
     CVAL VC      1    1      0.5287254199
     CVAL ZC      1    1      0.2492940998
     CVAL OMEGA   1    1      0.3804518363
;
;    REGRESSION SUMMARY
;     ITERATION                =    1548.0000
;     NUMBER OF PARMS UNFIT:   =                0.
;     SUM OF SQUARES           =   0.37979416E-03
;
     CVAL PLXANT  1    1       20.97926728     /2        -3513.104077     /
                  3          -64.27514879     /4        0.0000000000E+00/
                  5          0.0000000000E+00/6        0.0000000000E+00/
                  7          0.0000000000E+00/8         284.9000000     /
```

```
                  9          364.9000000
;
;
;    REGRESSION SUMMARY
;     ITERATION                =    63.000000
;     NUMBER OF PARMS UNFIT: =                0.
;     SUM OF SQUARES           =   0.34543831E-15
;
      CVAL CPIG    1    1      -15735.31347     /2          787.9762754     /
                   3          -0.3017469505     /4         0.0000000000E+00/
                   5           0.0000000000E+00/6         0.0000000000E+00/
                   7           255.3722222      /8          922.0388889     /
                   9           29629.03519      /10         533.2783800     /
                   11          1.000000000
;
      CVAL DHFORM  1    1      -186172507.8
      CVAL DGFORM  1    1       58331118.91
      CVAL TB      1    1       435.8722222
      CVAL VB      1    1      0.2052125734
      CVAL DHVLWT  1    1       37771528.46     /2          435.8722222     /
                   3           0.3800000000     /4         0.0000000000E+00/
                   5           0.0000000000E+00
;
;
;    REGRESSION SUMMARY
;     ITERATION                =    7.0000000
;     NUMBER OF PARMS UNFIT: =                0.
;     SUM OF SQUARES           =   0.72323879E-04
;
      CVAL RKTZRA  1    1      0.2545433310
      CVAL MUP     1    1      0.0000000000E+00
;
;    REGRESSION SUMMARY
;     ITERATION                =    37.000000
;     NUMBER OF PARMS UNFIT: =                0.
;     SUM OF SQUARES           =   0.16447130E-02
;
      CVAL MULAND  1    1       118.1029182     /2         -8618.953396     /
                   3          -20.82260320     /4          473.3867926     /
                   5           610.4198115
;
;
;   SUMMARY FOR COMPONENT BP374
;      VOLUME AVERAGE BOILING POINT (DEG K) =   463.650
;      AVERAGE MOLE WEIGHT                  =   157.567
;      SLOPE OF THE TBP CURVE               = 0.000000E+00
;      CUBIC AVERAGE BOILING POINT (DEG K)  =   463.650
;      MOLAL AVERAGE BOILING POINT (DEG K)  =   463.650
;      MEAN  AVERAGE BOILING POINT (DEG K)  =   463.650
;      UOP (WATSON) K CHAR. FACTOR          =   11.8150
;      API GRAVITY                          =   46.0700
;      SG GRAVITY  (60/60 F)                = 0.796869
;      PERCENT AROMATICS                    =   19.8892
;      PERCENT NAPTHENES                    =   33.3386
;      PERCENT PARAFINS                     =   46.7722
;      SYSOP SELECTED                       =   4.00000
;
PROP-DATA
  COMP-LIST BP374
      CVAL MW      1    1       157.5668619
      CVAL TC      1    1       651.1994778
      CVAL PC      1    1       2230426.910
      CVAL VC      1    1      0.5897697862
      CVAL ZC      1    1      0.2429568871
      CVAL OMEGA   1    1      0.4263734931
;
;    REGRESSION SUMMARY
;     ITERATION                =    1718.0000
```

```
;     NUMBER OF PARMS UNFIT: =                0.
;     SUM OF SQUARES         =  0.37564425E-03
;
      CVAL PLXANT 1    1       21.10882317     /2       -3774.961827     /
                   3          -69.75429939     /4       0.0000000000E+00/
                   5          0.0000000000E+00/6        0.0000000000E+00/
                   7          0.0000000000E+00/8         334.9000000     /
                   9           414.9000000
;
;
;    REGRESSION SUMMARY
;     ITERATION              =    84.000000
;     NUMBER OF PARMS UNFIT: =                0.
;     SUM OF SQUARES         =  0.42318661E-15
;
      CVAL CPIG   1    1     -15456.15179     /2         872.1780983     /
                   3         -0.3349530380     /4       0.0000000000E+00/
                   5          0.0000000000E+00/6        0.0000000000E+00/
                   7           255.3722222     /8         922.0388889     /
                   9           34900.36838     /10        589.4516824     /
                   11          1.000000000
;
      CVAL DHFORM 1    1      -202697802.5
      CVAL DGFORM 1    1       69516418.21
      CVAL TB     1    1       463.6500000
      CVAL VB     1    1      0.2303106469
      CVAL DHVLWT 1    1       40533991.24     /2         463.6500000     /
                   3          0.3800000000     /4       0.0000000000E+00/
                   5          0.0000000000E+00
;
;
;    REGRESSION SUMMARY
;     ITERATION              =    7.0000000
;     NUMBER OF PARMS UNFIT: =                0.
;     SUM OF SQUARES         =  0.13140176E-03
;
      CVAL RKTZRA 1    1      0.2499284090
      CVAL MUP    1    1      0.0000000000E+00
;
;    REGRESSION SUMMARY
;     ITERATION              =    37.000000
;     NUMBER OF PARMS UNFIT: =                0.
;     SUM OF SQUARES         =  0.19329131E-02
;
      CVAL MULAND 1    1       126.3882929     /2       -9497.811860     /
                   3          -21.82740898     /4         494.9116031     /
                   5           638.1754683
;
;
;   SUMMARY FOR COMPONENT BP424
;      VOLUME AVERAGE BOILING POINT (DEG K) =   491.428
;      AVERAGE MOLE WEIGHT                  =   174.749
;      SLOPE OF THE TBP CURVE               = 0.000000E+00
;      CUBIC AVERAGE BOILING POINT (DEG K)  =   491.428
;      MOLAL AVERAGE BOILING POINT (DEG K)  =   491.428
;      MEAN  AVERAGE BOILING POINT (DEG K)  =   491.428
;      UOP (WATSON) K CHAR. FACTOR          =   11.7974
;      API GRAVITY                          =   42.4000
;      SG GRAVITY  (60/60 F)                = 0.813686
;      PERCENT AROMATICS                    =   18.4543
;      PERCENT NAPTHENES                    =   34.8047
;      PERCENT PARAFINS                     =   46.7410
;      SYSOP SELECTED                       =   4.00000
;
PROP-DATA
  COMP-LIST BP424
     CVAL MW     1    1       174.7488457
     CVAL TC     1    1       678.9631101
```

```
      CVAL PC       1    1        2046424.655
      CVAL VC       1    1       0.6540820488
      CVAL ZC       1    1       0.2371125566
      CVAL OMEGA    1    1       0.4741677501
;
;    REGRESSION SUMMARY
;     ITERATION                 =    1883.0000
;     NUMBER OF PARMS UNFIT:    =                0.
;     SUM OF SQUARES            =   0.37239392E-03
;
      CVAL PLXANT   1    1        21.24202054     /2        -4040.305846     /
                    3           -75.62535664     /4        0.0000000000E+00/
                    5           0.0000000000E+00/6         0.0000000000E+00/
                    7           0.0000000000E+00/8          384.9000000     /
                    9            464.9000000
;
;
;    REGRESSION SUMMARY
;     ITERATION                 =    105.00000
;     NUMBER OF PARMS UNFIT:    =                0.
;     SUM OF SQUARES            =   0.51398802E-15
;
      CVAL CPIG     1    1      -14877.00033     /2          960.0819410     /
                    3         -0.3696476306     /4        0.0000000000E+00/
                    5           0.0000000000E+00/6        0.0000000000E+00/
                    7            255.3722222     /8          922.0388889     /
                    9            40695.47178     /10         648.0705904     /
                    11           1.000000000
;
      CVAL DHFORM   1    1      -215891379.6
      CVAL DGFORM   1    1       83612030.62
      CVAL TB       1    1       491.4277778
      CVAL VB       1    1       0.2570688772
      CVAL DHVLWT   1    1       43319825.43     /2          491.4277778     /
                    3           0.3800000000     /4        0.0000000000E+00/
                    5           0.0000000000E+00
;
;
;    REGRESSION SUMMARY
;     ITERATION                 =    7.0000000
;     NUMBER OF PARMS UNFIT:    =                0.
;     SUM OF SQUARES            =   0.21097444E-03
;
      CVAL RKTZRA   1    1       0.2456195606
      CVAL MUP      1    1       0.0000000000E+00
;
;    REGRESSION SUMMARY
;     ITERATION                 =    37.000000
;     NUMBER OF PARMS UNFIT:    =                0.
;     SUM OF SQUARES            =   0.22710492E-02
;
      CVAL MULAND   1    1        134.9452861     /2        -10430.30200     /
                    3           -22.86561436     /4         516.0119637     /
                    5            665.3838379
;
;
;   SUMMARY FOR COMPONENT BP475
;      VOLUME AVERAGE BOILING POINT (DEG K) =   519.261
;      AVERAGE MOLE WEIGHT                  =   194.045
;      SLOPE OF THE TBP CURVE               = 0.000000E+00
;      CUBIC AVERAGE BOILING POINT (DEG K)  =   519.261
;      MOLAL AVERAGE BOILING POINT (DEG K)  =   519.261
;      MEAN  AVERAGE BOILING POINT (DEG K)  =   517.800
;      UOP (WATSON) K CHAR. FACTOR          =   11.8115
;      API GRAVITY                          =   39.4400
;      SG GRAVITY  (60/60 F)                = 0.827776
;      PERCENT AROMATICS                    =   18.4490
;      PERCENT NAPTHENES                    =   35.5597
```

```
;      PERCENT PARAFINS                          =   45.9912
;      SYSOP SELECTED                            =   4.00000
;
PROP-DATA
  COMP-LIST BP475
      CVAL MW       1    1        194.0446714
      CVAL TC       1    1        705.6792434
      CVAL PC       1    1        1874843.634
      CVAL VC       1    1       0.7245985772
      CVAL ZC       1    1       0.2315410125
      CVAL OMEGA    1    1       0.5263636183
;
;    REGRESSION SUMMARY
;     ITERATION                  =    2053.0000
;     NUMBER OF PARMS UNFIT:     =                 0.
;     SUM OF SQUARES             =   0.37025544E-03
;
      CVAL PLXANT   1    1        21.37752016     /2       -4305.994140     /
                    3           -82.21176104     /4       0.0000000000E+00/
                    5           0.0000000000E+00/6        0.0000000000E+00/
                    7           0.0000000000E+00/8         435.0000000     /
                    9            515.0000000
;
;
;    REGRESSION SUMMARY
;     ITERATION                  =    126.00000
;     NUMBER OF PARMS UNFIT:     =                 0.
;     SUM OF SQUARES             =   0.62061274E-15
;
      CVAL CPIG     1    1       -13511.21343     /2         1055.096721     /
                    3           -0.4067784755     /4       0.0000000000E+00/
                    5            0.0000000000E+00/6       0.0000000000E+00/
                    7            255.3722222     /8         922.0388889     /
                    9            47643.47449     /10        711.7440498     /
                    11           1.000000000
;
      CVAL DHFORM   1    1       -215223961.9
      CVAL DGFORM   1    1        103716630.8
      CVAL TB       1    1        519.2611111
      CVAL VB       1    1       0.2870122619
      CVAL DHVLWT   1    1        46131247.18     /2         519.2611111     /
                    3           0.3800000000     /4       0.0000000000E+00/
                    5           0.0000000000E+00
;
;
;    REGRESSION SUMMARY
;     ITERATION                  =    7.0000000
;     NUMBER OF PARMS UNFIT:     =                 0.
;     SUM OF SQUARES             =   0.30849307E-03
;
      CVAL RKTZRA   1    1       0.2415432282
      CVAL MUP      1    1       0.0000000000E+00
;
;    REGRESSION SUMMARY
;     ITERATION                  =    37.000000
;     NUMBER OF PARMS UNFIT:     =                 0.
;     SUM OF SQUARES             =   0.26868645E-02
;
      CVAL MULAND   1    1        144.1422313     /2       -11437.15950     /
                    3           -23.98895836     /4         536.3162250     /
                    5            691.5656586
;
;
;  SUMMARY FOR COMPONENT BP525
;      VOLUME AVERAGE BOILING POINT (DEG K) =   547.094
;      AVERAGE MOLE WEIGHT                  =   215.354
;      SLOPE OF THE TBP CURVE               = 0.000000E+00
;      CUBIC AVERAGE BOILING POINT (DEG K)  =   547.094
```

```
;      MOLAL AVERAGE BOILING POINT (DEG K)  =   547.094
;      MEAN  AVERAGE BOILING POINT (DEG K)  =   517.800
;      UOP (WATSON) K CHAR. FACTOR          =   11.8235
;      API GRAVITY                          =   36.6600
;      SG GRAVITY  (60/60 F)                =  0.841461
;      PERCENT AROMATICS                    =   25.4704
;      PERCENT NAPTHENES                    =   31.3743
;      PERCENT PARAFINS                     =   43.1553
;      SYSOP SELECTED                       =   4.00000
;
PROP-DATA
  COMP-LIST BP525
     CVAL MW      1    1       215.3536475
     CVAL TC      1    1       732.0027723
     CVAL PC      1    1       1726024.936
     CVAL VC      1    1      0.7982679251
     CVAL ZC      1    1      0.2263892295
     CVAL OMEGA   1    1      0.5807696600
;
;    REGRESSION SUMMARY
;     ITERATION                =    2223.0000
;     NUMBER OF PARMS UNFIT: =                0.
;     SUM OF SQUARES           =  0.36844507E-03
;
     CVAL PLXANT  1    1       21.51843597     /2       -4577.492317     /
                  3           -89.04146066     /4       0.00000000000E+00/
                  5           0.00000000000E+00/6       0.00000000000E+00/
                  7           0.00000000000E+00/8        485.1000000     /
                  9            565.1000000
;
;
;    REGRESSION SUMMARY
;     ITERATION                =    147.00000
;     NUMBER OF PARMS UNFIT: =                0.
;     SUM OF SQUARES           =  0.74284249E-15
;
     CVAL CPIG    1    1      -11803.51835     /2         1153.508129     /
                  3          -0.4152912707     /4       0.00000000000E+00/
                  5           0.00000000000E+00/6       0.00000000000E+00/
                  7            255.3722222     /8         922.0388889     /
                  9           5511.14646      /10        777.6476633     /
                  11           1.000000000
;
     CVAL DHFORM  1    1      -186914718.7
     CVAL DGFORM  1    1       113525607.2
     CVAL TB      1    1       547.0944444
     CVAL VB      1    1      0.3188126349
     CVAL DHVLWT  1    1       40964194.83     /2        547.0944444     /
                  3           0.3800000000     /4       0.00000000000E+00/
                  5           0.00000000000E+00
;
;
;    REGRESSION SUMMARY
;     ITERATION                =    7.0000000
;     NUMBER OF PARMS UNFIT: =                0.
;     SUM OF SQUARES           =  0.41610859E-03
;
     CVAL RKTZRA  1    1      0.2377557894
     CVAL MUP     1    1      0.00000000000E+00
;
;    REGRESSION SUMMARY
;     ITERATION                =    37.000000
;     NUMBER OF PARMS UNFIT: =                0.
;     SUM OF SQUARES           =  0.31741258E-02
;
     CVAL MULAND  1    1       153.6305521     /2       -12504.64628     /
                  3           -25.14670850     /4        556.3221070     /
                  5            717.3627169
```

```
;
;
;   SUMMARY FOR COMPONENT BP575
;      VOLUME AVERAGE BOILING POINT (DEG K) =   574.872
;      AVERAGE MOLE WEIGHT                  =   238.929
;      SLOPE OF THE TBP CURVE               = 0.000000E+00
;      CUBIC AVERAGE BOILING POINT (DEG K)  =   574.872
;      MOLAL AVERAGE BOILING POINT (DEG K)  =   574.872
;      MEAN  AVERAGE BOILING POINT (DEG K)  =   517.800
;      UOP (WATSON) K CHAR. FACTOR          =   11.8394
;      API GRAVITY                          =   34.1300
;      SG GRAVITY  (60/60 F)                = 0.854314
;      PERCENT AROMATICS                    =   33.4600
;      PERCENT NAPTHENES                    =   25.8704
;      PERCENT PARAFINS                     =   40.6696
;      SYSOP SELECTED                       =   4.00000
;
PROP-DATA
  COMP-LIST BP575
      CVAL MW      1    1       238.9288652
      CVAL TC      1    1       757.7707736
      CVAL PC      1    1       1594344.961
      CVAL VC      1    1      0.87563307 97
      CVAL ZC      1    1      0.2215844830
      CVAL OMEGA   1    1      0.6381040569
;
;    REGRESSION SUMMARY
;     ITERATION                =    2398.0000
;     NUMBER OF PARMS UNFIT: =                0.
;     SUM OF SQUARES           =  0.36696847E-03
;
      CVAL PLXANT  1    1       21.66451631     /2       -4853.946744     /
                   3           -96.15472758     /4       0.0000000000E+00/
                   5          0.0000000000E+00/6       0.0000000000E+00/
                   7          0.0000000000E+00/8        535.1000000     /
                   9           615.1000000
;
;
;    REGRESSION SUMMARY
;     ITERATION                =    168.00000
;     NUMBER OF PARMS UNFIT: =                0.
;     SUM OF SQUARES           =  0.88049710E-15
;
      CVAL CPIG    1    1      -9620.648464     /2         1255.871869     /
                   3          -0.4853028471     /4        0.0000000000E+00/
                   5           0.0000000000E+00/6        0.0000000000E+00/
                   7            255.3722222     /8         922.0388889     /
                   9            63339.31856     /10        846.2385199     /
                   11           1.000000000
;
      CVAL DHFORM  1    1      -154323072.6
      CVAL DGFORM  1    1       124469906.9
      CVAL TB      1    1       574.8722222
      CVAL VB      1    1      0.3528859529
      CVAL DHVLWT  1    1       51811455.50     /2        574.8722222     /
                   3           0.3800000000     /4       0.0000000000E+00/
                   5          0.0000000000E+00
;
;
;    REGRESSION SUMMARY
;     ITERATION                =    7.0000000
;     NUMBER OF PARMS UNFIT: =                0.
;     SUM OF SQUARES           =  0.53108048E-03
;
      CVAL RKTZRA  1    1      0.2342367825
      CVAL MUP     1    1      0.0000000000E+00
;
;    REGRESSION SUMMARY
```

```
;     ITERATION                =    37.000000
;     NUMBER OF PARMS UNFIT: =              0.
;     SUM OF SQUARES           =  0.37492264E-02
;
      CVAL MULAND 1    1       163.4955236     /2       -13638.07707     /
                  3           -26.35087233     /4        575.9057879     /
                  5            742.6153581
;
```

Figure C.4
ASPEN SYSOP4 simulation input file

```
NEW
; (DO YOU HAVE "NEW" ABOVE THIS LINE?)
;
;         CODES FOR VAX/VMS
;
;:MAIL (ON A BATCH JOB; DO YOU WANT MAIL(Y), NOTIFY(N) Y/N) = N
;:CODE (PROJECT) = AI
;:OLDID = MS1C
;:NEWID = MS1C
;:DELETE FILES (EXCEPT .LOG, .HIS, .REP, .INP - G BUILDS PLD; Y/N/G) = Y
;:VERSION (REFERS TO TEST(T) OR PRODUCTION(P)) = T
;:BUILD A NEW INPUT TRANSLATOR (Y/N) = N
;:PDF LENGTH (800 MAX) = 790
;:TABLE ( PATHNAME OF USER SDF ) = NULL
;:QUEUE ( A:ASPEN ) = A
;:SUBMIT (Y IF IMMEDIATE, N IF SPECIFYING TIME) = Y
;:
;:KEY =                          ARG =
;:
;:   LISTED BELOW ARE THE POSSIBLE ENTRIES FOR 'KEY' AND THEIR ASSOCIATED
;:   FILE UNIT NUMBERS.  THE ACTUAL ENTRY FOR 'ARG' IS THE FILENAME OF THE
;:   FILE CONTAINING THE INSERT OR DATABANK.
;:
;:   KEY = INSERT                ARG = FOR019
;:   KEY = USRPP1A               ARG = FOR021
;:   KEY = USRPP1B               ARG = FOR022
;:   KEY = USRPP2A               ARG = FOR023
;:   KEY = USRPP2B               ARG = FOR024
;:   KEY = USRPP2C               ARG = FOR025
;:   KEY = USRCOST               ARG = FOR026
;:
;:END VAX/VMS PROCS
;
;
;
TITLE 'ASPEN RUN OF ASP1C.INP'
;
DESCRIPTION &
 "ALLIED CORPORATION
 ASPEN SIMULATION OF ASP1C.INP
 PENG-ROBINSON:SYSOP4 (50/50)
 S. E. SUND  RUN=1C  DATE 3/89"
;
IN-UNITS ENG
OUT-UNITS ENG
;
;
;        MXIO    :  Maximum number of INTEGER OVERFLOWS
;        MXDO    :  Maximum number of FLOATING POINT OVERFLOWS
;        MXDU    :  Maximum number of FLOATING POINT UNDERFLOWS
;        MXID    :  Maximum number of INTEGER DIVIDES BY ZERO
;        MXDD    :  Maximum number of FLOATING POINT DIVIDES BY ZERO
;        MXOM    :  Maximum number of FLOATING POINT OVERFLOWS IN MATH LIBRARY
;        MXUM    :  Maximum number of FLOATING POINT UNDERFLOWS IN MATH LIBRARY
;        MXSL    :  Maximum number of SIGNIFICANCE LOST IN MATH LIBRARY ERRORS
;        MXLZ    :  Maximum number of LOGZERNEG ERRORS IN MATH LIBRARY
;        MXSN    :  Maximum number of SQUROONEG ERRORS IN MATH LIBRARY
;        MXUE    :  Maximum number of UNDEFINED EXPONENTIATION ERRORS
;
RUN-CONTROL MAX-TIME=54000.  MAX-ERRORS=5000 &
```

```
  MXIO=100 MXDO=100 &
  MXDU=100 MXID=100 MXDD=100 MXOM=100 MXUM=100 MXSL=100 MXLZ=100 MXSN=100
;
HISTORY MSG-LEVEL PROPERTIES=2  SIMULATION=4
;
PROPERTY-REPORT ALL
STREAM-REPORT
 STANDARD OPTIONS=ALL
 SUPPLEMENTAL 1 OPTIONS=MASS-FLOW
;
;
SIM-OPTIONS NMB-RESULTS=2  SIZE-RESULTS=0
;
;
;---------------------------------------------------------------------
;
;          PHYSICAL PROPERTY DATA
;
;---------------------------------------------------------------------
;
COMPONENTS BP225                        BF3/
           BP275                        BF3/
           BP324                        BF3/
           BP374                        BF3/
           BP424                        BF3/
           BP475                        BF3/
           BP525                        BF3/
           BP575                        BF3
;
; TITLE   TEST RUN OF PROGRAM COMPEST
;   MASTERS OF SCIENCE
;   N.  J.  I.  T.   CHEMICAL ENGINEERING DEPARTMENT
;   STEVEN E. SUND
;   FOR PARTIAL FULFILLMENT OF A
;   MASTERS OF SCIENCE IN CHE ENG.
;   FALL 1988   SPRING 1989
;   ADVISOR DR. E. C. ROCHE
;    FOR SYSOP4 PENG ROBINSON
;
;
;  SUMMARY FOR COMPONENT BP225
;     VOLUME AVERAGE BOILING POINT (DEG K) =  380.761
;     AVERAGE MOLE WEIGHT                  =  115.398
;     SLOPE OF THE TBP CURVE               = 0.000000E+00
;     CUBIC AVERAGE BOILING POINT (DEG K)  =  380.761
;     MOLAL AVERAGE BOILING POINT (DEG K)  =  380.761
;     MEAN  AVERAGE BOILING POINT (DEG K)  =  380.761
;     UOP (WATSON) K CHAR. FACTOR          =  11.9652
;     API GRAVITY                          =  60.5300
;     SG GRAVITY  (60/60 F)                = 0.736864
;     PERCENT AROMATICS                    =  8.84911
;     PERCENT NAPTHENES                    =  35.1106
;     PERCENT PARAFINS                     =  56.0400
;     SYSOP SELECTED                       =  4.00000
;
PROP-DATA
  COMP-LIST BP225
     CVAL MW      1    1       115.3981836
     CVAL TC      1    1       563.8331613
     CVAL PC      1    1       2932997.331
     CVAL VC      1    1      0.4208001854
     CVAL ZC      1    1      0.2632750582
     CVAL OMEGA   1    1      0.2971405428
;
;   REGRESSION SUMMARY
;    ITERATION               =    1238.0000
;    NUMBER OF PARMS UNFIT: =              0.
;    SUM OF SQUARES          =  0.39046387E-03
```

```
;
     CVAL PLXANT 1    1       20.73581523     /2       -3010.526307     /
                 3           -53.90448885     /4       0.0000000000E+00/
                 5           0.0000000000E+00/6       0.0000000000E+00/
                 7           0.0000000000E+00/8        185.7000000     /
                 9            265.7000000
;
;
;    REGRESSION SUMMARY
;     ITERATION                 =    21.000000
;     NUMBER OF PARMS UNFIT:    =           0.
;     SUM OF SQUARES            =   0.22482929E-15
;
     CVAL CPIG   1    1      -14969.63646     /2         636.4331858     /
                 3          -0.2415604390     /4       0.0000000000E+00/
                 5           0.0000000000E+00/6       0.0000000000E+00/
                 7            255.3722222     /8         922.0388889     /
                 9            21346.32947     /10        432.5373873     /
                 11           1.000000000
;
     CVAL DHFORM 1    1      -167093238.4
     CVAL DGFORM 1    1       33212999.57
     CVAL TB     1    1       380.7611111
     CVAL VB     1    1      0.1616009320
     CVAL DHVLWT 1    1       32361763.25     /2         380.7611111     /
                 3           0.3800000000     /4       0.0000000000E+00/
                 5           0.0000000000E+00
;
;
;    REGRESSION SUMMARY
;     ITERATION                 =    5.0000000
;     NUMBER OF PARMS UNFIT:    =           0.
;     SUM OF SQUARES            =   0.12979604E-04
;
     CVAL RKTZRA 1    1      0.2645251387
     CVAL MUP    1    1      0.0000000000E+00
;
;    REGRESSION SUMMARY
;     ITERATION                 =    37.000000
;     NUMBER OF PARMS UNFIT:    =           0.
;     SUM OF SQUARES            =   0.12078411E-02
;
     CVAL MULAND 1    1       102.8439674     /2       -7038.655849     /
                 3           -18.98690027     /4        428.5132026     /
                 5            552.5564961
;
;
;  SUMMARY FOR COMPONENT BP275
;      VOLUME AVERAGE BOILING POINT (DEG K) =   408.372
;      AVERAGE MOLE WEIGHT                  =   128.204
;      SLOPE OF THE TBP CURVE               = 0.000000E+00
;      CUBIC AVERAGE BOILING POINT (DEG K)  =   408.372
;      MOLAL AVERAGE BOILING POINT (DEG F)  =   408.372
;      MEAN  AVERAGE BOILING POINT (DEG K)  =   408.372
;      UOP (WATSON) K CHAR. FACTOR          =   11.9154
;      API GRAVITY                          =   55.3200
;      SG GRAVITY  (60/60 F)                = 0.757414
;      PERCENT AROMATICS                    =   15.3800
;      PERCENT NAPTHENES                    =   34.5340
;      PERCENT PARAFINS                     =   50.0859
;      SYSOP SELECTED                       =   4.00000
;
PROP-DATA
  COMP-LIST BP275
     CVAL MW     1    1       128.2036122
     CVAL TC     1    1       593.3872478
     CVAL PC     1    1       2659001.461
     CVAL VC     1    1      0.4747008866
```

```
      CVAL ZC       1    1       0.2558427720
      CVAL OMEGA    1    1       0.3392753513
 ;
 ;    REGRESSION SUMMARY
 ;     ITERATION                  =    1393.0000
 ;     NUMBER OF PARMS UNFIT:     =          0.
 ;     SUM OF SQUARES             =   0.38543110E-03
 ;
      CVAL PLXANT 1    1        20.85607706     /2        -3259.027149     /
                  3            -59.09760168    /4        0.0000000000E+00/
                  5           0.0000000000E+00/6        0.0000000000E+00/
                  7           0.0000000000E+00/8         235.4000000     /
                  9            315.4000000
 ;
 ;
 ;    REGRESSION SUMMARY
 ;     ITERATION                  =    42.000000
 ;     NUMBER OF PARMS UNFIT:     =          0.
 ;     SUM OF SQUARES             =   0.28200766E-15
 ;
      CVAL CPIG     1    1      -15259.99359     /2         712.2214912     /
                  3           -0.2714361679     /4        0.0000000000E+00/
                  5           0.0000000000E+00/6        0.0000000000E+00/
                  7            255.3722222     /8         922.0388889     /
                  9            25547.49099     /10        483.1080850     /
                  11           1.000000000
 ;
      CVAL DHFORM 1    1      -172921695.8
      CVAL DGFORM 1    1       47066760.39
      CVAL TB     1    1       408.3722222
      CVAL VB     1    1      0.1853769161
      CVAL DHVLWT 1    1       35097971.90     /2         408.3722222     /
                  3           0.3800000000     /4        0.0000000000E+00/
                  5           0.0000000000E+00
 ;
 ;
 ;    REGRESSION SUMMARY
 ;     ITERATION                  =    7.0000000
 ;     NUMBER OF PARMS UNFIT:     =          0.
 ;     SUM OF SQUARES             =   0.34044353E-04
 ;
      CVAL RKTZRA 1    1      0.2593181988
      CVAL MUP    1    1      0.0000000000E+00
 ;
 ;    REGRESSION SUMMARY
 ;     ITERATION                  =    37.000000
 ;     NUMBER OF PARMS UNFIT:     =          0.
 ;     SUM OF SQUARES             =   0.14154249E-02
 ;
      CVAL MULAND 1    1        110.5423513     /2        -7813.264935     /
                  3           -19.91686762     /4         456.9743064     /
                  5            581.5195029
 ;
 ;
 ;   SUMMARY FOR COMPONENT BP324
 ;      VOLUME AVERAGE BOILING POINT (DEG F) =   435.872
 ;      AVERAGE MOLE WEIGHT                  =   141.984
 ;      SLOPE OF THE TBP CURVE               = 0.000000E+00
 ;      CUBIC AVERAGE BOILING POINT (DEG K)  =   435.872
 ;      MOLAL AVERAGE BOILING POINT (DEG K)  =   435.872
 ;      MEAN  AVERAGE BOILING POINT (DEG K)  =   435.872
 ;      UOP (WATSON) K CHAR. FACTOR          =   11.8382
 ;      API GRAVITY                          =   50.1200
 ;      SG GRAVITY  (60/60 F)                = 0.779099
 ;      PERCENT AROMATICS                    =   19.2952
 ;      PERCENT NAPTHENES                    =   33.2572
 ;      PERCENT PARAFINS                     =   47.4476
 ;      SYSOP SELECTED                       =   4.00000
```

```
;
PROP-DATA
  COMP-LIST BP324
      CVAL MW       1    1        141.9841320
      CVAL TC       1    1        622.8773587
      CVAL PC       1    1        2441808.559
      CVAL VC       1    1       0.52872541999
      CVAL ZC       1    1       0.24929409988
      CVAL OMEGA    1    1       0.38045183630
;
;    REGRESSION SUMMARY
;     ITERATION                  =    1548.0000
;     NUMBER OF PARMS UNFIT:     =           0.
;     SUM OF SQUARES             =   0.37979416E-03
;
      CVAL PLXANT 1    1        20.97926728     /2        -3513.104077     /
                  3            -64.27514879     /4        0.00000000000E+00/
                  5           0.00000000000E+00/6        0.00000000000E+00/
                  7           0.00000000000E+00/8         284.9000000     /
                  9            364.9000000
;
;
;    REGRESSION SUMMARY
;     ITERATION                  =    63.000000
;     NUMBER OF PARMS UNFIT:     =           0.
;     SUM OF SQUARES             =   0.34543831E-15
;
      CVAL CPIG   1    1       -15735.31347     /2          787.9762754     /
                  3           -0.3017469505     /4        0.00000000000E+00/
                  5            0.00000000000E+00/6        0.00000000000E+00/
                  7            255.3722222     /8          922.0388889     /
                  9            29629.03519     /10         533.2783800     /
                  11           1.000000000
;
      CVAL DHFORM 1    1       -186172507.8
      CVAL DGFORM 1    1        58331118.91
      CVAL TB     1    1        435.8722222
      CVAL VB     1    1       0.20521257340
      CVAL DHVLWT 1    1        37771528.46     /2          435.8722222     /
                  3            0.3800000000     /4        0.00000000000E+00/
                  5           0.00000000000E+00
;
;
;    REGRESSION SUMMARY
;     ITERATION                  =    7.0000000
;     NUMBER OF PARMS UNFIT:     =           0.
;     SUM OF SQUARES             =   0.72323879E-04
;
      CVAL RKTZRA 1    1       0.25454333100
      CVAL MUP    1    1       0.00000000000E+00
;
;    REGRESSION SUMMARY
;     ITERATION                  =    37.000000
;     NUMBER OF PARMS UNFIT:     =           0.
;     SUM OF SQUARES             =   0.16447130E-02
;
      CVAL MULAND 1    1        118.1029102     /2        -8618.953396     /
                  3            -20.82260320     /4         473.3867926     /
                  5            610.4198115
;
;
;  SUMMARY FOR COMPONENT BP374
;     VOLUME AVERAGE BOILING POINT (DEG K) =   463.650
;     AVERAGE MOLE WEIGHT                  =   157.567
;     SLOPE OF THE TBP CURVE               = 0.000000E+00
;     CUBIC AVERAGE BOILING POINT (DEG K)  =   463.650
;     MOLAL AVERAGE BOILING POINT (DEG K)  =   463.650
;     MEAN  AVERAGE BOILING POINT (DEG K)  =   463.650
```

```
;      UOP (WATSON) K CHAR. FACTOR              =   11.8150
;      API GRAVITY                              =   46.0700
;      SG GRAVITY  (60/60 F)                    =  0.796869
;      PERCENT AROMATICS                        =   19.8892
;      PERCENT NAPTHENES                        =   33.3386
;      PERCENT PARAFINS                         =   46.7722
;      SYSOP SELECTED                           =   4.00000
;
PROP-DATA
  COMP-LIST BP374
     CVAL MW      1    1       157.5668619
     CVAL TC      1    1       651.1994778
     CVAL PC      1    1       2230426.910
     CVAL VC      1    1      0.5897697862
     CVAL ZC      1    1      0.2429568871
     CVAL OMEGA   1    1      0.4263734931
;
;    REGRESSION SUMMARY
;     ITERATION                =    1718.0000
;     NUMBER OF PARMS UNFIT: =                 0.
;     SUM OF SQUARES           =   0.37564425E-03
;
     CVAL PLXANT  1    1       21.10882317     /2       -3774.961827     /
                  3           -69.75429939     /4       0.0000000000E+00/
                  5          0.0000000000E+00/6       0.0000000000E+00/
                  7          0.0000000000E+00/8        334.9000000     /
                  9           414.9000000
;
;
;    REGRESSION SUMMARY
;     ITERATION                =    84.000000
;     NUMBER OF PARMS UNFIT: =                 0.
;     SUM OF SQUARES           =   0.42318661E-15
;
     CVAL CPIG    1    1      -15456.15179     /2         872.1780983     /
                  3          -0.3349530380     /4        0.0000000000E+00/
                  5          0.0000000000E+00/6        0.0000000000E+00/
                  7           255.3722222     /8         922.0388889     /
                  9           34900.36838     /10        589.4516824     /
                  11          1.000000000
;
     CVAL DHFORM  1    1      -202607802.5
     CVAL DGFORM  1    1       69516418.21
     CVAL TB      1    1       463.6500000
     CVAL VB      1    1      0.2303106469
     CVAL DHVLWT  1    1       40533991.24     /2        463.6500000     /
                  3           0.3800000000     /4       0.0000000000E+00/
                  5          0.0000000000E+00
;
;
;    REGRESSION SUMMARY
;     ITERATION                =    7.0000000
;     NUMBER OF PARMS UNFIT: =                 0.
;     SUM OF SQUARES           =   0.13140176E-03
;
     CVAL RKTZRA  1    1      0.2499284090
     CVAL MUP     1    1      0.0000000000E+00
;
;    REGRESSION SUMMARY
;     ITERATION                =    37.000000
;     NUMBER OF PARMS UNFIT: =                 0.
;     SUM OF SQUARES           =   0.19329131E-02
;
     CVAL MULAND  1    1       126.3882929     /2       -9497.811860     /
                  3           -21.82740898     /4        494.9116031     /
                  5           638.1754883
;
;
```

```
;   SUMMARY FOR COMPONENT BP424
;      VOLUME AVERAGE BOILING POINT (DEG K) =   491.428
;      AVERAGE MOLE WEIGHT                  =   174.749
;      SLOPE OF THE TBP CURVE               = 0.000000E+00
;      CUBIC AVERAGE BOILING POINT (DEG K)  =   491.428
;      MOLAL AVERAGE BOILING POINT (DEG K)  =   491.428
;      MEAN  AVERAGE BOILING POINT (DEG K)  =   491.428
;      UOP (WATSON) K CHAR. FACTOR          =   11.7974
;      API GRAVITY                          =   42.4000
;      SG GRAVITY  (60/60 F)                = 0.813686
;      PERCENT AROMATICS                    =   18.4543
;      PERCENT NAPTHENES                    =   34.8047
;      PERCENT PARAFINS                     =   46.7410
;      SYSOP SELECTED                       =   4.00000
;
PROP-DATA
  COMP-LIST BP424
     CVAL MW      1    1       174.7488457
     CVAL TC      1    1       678.9631101
     CVAL PC      1    1       2046424.655
     CVAL VC      1    1      0.6540820488
     CVAL ZC      1    1      0.2371125566
     CVAL OMEGA   1    1      0.4741677501
;
;    REGRESSION SUMMARY
;     ITERATION                =    1883.0000
;     NUMBER OF PARMS UNFIT: =                0.
;     SUM OF SQUARES           =  0.37239392E-03
;
     CVAL PLXANT 1    1       21.24202054     /2       -4040.305846     /
                 3           -75.62535664     /4       0.0000000000E+00/
                 5          0.0000000000E+00/6       0.0000000000E+00/
                 7          0.0000000000E+00/8        384.9000000     /
                 9           464.9000000
;
;
;    REGRESSION SUMMARY
;     ITERATION                =    105.00000
;     NUMBER OF PARMS UNFIT: =                0.
;     SUM OF SQUARES           =  0.51398802E-15
;
     CVAL CPIG    1    1      -14877.00033     /2         960.0819410     /
                 3          -0.3696476306     /4       0.0000000000E+00/
                 5          0.0000000000E+00/6       0.0000000000E+00/
                 7           255.3722222     /8         922.0388889     /
                 9           40695.47178     /10        648.0705904     /
                 11          1.000000000
;
     CVAL DHFORM 1    1      -215891379.6
     CVAL DGFORM 1    1       83612030.62
     CVAL TB      1    1       491.4277778
     CVAL VB      1    1      0.2570686772
     CVAL DHVLWT 1    1       43319825.43     /2        491.4277778     /
                 3          0.3800000000     /4       0.0000000000E+00/
                 5          0.0000000000E+00
;
;
;    REGRESSION SUMMARY
;     ITERATION                =    7.0000000
;     NUMBER OF PARMS UNFIT: =                0.
;     SUM OF SQUARES           =  0.21097444E-03
;
     CVAL RKTZRA 1    1      0.2456195606
     CVAL MUP     1    1      0.0000000000E+00
;
;    REGRESSION SUMMARY
;     ITERATION                =    37.000000
;     NUMBER OF PARMS UNFIT: =                0.
```

```
;     SUM OF SQUARES              =  0.22710492E-02
;
      CVAL MULAND 1    1          134.9452861     /2        -10430.30200     /
                  3              -22.86561436     /4          516.0119637     /
                  5               665.3838479
;
;
;   SUMMARY FOR COMPONENT BP475
;      VOLUME AVERAGE BOILING POINT (DEG K) =   519.261
;      AVERAGE MOLE WEIGHT                  =   194.045
;      SLOPE OF THE TBP CURVE               = 0.000000E+00
;      CUBIC AVERAGE BOILING POINT (DEG K)  =   519.261
;      MOLAL AVERAGE BOILING POINT (DEG K)  =   519.261
;      MEAN  AVERAGE BOILING POINT (DEG K)  =   517.800
;      UOP (WATSON) K CHAR. FACTOR          =   11.8115
;      API GRAVITY                          =   39.4400
;      SG GRAVITY  (60/60 F)                = 0.827776
;      PERCENT AROMATICS                    =   18.4490
;      PERCENT NAPTHENES                    =   35.5597
;      PERCENT PARAFINS                     =   45.9912
;      SYSOP SELECTED                       =   4.00000
;
PROP-DATA
  COMP-LIST BP475
      CVAL MW      1    1        194.0446714
      CVAL TC      1    1        705.6792434
      CVAL PC      1    1        1874843.634
      CVAL VC      1    1       0.7245985772
      CVAL ZC      1    1       0.2315410125
      CVAL OMEGA   1    1       0.5263636183
;
;    REGRESSION SUMMARY
;     ITERATION                =    2053.0000
;     NUMBER OF PARMS UNFIT: =                0.
;     SUM OF SQUARES           =  0.37025541E-03
;
      CVAL PLXANT 1    1        21.37752016     /2        -4305.994140     /
                  3             -82.21176104     /4        0.0000000000E+00/
                  5             0.0000000000E+00/6        0.0000000000E+00/
                  7             0.0000000000E+00/8         435.0000000     /
                  9              515.0000000
;
;
;    REGRESSION SUMMARY
;     ITERATION                =    126.00000
;     NUMBER OF PARMS UNFIT: =                0.
;     SUM OF SQUARES           =  0.62061274E-15
;
      CVAL CPIG    1    1       -13511.21343     /2         1055.096721     /
                  3             -0.4067784755     /4        0.0000000000E+00/
                  5             0.0000000000E+00/6        0.0000000000E+00/
                  7              255.3722222     /8         922.0386869     /
                  9              4743.47149     /10         711.7446498     /
                  11             1.000000000
;
      CVAL DHFORM 1    1       -215223961.9
      CVAL DGFORM 1    1        103716630.8
      CVAL TB      1    1        519.2611111
      CVAL VB      1    1       0.2870122619
      CVAL DHVLWT 1    1        46131247.18     /2         519.2611111     /
                  3             0.3800000000     /4        0.0000000000E+00/
                  5             0.0000000000E+00
;
;
;    REGRESSION SUMMARY
;     ITERATION                =    7.0000000
;     NUMBER OF PARMS UNFIT: =                0.
;     SUM OF SQUARES           =  0.30849307E-03
```

```
;
     CVAL RKTZRA 1    1      0.2415432282
     CVAL MUP    1    1      0.0000000000E+00
;
;    REGRESSION SUMMARY
;     ITERATION                =    37.000000
;     NUMBER OF PARMS UNFIT: =                0.
;     SUM OF SQUARES           =   0.26868645E-02
;
     CVAL MULAND 1    1       144.1422313    /2       -11437.15950    /
                 3           -23.98895836    /4        536.3162250    /
                 5            691.5656586
;
;
;   SUMMARY FOR COMPONENT BP525
;      VOLUME AVERAGE BOILING POINT (DEG K) =   547.094
;      AVERAGE MOLE WEIGHT                  =   215.354
;      SLOPE OF THE TBP CURVE               = 0.000000E+00
;      CUBIC AVERAGE BOILING POINT (DEG K)  =   547.094
;      MOLAL AVERAGE BOILING POINT (DEG K)  =   547.094
;      MEAN  AVERAGE BOILING POINT (DEG K)  =   517.800
;      UOP (WATSON) K CHAR. FACTOR          =   11.8235
;      API GRAVITY                          =   36.6600
;      SG GRAVITY  (60/60 F)                = 0.841461
;      PERCENT AROMATICS                    =   25.4704
;      PERCENT NAPTHENES                    =   31.3743
;      PERCENT PARAFINS                     =   43.1553
;      SYSOP SELECTED                       =   4.00000
;
PROP-DATA
  COMP-LIST BP525
     CVAL MW     1    1       215.3536475
     CVAL TC     1    1       732.0027723
     CVAL PC     1    1       1726024.936
     CVAL VC     1    1      0.7982679251
     CVAL ZC     1    1      0.2263892265
     CVAL OMEGA  1    1      0.5807696600
;
;    REGRESSION SUMMARY
;     ITERATION                =    2223.0000
;     NUMBER OF PARMS UNFIT: =                0.
;     SUM OF SQUARES           =   0.36844507E-03
;
     CVAL PLXANT 1    1       21.51843597    /2       -4577.492317    /
                 3           -89.04146066    /4       0.0000000000E+00/
                 5           0.0000000000E+00/6       0.0000000000E+00/
                 7           0.0000000000E+00/8        485.1000000    /
                 9            565.1000000
;
;
;    REGRESSION SUMMARY
;     ITERATION                =    147.00000
;     NUMBER OF PARMS UNFIT: =                0.
;     SUM OF SQUARES           =   0.74284249E-15
;
     CVAL CPIG   1    1      -11803.51835    /2        1153.508129    /
                 3          -0.4452912707    /4       0.0000000000E+00/
                 5           0.0600000000E+00/6       0.0000000000E+00/
                 7            255.3722222    /8        922.0388889    /
                 9            55141.14646    /10       777.6476633    /
                 11           1.000000000
;
     CVAL DHFORM 1    1      -186514718.7
     CVAL DGFORM 1    1       113525607.2
     CVAL TB     1    1       547.0944444
     CVAL VB     1    1      0.3188126349
     CVAL DHVLWT 1    1       48964194.83    /2        547.0944444    /
                 3           0.3800000000    /4       0.0000000000E+00/
```

```
                5          0.0000000000E+00
;
;
;    REGRESSION SUMMARY
;     ITERATION                =    7.0000000
;     NUMBER OF PARMS UNFIT:  =              0.
;     SUM OF SQUARES           =  0.41810859E-03
;
      CVAL RKTZRA 1    1      0.2377557894
      CVAL MUP    1    1      0.0000000000E+00
;
;    REGRESSION SUMMARY
;     ITERATION                =    37.000000
;     NUMBER OF PARMS UNFIT:  =              0.
;     SUM OF SQUARES           =  0.31741258E-02
;
      CVAL MULAND 1    1       153.6305521     /2       -12504.64628     /
                  3           -25.14670850     /4        556.3221070     /
                  5            717.3627169
;
;
;   SUMMARY FOR COMPONENT BP575
;      VOLUME AVERAGE BOILING POINT (DEG K) =  574.872
;      AVERAGE MOLE WEIGHT                  =  238.929
;      SLOPE OF THE TBP CURVE               = 0.000000E+00
;      CUBIC AVERAGE BOILING POINT (DEG K)  =  574.872
;      MOLAL AVERAGE BOILING POINT (DEG K)  =  574.872
;      MEAN  AVERAGE BOILING POINT (DEG K)  =  517.800
;      UOP (WATSON) K CHAR. FACTOR          =  11.8394
;      API GRAVITY                          =  34.1300
;      SG GRAVITY  (60/60 F)                = 0.854314
;      PERCENT AROMATICS                    =  33.4600
;      PERCENT NAPTHENES                    =  25.8704
;      PERCENT PARAFINS                     =  40.6696
;      SYSOP SELECTED                       =  1.00000
;
PROP-DATA
  COMP-LIST BP575
      CVAL MW      1    1       238.9288652
      CVAL TC      1    1       757.7707736
      CVAL PC      1    1       1594344.961
      CVAL VC      1    1      0.8756330797
      CVAL ZC      1    1      0.2215844830
      CVAL OMEGA   1    1      0.6381040569
;
;    REGRESSION SUMMARY
;     ITERATION                =    2398.0000
;     NUMBER OF PARMS UNFIT:  =              0.
;     SUM OF SQUARES           =  0.36696847E-03
;
      CVAL PLXANT 1    1       21.66451631     /2       -4853.946744     /
                  3           -96.15472758     /4       0.0000000000E+00/
                  5           0.0000000000E+00/6       0.0000000000E+00/
                  7           0.0000000000E+00/8        535.1000000     /
                  9            615.1000000
;
;
;    REGRESSION SUMMARY
;     ITERATION                =    168.00000
;     NUMBER OF PARMS UNFIT:  =              0.
;     SUM OF SQUARES           =  0.88049710E-15
;
      CVAL CPIG   1    1      -9620.648464     /2         1255.871869     /
                  3          -0.4853028471     /4       0.0000000000E+00/
                  5           0.0000000000E+00/6       0.0000000000E+00/
                  7            255.3722222     /8         922.0388889     /
                  9            63339.31856     /10        846.2385199     /
                  11           1.000000000
```

```
;
      CVAL DHFORM 1    1       -154323072.6
      CVAL DGFORM 1    1        124469908.9
      CVAL TB     1    1        574.8722222
      CVAL VB     1    1       0.3528859529
      CVAL DHVLWT 1    1        51811455.50     /2        574.8722222     /
                  3             0.3800000000     /4       0.0000000000E+00/
                  5            0.0000000000E+00
;
;
;    REGRESSION SUMMARY
;     ITERATION                =    7.0000000
;     NUMBER OF PARMS UNFIT:   =                0.
;     SUM OF SQUARES           =   0.53108048E-03
;
      CVAL RKTZRA 1    1       0.2342367825
      CVAL MUP    1    1      0.0000000000E+00
;
;    REGRESSION SUMMARY
;     ITERATION                =    37.000000
;     NUMBER OF PARMS UNFIT:   =                0.
;     SUM OF SQUARES           =   0.37492264E-02
;
      CVAL MULAND 1    1        163.4955236     /2       -13638.07707     /
                  3            -26.35087233     /4        575.9057879     /
                  5             742.6153581
;
DEF-STREAMS HEAT H01
;
PROPERTIES SYSOP4 GLOBAL
;
PROP-SOURCES
        GLOBAL ASPENPCD COMPS=ALL
;-----------------------------------------------------------------------
;
;         BLOCK INPUT
;
;-----------------------------------------------------------------------
;
FLOWSHEET
   BLOCK  FLA1  IN=S01                    OUT=S02 S03 H01
;
;-----------------------------------------------------------------------
;
;          FEED STREAMS & RECYCLES
;
;-----------------------------------------------------------------------
;
;    FEED STREAMS
;
STREAM S01 TEMP=400. PRES=14.696
  MOLE-FLOW BP225 22.6 / BP275 23.5 /
            BP324 22.4 / BP374 20.0 /
            BP424 17.4 / BP475 15.8 /
            BP525 14.7 / BP575 13.8
;
; 50/50 VAP. LIQ. SPLIT
;
BLOCK  FLA1  FLASH2
 PARAM PRES=-1 V=0.5
```

Figure C.5

Process Flow Diagram for Simulation
Comparison of Aspen Version D and
PROCESS Version 3.02

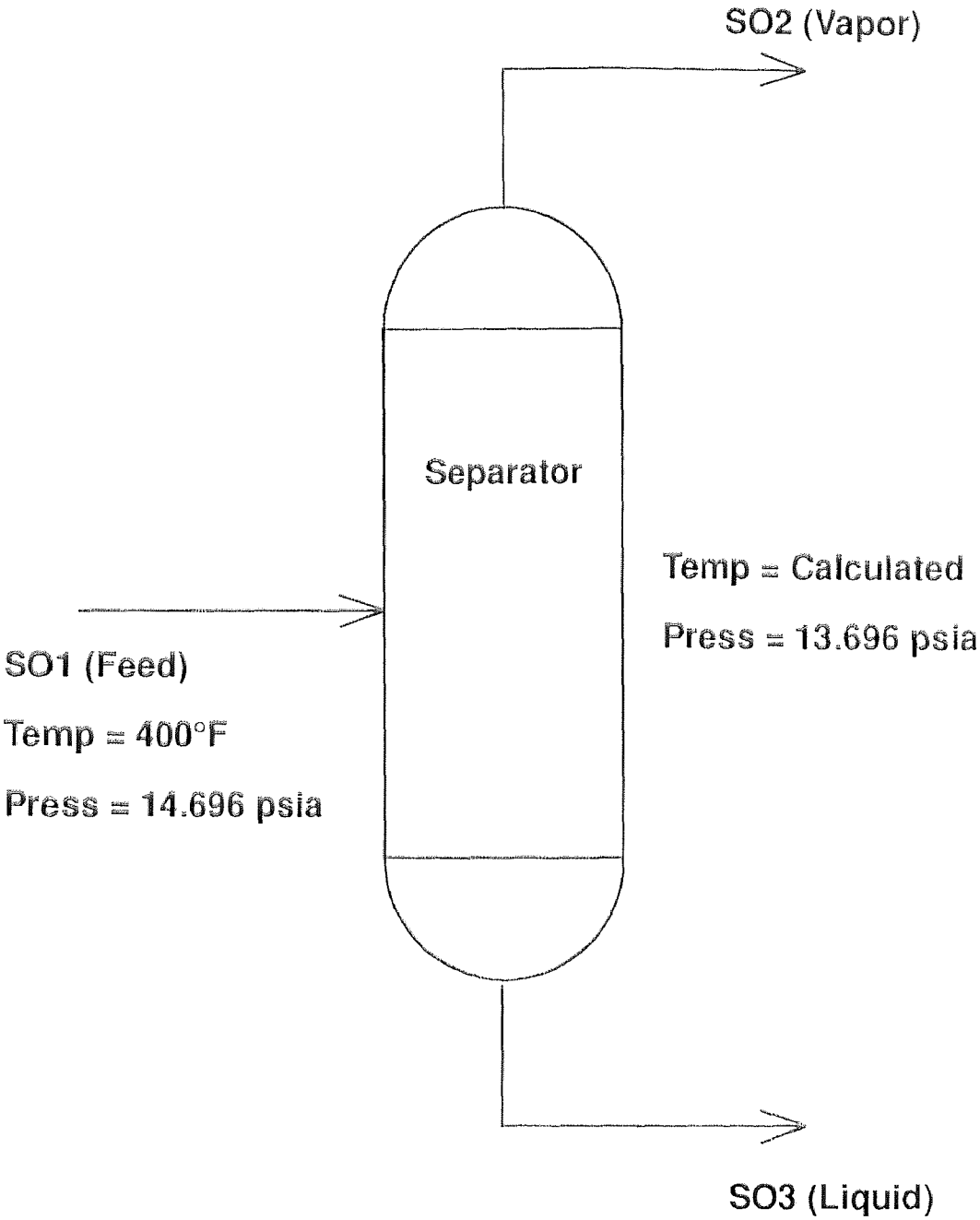

Figure C.6
ASPEN report summary for 50/50 split
simulation using SYSOP4

ASPEN(VER D)ALLIED SIGNAL CORP - SCIENTIFIC COMPUTATION DATE: 3/14/89 PAGE I
ASPEN RUN OF ASP1C.INP
DESCRIPTION

ALLIED CORPORATION ASPEN SIMULATION OF ASP1C.INP
PENG-ROBINSON:SYSOP4 (50/50) S. E. SUND RUN=1C DATE 3/89

RUN CONTROL INFORMATION

TYPE OF RUN: NEW

INPUT FILE NAME: ASP1C

INPUT PROBLEM DATA FILE NAME: MS1C UPDATE NO. 0

MAIN CALLING PROGRAM NAME: MS1C

CPU TIME USED DURING SIMULATION STEP: 1.54 SECONDS
SIMULATION REQUESTED FOR ENTIRE FLOWSHEET

TABLE OF CONTENTS

ASPEN(VER D)ALLIED SIGNAL CORP - SCIENTIFIC COMPUTATION DATE: 3/14/89 PAGE 1
ASPEN RUN OF ASP1C.INP
FLOWSHEET SECTION

FLOWSHEET CONNECTIVITY BY STREAMS

STREAM	SOURCE	DEST	STREAM	SOURCE	DEST
S02	FLA1	----	S03	FLA1	----
H01	FLA1	----	S01	----	FLA1

FLOWSHEET CONNECTIVITY BY BLOCKS

BLOCK	INLETS	OUTLETS
FLA1	S01	S02 S03 H01

COMPUTATIONAL SEQUENCE

SEQUENCE USED WAS:
FLA1

OVERALL FLOWSHEET BALANCE

*** MASS AND ENERGY BALANCE ***

	IN	OUT	RELATIVE DIFF.
CONVENTIONAL COMPONENTS (LBMOL/HR)			
BP225	22.6000	22.6000	0.166929E-09
BP275	23.5000	23.5000	0.129678E-09
BP324	22.4000	22.4000	0.765985E-10
BP374	20.0000	20.0000	0.821201E-11
BP424	17.4000	17.4000	-0.657424E-10
BP475	15.8000	15.8000	-0.131278E-09
BP525	14.7000	14.7000	-0.178534E-09
BP575	13.8000	13.8000	-0.207068E-09
TOTAL BALANCE			
MOLE(LBMOL/HR)	150.200	150.200	0.000000E+00
MASS(LB/HR)	24522.0	24522.0	-0.307795E-10
ENTHALPY(BTU/HR)	-0.100194E+08	-0.100194E+08	0.232381E-16

COMPONENTS

ID	TYPE	FORMULA	NAME OR ALIAS
BP225	C	MISSING	BF3
BP275	C	MISSING	BF3
BP324	C	MISSING	BF3
BP374	C	MISSING	BF3
BP424	C	MISSING	BF3
BP475	C	MISSING	BF3
BP525	C	MISSING	BF3
BP575	C	MISSING	BF3

OPTION SETS

KEY TO OPTION SET TABLES:
OPTION SET ID
MP KEYWORD MP ROUTE ID

```
ASPEN(VER D)ALLIED SIGNAL CORP - SCIENTIFIC COMPUTATION DATE:  3/14/89 PAGE    3
                                ASPEN RUN OF ASP1C.INP
                            PHYSICAL PROPERTIES SECTION

OPTION SETS (CONTINUED)


   SYSOP0                          SYSOP4
    PHILMX      PHILMX00            PHIVMX      PHIVMX04
    HVMX        HVMX00              PHILMX      PHILMX04
    HLMX        HLMX00              HVMX        HVMX04
    GVMX        GVMX00              HLMX        HLMX04
    GLMX        GLMX00              GVMX        GVMX04
    SVMX        SVMX00              GLMX        GLMX04
    SLMX        SLMX00              SVMX        SVMX04
    VVMX        VVMX00              SLMX        SLMX04
    VLMX        VLMX01              VVMX        VVMX04
    MUVMX       MUVMX01             VLMX        VLMX04
    MULMX       MULMX01             MUVMX       MUVMX02
    KVMX        KVMX01              MULMX       MULMX02
    KLMX        KLMX01              KVMX        KVMX02
    DVMX        DVMX01              KLMX        KLMX01
    DLMX        DLMX01              DVMX        DVMX02
    SIGLMX      SIGLMX01            DLMX        DLMX01
    PHIV        PHIV00              SIGLMX      SIGLMX01
    PHIL        PHIL00
    HV          HV00
    HL          HL00
    GV          GV00
    GL          GL00
    SV          SV00
    SL          SL00
    VV          VV00
    VL          VL01
    MUV         MUV01
    MUL         MUL01
    KV          KV01
    KL          KL01
    SIGL        SIGL01
    PHISMX      PHISMX02
    HSMX        HSMX02
    GSMX        GSMX02
    SSMX        SSMX01
    VSMX        VSMX02
    KSMX        KSMX01
    PHIS        PHIS02
    HS          HS02
    GS          GS02
    SS          SS02
    VS          VS01
    KS          KS01

MAJOR AND SUBORDINATE PROPERTY ROUTES

 KEY TO ROUTE TABLES:
  ROUTE ID    KEYWORD    METHOD CODE    MP/SP
              ASSOCIATED MODELS: NAME    PROPERTY    DATA SET    OPTION CODES
              ASSOCIATED MAJOR (SUBORDINATE) PROPERTIES: KEYWORD    ROUTE ID

 PHILMX00 PHILMX 2 MP
```

MAJOR AND SUBORDINATE PROPERTY ROUTES (CONTINUED)

```
          ASSOC. MP'S:      PHIL PHIL00

HVMX00    HVMX 3 MP

HLMX00    HLMX 3 MP
          ASSOC. SP'S:      DHLMX DHLMX00

GVMX00    GVMX 3 MP
          ASSOC. SP'S:      DGVMX DGVMX00

GLMX00    GLMX 3 MP
          ASSOC. SP'S:      DGLMX DGLMX00

SVMX00    SVMX 2 MP
          ASSOC. SP'S:      DSVMX DSVMX00

SLMX00    SLMX 2 MP
          ASSOC. SP'S:      DSLMX DSLMX00

VVMX00    VVMX 1 MP
          ASSOC. MODELS:    VV2IG VVMX 1

VLMX01    VLMX 1 MP
          ASSOC. MODELS:    VL2RKT VLMX 1

MUVMX01   MUVMX 1 MP
          ASSOC. MODELS:    MUV2BROK MUVMX 1

MULMX01   MULMX 1 MP
          ASSOC. MODELS:    MUL2ANDR MULMX 1

KVMX01    KVMX 1 MP
          ASSOC. MODELS:    KV2WMS KVMX 1

KLMX01    KLMX 1 MP
          ASSOC. MODELS:    KL2SRVR KLMX 1

DVMX01    DVMX 1 MP
          ASSOC. MODELS:    DV1CEWL DVMX 1

DLMX01    DLMX 1 MP
          ASSOC. MODELS:    DL1WCV DLMX 1

SIGLMX01  SIGLMX 1 MP
          ASSOC. MODELS:    SIG2HSS SIGLMX 1

PHIV00    PHIV 1 MP
          ASSOC. MODELS:    PHV0USR PHIV 1

PHIL00    PHIL 2 MP
          ASSOC. MODELS:    PL0XANT PL 1

HV00      HV 2 MP
```

MAJOR AND SUBORDINATE PROPERTY ROUTES (CONTINUED)

```
HL00        HL 2 MP
            ASSOC. SP'S:      DHL DHL00

GV00        GV 2 MP
            ASSOC. SP'S:      DGV DGV00

GL00        GL 2 MP
            ASSOC. SP'S:      DGL DGL00

SV00        SV 1 MP
            ASSOC. MP'S:      HV HV00 / GV GV00

SL00        SL 1 MP
            ASSOC. MP'S:      HL HL00 / GL GL00

VV00        VV 1 MP
            ASSOC. MODELS:    VV0IG VV 1

VL01        VL 1 MP
            ASSOC. MODELS:    VL0RKT VL 1

MUV01       MUV 1 MP
            ASSOC. MODELS:    MUV0BROK MUV 1

MUL01       MUL 1 MP
            ASSOC. MODELS:    MUL0ANDR MUL 1

KV01        KV 1 MP
            ASSOC. MODELS:    KV0STLTH KV 1

KL01        KL 1 MP
            ASSOC. MODELS:    KL0USR KL 1

SIGL01      SIGL 1 MP
            ASSOC. MODELS:    SIG0HSS SIGL 1

PHISMX02    PHISMX 2 MP
            ASSOC. MODELS:    PHS1IS PHISMX 1
            ASSOC. MP'S:      PHIS PHIS02

HSMX02      HSMX 2 MP
            ASSOC. MP'S:      HS HS02

GSMX02      GSMX 2 MP
            ASSOC. MP'S:      GS GS02

SSMX01      SSMX 1 MP
            ASSOC. MP'S:      HSMX HSMX02 / GSMX GSMX02

VSMX02      VSMX 2 MP
            ASSOC. MODELS:    VS2IS VSMX 1
            ASSOC. MP'S:      VS VS01
```

MAJOR AND SUBORDINATE PROPERTY ROUTES (CONTINUED)

```
KSMX01    KSMX 2 MP
          ASSOC. MP'S:      KS KS01

PHIS02    PHIS 2 MP
          ASSOC. MODELS:    PS0ANT PS 1

HS02      HS 1 MP
          ASSOC. MODELS:    HS0POL1 HS 1

GS02      GS 1 MP
          ASSOC. MODELS:    GS0POL1 GS 1

SS02      SS 1 MP
          ASSOC. MODELS:    SS0POL1 SS 1

VS01      VS 1 MP
          ASSOC. MODELS:    VS0POLY VS 1

KS01      KS 1 MP
          ASSOC. MODELS:    KS0POLY KS 1

PHIVMX04  PHIVMX 1 MP
          ASSOC. MODELS:    ESPR EOS 1

PHILMX04  PHILMX 1 MP
          ASSOC. MODELS:    ESPR EOS 1

HVMX04    HVMX 3 MP
          ASSOC. SP'S:      DHVMX DHVMX04

HLMX04    HLMX 3 MP
          ASSOC. SP'S:      DHLMX DHLMX04

GVMX04    GVMX 3 MP
          ASSOC. SP'S:      DGVMX DGVMX04

GLMX04    GLMX 3 MP
          ASSOC. SP'S:      DGLMX DGLMX04

SVMX04    SVMX 2 MP
          ASSOC. SP'S:      DSVMX DSVMX04

SLMX04    SLMX 2 MP
          ASSOC. SP'S:      DSLMX DSLMX04

VVMX04    VVMX 1 MP
          ASSOC. MODELS:    ESPR EOS 1

VLMX04    VLMX 1 MP
          ASSOC. MODELS:    ESPR EOS 1

MUVMX02   MUVMX 1 MP
          ASSOC. MODELS:    MUV2DNST MUVMX 1
```

MAJOR AND SUBORDINATE PROPERTY ROUTES (CONTINUED)

```
 MULMX02   MULMX 1 MP
           ASSOC. MODELS:    MUL2LEST MULMX 1

 KVMX02    KVMX 1 MP
           ASSOC. MODELS:    KV2STLTH KVMX 1

 DVMX02    DVMX 1 MP
           ASSOC. MODELS:    DV1DKK DVMX 1

 DHLMX00   DHLMX 2 SP
           ASSOC. SP'S:      DHL DHL00

 DGVMX00   DGVMX 1 SP
           ASSOC. MODELS:    ESIG EOS 1

 DGLMX00   DGLMX 2 SP
           ASSOC. SP'S:      DGL DGL00

 DSVMX00   DSVMX 1 SP
           ASSOC. MODELS:    ESIG EOS 1

 DSLMX00   DSLMX 2 SP
           ASSOC. SP'S:      DHLMX DHLMX00 / DGLMX DGLMX00

 DHL00     DHL 3 SP
           ASSOC. MODELS:    DHVLWTSN DHVL 1

 DGV00     DGV 2 SP

 DGL00     DGL 2 SP
           ASSOC. MP'S:      PHIL PHIL00

 DHVMX04   DHVMX 1 SP
           ASSOC. MODELS:    ESPR EOS 1

 DHLMX04   DHLMX 1 SP
           ASSOC. MODELS:    ESPR EOS 1

 DGVMX04   DGVMX 1 SP
           ASSOC. MODELS:    ESPR EOS 1

 DGLMX04   DGLMX 1 SP
           ASSOC. MODELS:    ESPR EOS 1

 DSVMX04   DSVMX 1 SP
           ASSOC. MODELS:    ESPR EOS 1

 DSLMX04   DSLMX 1 SP
           ASSOC. MODELS:    ESPR EOS 1

PARAMETER SOURCES

 GLOBAL
```

PARAMETER SOURCES (CONTINUED)

PASSWORD ASPENPCD
COMP-LIST ALL

PARAMETER VALUES

CONVENTIONAL COMPONENT - UNARY PARAMETER TABLE

PARAMETER NAME/SET/EL			COMPONENTS BP225	BP275	BP324	BP374	BP424
ZC	1		2.63275-01	2.55843-01	2.49294-01	2.42957-01	2.37113-01
TC	1		5.63833+02	5.93387+02	6.22877+02	6.51199+02	6.78963+02
PC	1		2.93300+06	2.65900+06	2.44181+06	2.23043+06	2.04642+06
MW	1		1.15398+02	1.28204+02	1.41984+02	1.57567+02	1.74749+02
PLXANT	1	1	2.07358+01	2.08561+01	2.09793+01	2.11088+01	2.12420+01
		2	-3.01053+03	-3.25903+03	-3.51310+03	-3.77496+03	-4.04031+03
		3	-5.39045+01	-5.90976+01	-6.42751+01	-6.97543+01	-7.56254+01
		4	0.0	0.0	0.0	0.0	0.0
		5	0.0	0.0	0.0	0.0	0.0
		6	0.0	0.0	0.0	0.0	0.0
		7	0.0	0.0	0.0	0.0	0.0
		8	1.85700+02	2.35400+02	2.84900+02	3.34900+02	3.84900+02
		9	2.65700+02	3.15400+02	3.64900+02	4.14900+02	4.64900+02
TB	1		3.80761+02	4.08372+02	4.35872+02	4.63650+02	4.91428+02
CPIG	1	1	-1.49696+04	-1.52600+04	-1.57353+04	-1.54562+04	-1.48770+04
		2	6.36433+02	7.12221+02	7.87976+02	8.72178+02	9.60082+02
		3	-2.41560-01	-2.71436-01	-3.01747-01	-3.34953-01	-3.69648-01
		4	0.0	0.0	0.0	0.0	0.0
		5	0.0	0.0	0.0	0.0	0.0
		6	0.0	0.0	0.0	0.0	0.0
		7	2.55372+02	2.55372+02	2.55372+02	2.55372+02	2.55372+02
		8	9.22039+02	9.22039+02	9.22039+02	9.22039+02	9.22039+02
		9	2.13463+04	2.55375+04	2.96290+04	3.49004+04	4.06955+04
		10	4.32537+02	4.83108+02	5.33278+02	5.80452+02	6.46071+02
		11	1.00000 00	1.00000 00	1.00000 00	1.00000 00	1.00000 00
DHVLWT	1	1	3.23618+07	3.56580+07	3.77715+07	4.05340+07	4.33196+07
		2	3.80761+02	4.08372+02	4.35872+02	4.63650+02	4.91428+02
		3	3.80000-01	3.80000-01	3.80000-01	3.80000-01	3.80000-01
		4	0.0	0.0	0.0	0.0	0.0
		5	0.0	0.0	0.0	0.0	0.0
OMEGA	1		2.97141-01	3.39275-01	3.80452-01	4.26373-01	4.74168-01
DHFORM	1		-1.67093+08	-1.72922+08	-1.86173+08	-2.02698+08	-2.15891+08
DGFORM	1		3.32130+07	4.70668+07	5.83311+07	6.95164+07	8.36120+07
VC	1		4.20800-01	4.74701-01	5.28725-01	5.89770-01	6.54082-01
RKTZRA	1		2.64525-01	2.59318-01	2.54543-01	2.49928-01	2.45620-01
VCRKT	1		MISSING	MISSING	MISSING	MISSING	MISSING
VB	1		1.61601-01	1.83377-01	2.05213-01	2.30311-01	2.57069-01
MUP	1		0.0	0.0	0.0	0.0	0.0
LJPAR	1	1	MISSING	MISSING	MISSING	MISSING	MISSING
		2	MISSING	MISSING	MISSING	MISSING	MISSING
STKPAR	1	1	MISSING	MISSING	MISSING	MISSING	MISSING
		2	MISSING	MISSING	MISSING	MISSING	MISSING
HULAND	1	1	1.02844+02	1.10542+02	1.18103+02	1.26388+02	1.34945+02
		2	-7.03866+03	-7.61326+03	-8.61895+03	-9.49781+03	-1.04303+04
		3	-1.89869+01	-1.99169+01	-2.08226+01	-2.18274+01	-2.28656+01

PARAMETER VALUES (CONTINUED)

		4	4.28513+02	4.50974+02	4.73387+02	4.94912+02	5.16012+02
		5	5.52556+02	5.81520+02	6.10420+02	6.38175+02	6.65384+02
DVBLNC	1		MISSING	MISSING	MISSING	MISSING	MISSING
DLWC	1		MISSING	MISSING	MISSING	MISSING	MISSING
CHI	1		MISSING	MISSING	MISSING	MISSING	MISSING
PHV0UA	1	1	MISSING	MISSING	MISSING	MISSING	MISSING
		2	MISSING	MISSING	MISSING	MISSING	MISSING
		3	MISSING	MISSING	MISSING	MISSING	MISSING
		4	MISSING	MISSING	MISSING	MISSING	MISSING
		5	MISSING	MISSING	MISSING	MISSING	MISSING
KL0UA	1	1	MISSING	MISSING	MISSING	MISSING	MISSING
		2	MISSING	MISSING	MISSING	MISSING	MISSING
		3	MISSING	MISSING	MISSING	MISSING	MISSING
		4	MISSING	MISSING	MISSING	MISSING	MISSING
		5	MISSING	MISSING	MISSING	MISSING	MISSING
PSANT	1	1	MISSING	MISSING	MISSING	MISSING	MISSING
		2	MISSING	MISSING	MISSING	MISSING	MISSING
		3	0.0	0.0	0.0	0.0	0.0
		4	0.0	0.0	0.0	0.0	0.0
		5	1.00000+03	1.00000+03	1.00000+03	1.00000+03	1.00000+03
CPSPOI	1	1	MISSING	MISSING	MISSING	MISSING	MISSING
		2	0.0	0.0	0.0	0.0	0.0
		3	0.0	0.0	0.0	0.0	0.0
		4	0.0	0.0	0.0	0.0	0.0
		5	0.0	0.0	0.0	0.0	0.0
		6	0.0	0.0	0.0	0.0	0.0
		7	1.00000+03	1.00000+03	1.00000+03	1.00000+03	1.00000+03
DHSFRM	1		MISSING	MISSING	MISSING	MISSING	MISSING
DGSFRM	1		MISSING	MISSING	MISSING	MISSING	MISSING
VSPOLY	1	1	MISSING	MISSING	MISSING	MISSING	MISSING
		2	0.0	0.0	0.0	0.0	0.0
		3	0.0	0.0	0.0	0.0	0.0
		4	0.0	0.0	0.0	0.0	0.0
		5	0.0	0.0	0.0	0.0	0.0
		6	0.0	0.0	0.0	0.0	0.0
		7	1.00000+03	1.00000+03	1.00000+03	1.00000+03	1.00000+03
KSPOLY	1	1	MISSING	MISSING	MISSING	MISSING	MISSING
		2	0.0	0.0	0.0	0.0	0.0
		3	0.0	0.0	0.0	0.0	0.0
		4	0.0	0.0	0.0	0.0	0.0
		5	0.0	0.0	0.0	0.0	0.0
		6	0.0	0.0	0.0	0.0	0.0
		7	1.00000+03	1.00000+03	1.00000+03	1.00000+03	1.00000+03
TCPR	1		MISSING	MISSING	MISSING	MISSING	MISSING
PCPR	1		MISSING	MISSING	MISSING	MISSING	MISSING
OMGPR	1		MISSING	MISSING	MISSING	MISSING	MISSING
CHARGE	1		0.0	0.0	0.0	0.0	0.0
CPAQ	1	1	MISSING	MISSING	MISSING	MISSING	MISSING
		2	MISSING	MISSING	MISSING	MISSING	MISSING
		3	0.0	0.0	0.0	0.0	0.0
		4	0.0	0.0	0.0	0.0	0.0
		5	0.0	0.0	0.0	0.0	0.0
		6	0.0	0.0	0.0	0.0	0.0
		7	0.0	0.0	0.0	0.0	0.0

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ASPEN RUN OF ASP1C.INP
PHYSICAL PROPERTIES SECTION

PARAMETER VALUES (CONTINUED)

	8	2.00000+03	2.00000+03	2.00000+03	2.00000+03	2.00000+03
	9	MISSING	MISSING	MISSING	MISSING	MISSING
	10	MISSING	MISSING	MISSING	MISSING	MISSING
	11	MISSING	MISSING	MISSING	MISSING	MISSING

PARAMETER		COMPONENTS		
NAME/SET/EL		BP475	BP525	BP575
ZC	1	2.31541-01	2.26389-01	2.21584-01
TC	1	7.05679+02	7.32003+02	7.57771+02
PC	1	1.87484+06	1.72602+06	1.59434+06
MW	1	1.94045+02	2.15354+02	2.38929+02
PLXANT	1 1	2.13775+01	2.15184+01	2.16645+01
	2	-4.30599+03	-4.57749+03	-4.85395+03
	3	-8.22118+01	-8.90415+01	-9.61547+01
	4	0.0	0.0	0.0
	5	0.0	0.0	0.0
	6	0.0	0.0	0.0
	7	0.0	0.0	0.0
	8	4.35000+02	4.85100+02	5.35100+02
	9	5.15000+02	5.65100+02	6.15100+02
TB	1	5.19261+02	5.47094+02	5.74872+02
CPIG	1 1	-1.35112+04	-1.18035+04	-9.62065+03
	2	1.05510+03	1.15351+03	1.25587+03
	3	-4.06778-01	-4.45291-01	-4.85303-01
	4	0.0	0.0	0.0
	5	0.0	0.0	0.0
	6	0.0	0.0	0.0
	7	2.55372+02	2.55372+02	2.55372+02
	8	9.22039+02	9.22039+02	9.22039+02
	9	4.76435+04	5.51411+04	6.33393+04
	10	7.11744+02	7.77648+02	8.46239+02
	11	1.00000 00	1.00000 00	1.00000 00
DHVLWT	1 1	4.61312+07	4.89642+07	5.18115+07
	2	5.19261+02	5.47094+02	5.74872+02
	3	3.80000-01	3.80000-01	3.80000-01
	4	0.0	0.0	0.0
	5	0.0	0.0	0.0
OMEGA	1	5.26364-01	5.80770-01	6.38104-01
DHFORM	1	-2.15224+08	-1.86515+08	-1.54323+08
DGFORM	1	1.03717+08	1.13526+08	1.24470+08
VC	1	7.24599-01	7.98268-01	8.75633-01
RKTZRA	1	2.41543-01	2.37756-01	2.34237-01
VCRKT	1	MISSING	MISSING	MISSING
VB	1	2.87012-01	3.18813-01	3.52886-01
MUP	1	0.0	0.0	0.0
LJPAR	1 1	MISSING	MISSING	MISSING
	2	MISSING	MISSING	MISSING
STKPAR	1 1	MISSING	MISSING	MISSING
	2	MISSING	MISSING	MISSING
MULAND	1 1	1.44142+02	1.53631+02	1.63496+02
	2	-1.14372+04	-1.25046+04	-1.36381+04
	3	-2.39896+01	-2.51467+01	-2.63509+01
	4	5.36316+02	5.56322+02	5.75906+02
	5	6.91566+02	7.17363+02	7.42615+02

PARAMETER VALUES (CONTINUED)

DVBLNC	1		MISSING	MISSING	MISSING
DLWC	1		MISSING	MISSING	MISSING
CHI	1		MISSING	MISSING	MISSING
PHVOUA	1	1	MISSING	MISSING	MISSING
		2	MISSING	MISSING	MISSING
		3	MISSING	MISSING	MISSING
		4	MISSING	MISSING	MISSING
		5	MISSING	MISSING	MISSING
KLOUA	1	1	MISSING	MISSING	MISSING
		2	MISSING	MISSING	MISSING
		3	MISSING	MISSING	MISSING
		4	MISSING	MISSING	MISSING
		5	MISSING	MISSING	MISSING
PSANT	1	1	MISSING	MISSING	MISSING
		2	MISSING	MISSING	MISSING
		3	0.0	0.0	0.0
		4	0.0	0.0	0.0
		5	1.00000+03	1.00000+03	1.00000+03
CPSPOI	1	1	MISSING	MISSING	MISSING
		2	0.0	0.0	0.0
		3	0.0	0.0	0.0
		4	0.0	0.0	0.0
		5	0.0	0.0	0.0
		6	0.0	0.0	0.0
		7	1.00000+03	1.00000+03	1.00000+03
DHSFRM	1		MISSING	MISSING	MISSING
DGSFRM	1		MISSING	MISSING	MISSING
VSPOLY	1	1	MISSING	MISSING	MISSING
		2	0.0	0.0	0.0
		3	0.0	0.0	0.0
		4	0.0	0.0	0.0
		5	0.0	0.0	0.0
		6	0.0	0.0	0.0
		7	1.00000+03	1.00000+03	1.00000+03
KSPOLY	1	1	MISSING	MISSING	MISSING
		2	0.0	0.0	0.0
		3	0.0	0.0	0.0
		4	0.0	0.0	0.0
		5	0.0	0.0	0.0
		6	0.0	0.0	0.0
		7	1.00000+03	1.00000+03	1.00000+03
TCPR	1		MISSING	MISSING	MISSING
PCPR	1		MISSING	MISSING	MISSING
OMGPR	1		MISSING	MISSING	MISSING
CHARGE	1		0.0	0.0	0.0
CPAQ	1	1	MISSING	MISSING	MISSING
		2	MISSING	MISSING	MISSING
		3	0.0	0.0	0.0
		4	0.0	0.0	0.0
		5	0.0	0.0	0.0
		6	0.0	0.0	0.0
		7	0.0	0.0	0.0
		8	2.00000+03	2.00000+03	2.00000+03
		9	MISSING	MISSING	MISSING

PARAMETER VALUES (CONTINUED)

10	MISSING	MISSING	MISSING
11	MISSING	MISSING	MISSING

CONVENTIONAL COMPONENT - BINARY PARAMETER TABLES

TABLE FOR RKTKIJ SET = 1 ELEMENT = 1

	BP225	BP275	BP324	BP374	BP424
BP225	MISSING	MISSING	MISSING	MISSING	MISSING
BP275	MISSING	MISSING	MISSING	MISSING	MISSING
BP324	MISSING	MISSING	MISSING	MISSING	MISSING
BP374	MISSING	MISSING	MISSING	MISSING	MISSING
BP424	MISSING	MISSING	MISSING	MISSING	MISSING
BP475	MISSING	MISSING	MISSING	MISSING	MISSING
BP525	MISSING	MISSING	MISSING	MISSING	MISSING
BP575	MISSING	MISSING	MISSING	MISSING	MISSING

	BP475	BP525	BP575
BP225	MISSING	MISSING	MISSING
BP275	MISSING	MISSING	MISSING
BP324	MISSING	MISSING	MISSING
BP374	MISSING	MISSING	MISSING
BP424	MISSING	MISSING	MISSING
BP475	MISSING	MISSING	MISSING
BP525	MISSING	MISSING	MISSING
BP575	MISSING	MISSING	MISSING

TABLE FOR PRKIJ SET = 1 ELEMENT = 1

	BP225	BP275	BP324	BP374	BP424
BP225	0.0	0.0	0.0	0.0	0.0
BP275	0.0	0.0	0.0	0.0	0.0
BP324	0.0	0.0	0.0	0.0	0.0
BP374	0.0	0.0	0.0	0.0	0.0
BP424	0.0	0.0	0.0	0.0	0.0
BP475	0.0	0.0	0.0	0.0	0.0
BP525	0.0	0.0	0.0	0.0	0.0
BP575	0.0	0.0	0.0	0.0	0.0

	BP475	BP525	BP575
BP225	0.0	0.0	0.0
BP275	0.0	0.0	0.0
BP324	0.0	0.0	0.0
BP374	0.0	0.0	0.0
BP424	0.0	0.0	0.0
BP475	0.0	0.0	0.0
BP525	0.0	0.0	0.0
BP575	0.0	0.0	0.0

```
ASPEN(VER D)ALLIED SIGNAL CORP - SCIENTIFIC COMPUTATION DATE:  3/14/89 PAGE  13
                              ASPEN RUN OF ASP1C.INP
                           UNIT OPERATIONS BLOCK SECTION

FLASH:2-OUTL (FLASH2):  FLA1
  INPUT STREAM(S):  S01
  OUTPUT STREAM(S): S02          S03          H01
  PROPERTY OPTION SET SYSOP4

                        *** MASS AND ENERGY BALANCE ***
                                   IN                  OUT          RELATIVE DIFF.
   CONVENTIONAL COMPONENTS (LBMOL/HR)
      BP225                      22.6000             22.6000          0.166929E-09
      BP275                      23.5000             23.5000          0.129678E-09
      BP324                      22.4000             22.4000          0.765985E-10
      BP374                      20.0000             20.0000          0.821201E-11
      BP424                      17.4000             17.4000         -0.657424E-10
      BP475                      15.8000             15.8000         -0.131278E-09
      BP525                      14.7000             14.7000         -0.178534E-09
      BP575                      13.8000             13.8000         -0.207068E-09
   TOTAL BALANCE
      MOLE(LBMOL/HR)             150.200             150.200          0.000000E+00
      MASS(LB/HR    )            24522.0             24522.0         -0.307795E-10
      ENTHALPY(BTU/HR  )      -0.100194E+08       -0.100194E+08       0.232381E-16

                             *** INPUT DATA ***
  TWO     PHASE   PV   FLASH
  PRESSURE DROP           PSIA                                      -1.0000
  VAPOR FRACTION                                                    0.50000
  MAXIMUM ITERATION NO.                                              30
  CONVERGENCE TOLERANCE                                             0.10000E-03
  LIQUID ENTRAINMENT                                                0.00000E+00
  SOLID SPLIT FRACTIONS:
  SUBSTREAM NO. =     1    MIXED SUBSTREAM, NO SOLID SPLITS.

                             *** RESULTS ***
  OUTPUT TEMPERATURE      F                                          375.19
  OUTPUT PRESSURE         PSIA                                       13.696
  HEAT DUTY               BTU/HR                                  -0.67418E+06
  VAPOR FRACTION                                                    0.50000


     V-L PHASE EQUILIBRIUM :

     COMP            F(I)            X(I)            Y(I)            K(I)
     BP225         0.15047      0.43288E-01      0.25764          5.9512
     BP275         0.15646      0.69882E-01      0.24303          3.4776
     BP324         0.14913         0.10039       0.19788          1.9711
     BP374         0.13316         0.12849       0.13782          1.0726
     BP424         0.11585         0.14834       0.83347E-01      0.56187
     BP475         0.10519         0.16412       0.46266E-01      0.28193
     BP525      0.97870E-01        0.17243       0.23310E-01      0.13520
     BP575      0.91877E-01        0.17306       0.10696E-01      0.61818E-01
```

DESCRIPTION OF STREAM CLASS HEAT

STREAM CLASS : HEAT
STREAM ATTR : HEAT

DESCRIPTION OF STREAM CLASS CONVEN

STREAM CLASS : CONVEN
SUBSTREAMS : MIXED
SUBSTRM CLASS: MIXED

H01

STREAM ID	H01
FROM :	FLA1
TO :	
CLASS:	HEAT

STREAM ATTRIBUTES:
HEAT

Q	BTU/HR	.67418+06

ASPEN(VER D)ALLIED SIGNAL CORP - SCIENTIFIC COMPUTATION DATE: 3/14/89 PAGE 16
ASPEN RUN OF ASP1C.INP
STREAM SECTION

S02 S03 S01

STREAM ID		S02	S03	S01
FROM :		FLA1	FLA1	
TO :				FLA1
CLASS:		CONVEN	CONVEN	CONVEN
SUBSTREAM: MIXED		STRUCTURE: CONVENTIONAL		
BP225	LBMOL/HR	19.3490	3.2509	22.6000
BP275	LBMOL/HR	18.2518	5.2481	23.5000
BP324	LBMOL/HR	14.8607	7.5392	22.4000
BP374	LBMOL/HR	10.3504	9.6495	20.0000
BP424	LBMOL/HR	6.2593	11.1406	17.4000
BP475	LBMOL/HR	3.4746	12.3253	15.8000
BP525	LBMOL/HR	1.7505	12.9494	14.7000
BP575	LBMOL/HR	0.8033	12.9966	13.8000
TOTAL	LBMOL/HR	75.1000	75.1000	150.2000
TEMP	F	375.1903	375.1903	400.0000
PRES	PSIA	13.6960	13.6960	14.6960
ENTHALPY	BTU/LBMOL	-.62186+05	-.80205+05	-.66707+05
VFRAC		1.0000	0.0	0.6314
LFRAC		0.0	1.0000	0.3685
ENTROPY	BTU/LBMOL-R	-164.4228	-210.8351	-182.4077
DENSITY	LBMOL/CUFT	0.0015	0.2197	0.0023
AVG MW		141.8196	184.7052	163.2624

H01

STREAM ID		H01
FROM :		FLA1
TO :		
CLASS:		HEAT

STREAM ATTRIBUTES:
HEAT

Q	BTU/HR	.67418+06

ASPEN(VER D)ALLIED SIGNAL CORP - SCIENTIFIC COMPUTATION DATE: 3/14/89 PAGE 18
ASPEN RUN OF ASP1C.INP
STREAM SECTION

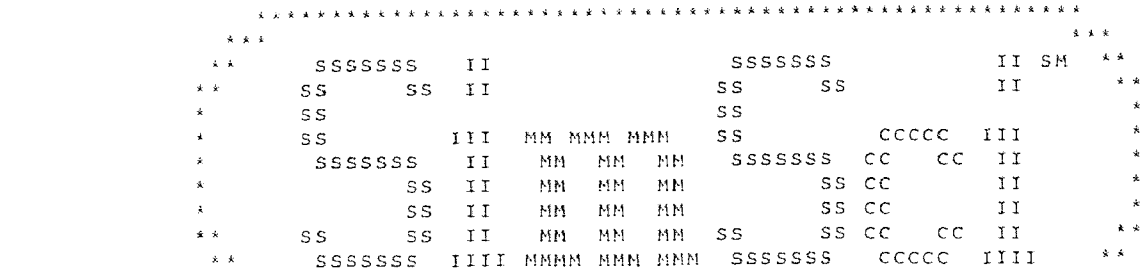
S02 S03 S01

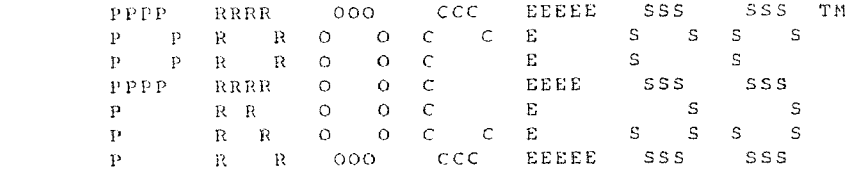
STREAM ID		S02	S03	S01
FROM :		FLA1	FLA1	
TO :				FLA1
CLASS:		CONVEN	CONVEN	CONVEN
SUBSTREAM: MIXED		STRUCTURE: CONVENTIONAL		
BP225	LB/HR	2232.8448	375.1541	2607.9989
BP275	LB/HR	2339.9559	672.8289	3012.7849
BP324	LB/HR	2109.9927	1070.4519	3180.4446
BP374	LB/HR	1630.8824	1520.4548	3151.3372
BP424	LB/HR	1093.8219	1946.8080	3040.6299
BP475	LB/HR	674.2290	2391.6768	3065.9058
BP525	LB/HR	376.9977	2788.7009	3165.6986
BP575	LB/HR	191.9322	3105.2861	3297.2183
TOTAL	LB/HR	.10651+05	.13871+05	.24522+05
TEMP	F	375.1903	375.1903	400.0000
PRES	PSIA	13.6960	13.6960	14.6960
ENTHALPY	BTU/LB	-438.4840	-434.2325	-408.5863
VFRAC		1.0000	0.0	0.6314
LFRAC		0.0	1.0000	0.3685
ENTROPY	BTU/LB-R	-1.1593	-1.1414	-1.1172
DENSITY	LB/CUFT	0.2251	40.5965	0.3846
AVG MW		141.8196	184.7052	163.2624

Figure C.7
PROCESS listing for 50/50 split
simulation using PR

```
VERSION 3.02, VAX      77                        TM
SIMULATION SCIENCES INC.                PROCESS    INPUT LISTING          PAGE    1

TITLE PROB=RUN 3C
 DESC COMPARISON PROBLEM NUMBER 3C RUN ON PROCESS
 DESC FOR STEVEN E. SUND  MS PROJECT CHECK
 DESC RUN MADE AT NJIT ON 3/89
 DESC DEW POINT CALCULATION
 DIMENSION XDENSITY=API
COMPONENT DATA
 PETROLEUM 1,BP225,,60.53,225.7/2,BP275,,55.32,275.4/*
           3,BP324,,50.12,324.9/4,BP374,,46.07,374.9/*
           5,BP424,,42.40,424.9/6,BP475,,39.44,475.0/*
           7,BP525,,36.66,525.1/8,BP575,,34.13,575.1
THERMO DATA
 METHOD SYSTEM=PR
STREAM DATA
 PROP STRM=S01,TEMPERATURE=400.0,PRESSURE=14.696,*
 COMP=22.6/23.5/22.4/20.0/17.4/15.8/14.7/13.8
UNIT OPERATION DATA
FLASH NAME=FLA1,UID=F1
  FEED S01
  PRODUCT V=S02,L=S03
  DEW   DP=1
END
```

```
 == PROCESS INDEX
       TM
PROCESS   SIMULATION PROGRAM - VERSION 3.02


       TM
PROCESS   OUTPUT DIRECTORY -                    RUN 3C
                                                14-MAR-89

INPUT PRINTOUT
GENERAL           - P.  1
COMPONENT         - P.  2          LIBRARY VERSION
THERMODYNAMIC     - P.  3
STREAM            - P.  4
UNIT    1, F1   , - P.  5
INPUT IN ORDER

UNIT    1, F1   ,      SOLVED
*** PROBLEM SOLUTION      REACHED ***

FLASH DRUMS/MIX/SPLIT SUMMARY      - P.  7
STREAM COMPONENT MOLAL  RATES      - P.  8
STREAM SUMMARY                     - P.  9

**SIMSCI ROYALTY IS     5.60 PROCESS CHARGE UNITS
```





VERSION 3.02

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		(800) 8-SIMSCI (CANADA)
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I PROBLEM AND PROCESS DESCRIPTION

1 PROBLEM DESCRIPTION

COMPARISON PROBLEM NUMBER 3C RUN ON PROCESS
FOR STEVEN E. SUND MS PROJECT CHECK
RUN MADE AT NJIT ON 3/89
DEW POINT CALCULATION

3 DIMENSIONAL UNITS - ENGLISH

TIME	- HR	WEIGHT	- LB	TEMP	- F	PRESSURE	- PSIA
ENERGY	- BTU	WORK	- HP	LIQ VOL	- CUFT	VAP VOL	- CUFT
VISC	- CP	TH COND	- BTUH	SURF TEN	- DYNE		

FORM FOR ENTERING COMPONENT LIQUID DENSITIES - API

4 TOLERANCES

PRODUCT CONVERGENCE ON COMPONENTS WITH X GT 0.0100	0.01000
TEMPERATURE	-1.000
PRESSURE	0.010
TOWER ENTHALPY BALANCES	0.00500
BUBBLE POINT RELATIONS	0.00100
COMPONENT BALANCES	0.00100
SPECIFICATIONS ON TEMPERATURE	-0.10000
PRESSURE	0.00500
STREAM RATE/PROPERTY	0.01000
PURITY/RECOVERY	0.01000
HEATER/COOLER DUTY	0.00100
OTHERS	0.00100

7 CALCULATIONAL OPTIONS

NUMBER OF TRIALS 10
COMPUTE WATER PROPERTIES ASSUMING SATURATED CONDITIONS

VERSION 3.02, VAX 77 TM
SIMULATION SCIENCES INC. PROCESS PAGE 2
PROJECT
PROBLEM RUN 3C INPUT 14-MAR-89

COMPONENT DATA LIBRARY
VERSION

II DEFINED COMPONENTS

NUMBER OF DEFINED COMPS = 8

PETROLEUM COMPONENT PROPERTIES GENERATED BY CAVETT CORRELATIONS

COMP NO	1	2	3	4
	BP225	BP275	BP324	BP374
COMP TYP	PETRO CUT	PETRO CUT	PETRO CUT	PETRO CUT
MOL WT	103.976	119.052	134.959	152.907
NBP, DEG F	225.700	275.400	324.900	374.900
STD COND.LIQ				
SP GR	0.7369	0.7574	0.7791	0.7969
DEG API	60.530	55.320	50.120	46.070
LBS/FT3	45.906	47.187	48.538	49.645
UOP K	11.9652	11.9154	11.8381	11.8150
TC, DEG F	545.059	600.239	655.611	709.087
PC, PSIA	435.131	406.196	381.216	352.802
VC,CC/G-MOLE	406.408	453.020	501.710	561.062
ZC	0.2627	0.2592	0.2560	0.2528
ACENTRIC FAC	0.353	0.398	0.438	0.477
H FORMATION	-43.068	-55.372	-70.280	-85.396
G FORMATION	0.000	0.000	0.000	0.000

COMP NO	5	6	7	8
	BP424	BP475	BP525	BP575
COMP TYP	PETRO CUT	PETRO CUT	PETRO CUT	PETRO CUT
MOL WT	172.682	194.969	219.498	246.330
NBP, DEG F	424.900	475.000	525.100	575.100
STD COND.LIQ				
SP GR	0.8137	0.8278	0.8415	0.8543
DEG API	42.400	39.440	36.660	34.130
LBS/FT3	50.692	51.570	52.423	53.223
UOP K	11.7974	11.8115	11.8234	11.8394
TC, DEG F	761.256	811.156	859.799	906.908
PC, PSIA	324.929	296.008	268.930	243.643
VC,CC/G-MOLE	628.703	709.468	800.833	904.058
ZC	0.2498	0.2467	0.2436	0.2406
ACENTRIC FAC	0.515	0.554	0.592	0.630
H FORMATION	-99.238	-92.528	-83.424	-72.752
G FORMATION	0.000	0.000	0.000	0.000

III THERMODYNAMIC AND TRANSPORT DATA

1 SUMMARY

SET 1

KVALUE	PENG-ROBINSN
** LIQUID **	
ENTHALPY	PENG-ROBINSN
ENTROPY	PENG-ROBINSN
DENSITY	API
** VAPOR **	
ENTHALPY	PENG-ROBINSN
ENTROPY	PENG-ROBINSN
DENSITY	PENG-ROBINSN

IV STREAM DATA

1 STREAM S01 , , IS OF MIXED PHASE

COMPONENT	MOLAR COMPOSITION
1 BP225	22.6000
2 BP275	23.5000
3 BP324	22.4000
4 BP374	20.0000
5 BP424	17.4000
6 BP475	15.8000
7 BP525	14.7000
8 BP575	13.8000
TOTAL RATE, LB MOLS/HR	150.2000
TEMPERATURE, DEG F	400.0000
PRESSURE, PSIA	14.6960

1 UNIT F1 , FLA1 , IS A FLASH DRUM

1 FEED STREAMS

1 STREAM S01

2 PRODUCT STREAMS

1 STREAM S02 IS OF VAPOR PHASE
2 STREAM S03 IS OF LIQUID PHASE

3 THERMO AND TRANSPORT DATA SETS USED

K-VALUES - SET 1
ENTHALPY LIQUID - SET 1 VAPOR - SET 1
DENSITY LIQUID - SET 1 VAPOR - SET 1

4 UNIT SPECIFICATIONS

1 HOLD PRESSURE DROP AT 1.000 PSIA

2 HOLD UNIT AT DEW POINT CONDITION
RELATIVE TOLERANCE IS 0.000000E+00

*** ALL INPUT DATA IN ORDER ***

**** PROBLEM SOLUTION REACHED ****

SUMMARY OF FLASH DRUMS,MIXER/SPLITTERS AND VALVES

UNIT ID	F1	
NUMBER	1	
NAME	FLA1	
TYPE	FLASH	
FEEDS	S01	
PRODUCTS	S02	(V)
	S03	(L)
TEMP, DEG F	447.8649	
PRESSURE, PSIA	13.6960	
FRACTION LIQUID	0.00000	
DUTY, MM BTU /HR	1.78057	

STREAM COMPONENT FLOW RATES - LB MOLS/HR

STREAM ID	S01	S02	S03
NAME / PHASE	MIXED	VAPOR	LIQUID
1 BP225	22.6000	22.6000	0.0134
2 BP275	23.5000	23.5000	0.0221
3 BP324	22.4000	22.4000	0.0346
4 BP374	20.0000	20.0000	0.0528
5 BP424	17.4000	17.4000	0.0811
6 BP475	15.8000	15.8000	0.1344
7 BP525	14.7000	14.7000	0.2351
8 BP575	13.8000	13.8000	0.4265
TOTALS, LB MOLS/HR	150.2000	150.2000	1.0000
TEMPERATURE, DEG F	400.0000	447.8649	447.8649
PRESSURE, PSIA	14.6960	13.6960	13.6960
H, MM BTU /HR	5.6391	7.4197	0.0423
MOLECULAR WEIGHT	159.3872	159.3872	213.6433
MOL FRAC LIQUID	0.3595	0.0000	1.0000
RECYCLE CONVERGENCE	0.0000	0.0000	0.0000

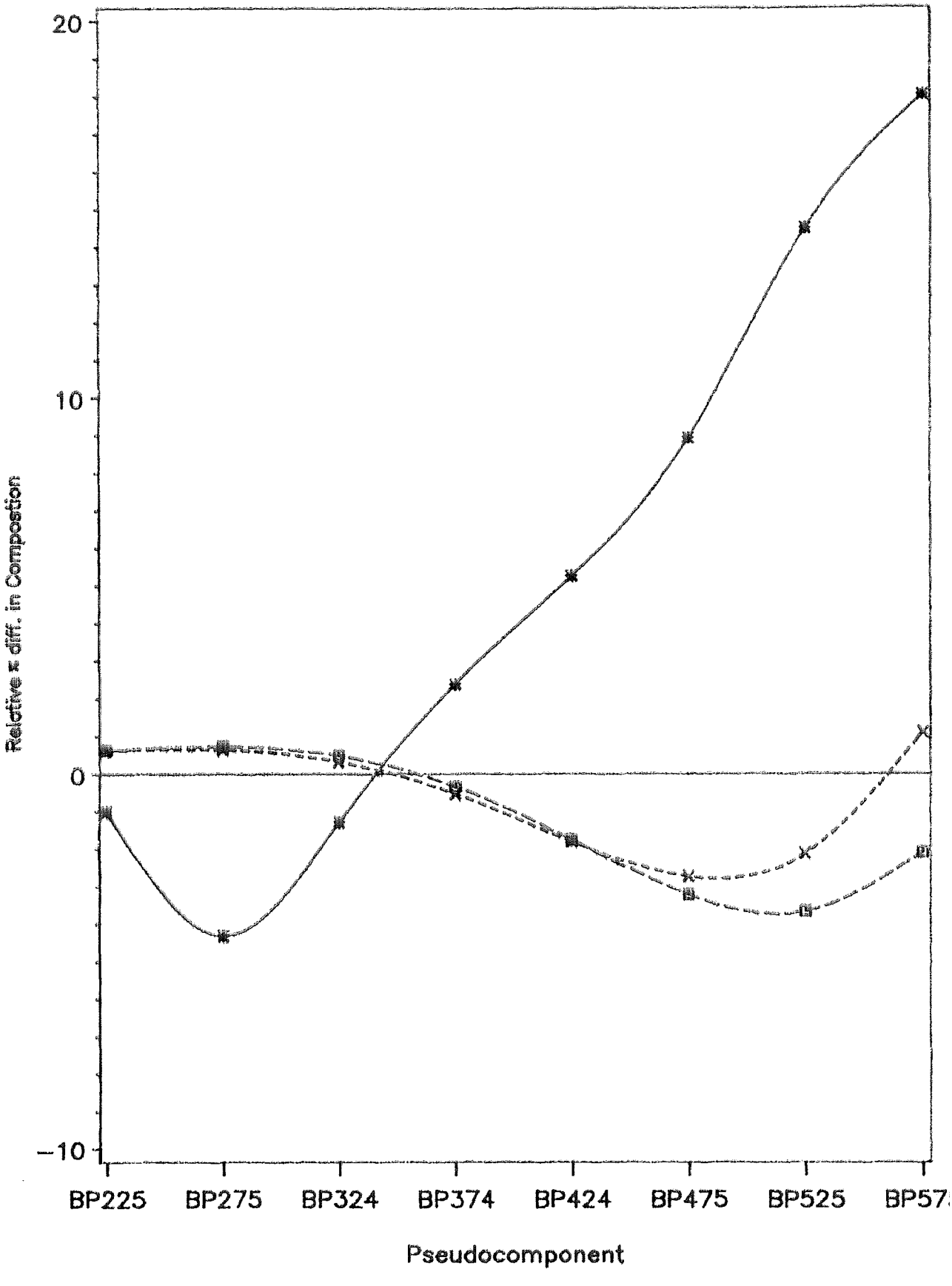
STREAM SUMMARY

STREAM ID	S01	S02	S03
NAME			
PHASE	MIXED	VAPOR	LIQUID
FROM UNIT/TRAY	0/ 0	1/ 0	1/ 0
TO UNIT/TRAY	1/ 0	0/ 0	0/ 0
LB MOLS/HR	150.200	150.200	1.000
TEMPERATURE, DEG F	400.000	447.865	447.865
PRESSURE, PSIA	14.696	13.696	13.696
H, MM BTU /HR	5.639	7.420	0.042
M BTU /LB MOLE	37.544	49.399	42.349
BTU /LB	235.552	309.929	198.221
MOL FRAC LIQUID	0.35950	0.00000	1.00000
M LBS/HR	23.940	23.940	0.214
MOLECULAR WEIGHT	159.387	159.387	213.643
STD LIQ FT3/HR	478.789	478.789	4.088
DEG API	44.804	44.804	37.168
SP GR	0.8026	0.8026	0.8389
LBS/FT3	50.0011	50.0011	52.2649
WATSON K	11.846	11.846	11.830
REDUCED TEMP (TR)	0.736	0.776	0.698
REDUCED PRES (PR)	0.042	0.039	0.049
ACENTRIC FACTOR	0.478	0.478	0.578
VAPOR			
M LBS/HR	13.541	23.940	0.000
MOLECULAR WEIGHT	140.757	159.387	0.000
STD LIQ FT3/HR	276.918	478.789	0.000
STD M FT3/HR	36.508	56.999	0.000
ACTUAL M FT3/HR	58.145	102.848	0.000
LBS/M FT3	232.889	232.770	0.000
Z	0.96283	0.96298	0.00000
CP,BTU /LB MOL F	7.6640E+01	9.0278E+01	0.0000E+00
LIQUID			
M LBS/HR	10.399	0.000	0.214
MOLECULAR WEIGHT	192.580	0.000	213.643
STD LIQ FT3/HR	201.871	0.000	4.088
ACTUAL GPM	30.0549	0.0000	0.6203
FT3/HR	241.066	0.000	4.976
LBS/FT3	43.137	0.000	42.937
Z	0.00711	0.00000	0.00700
CP,BTU /LB MOL F	1.2081E+02	0.0000E+00	1.3815E+02

STD VAPOR CONDITIONS ARE 60.0 DEG F AND 14.696 PSIA
STD VAPOR VOLUME IS 379.490 FT3/LB MOLE
NOTE: TR AND PR ARE PSEUDOCRITICALS CALCULATED VIA KAYS RULE

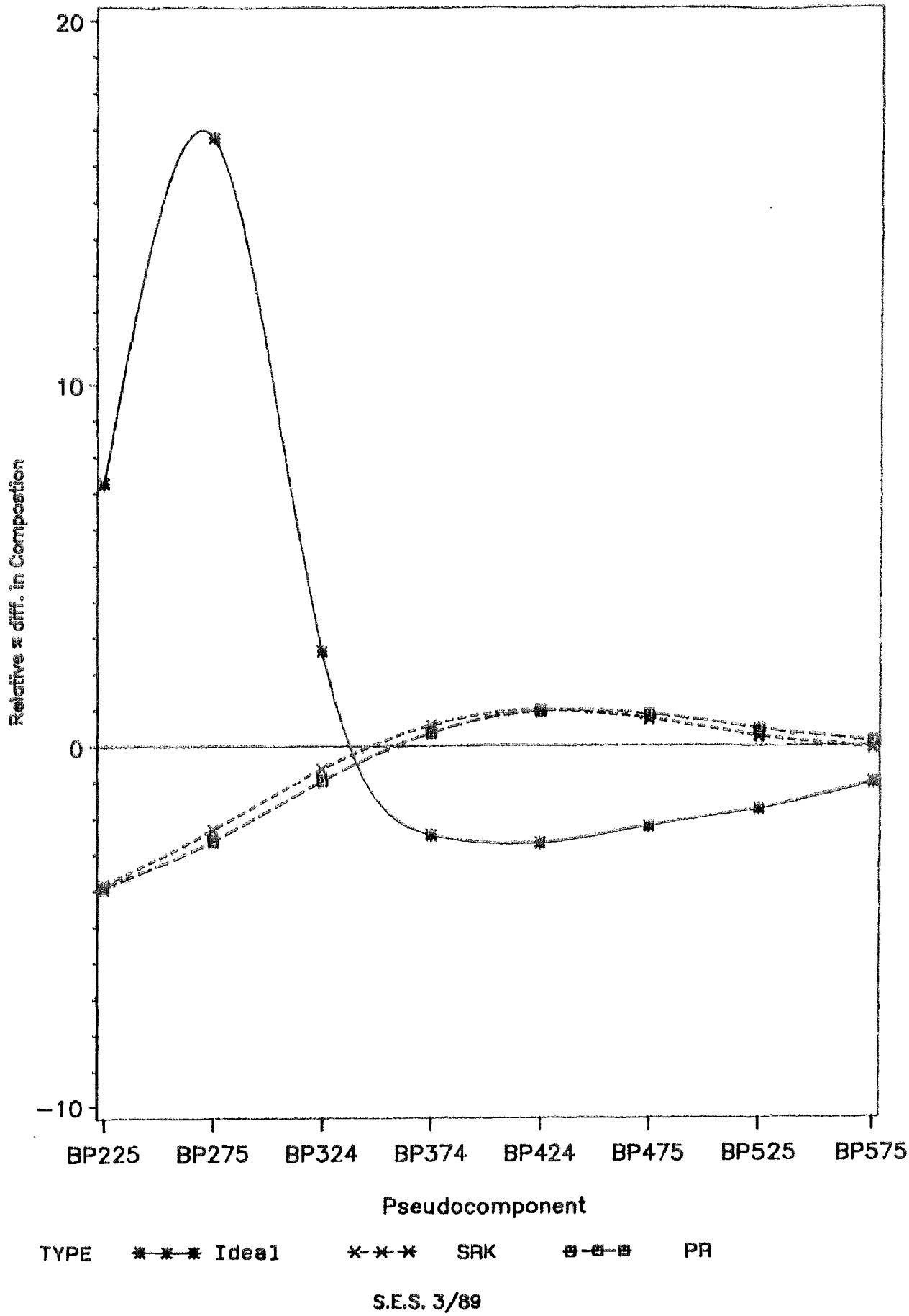
SIMSCI ROYALTY FOR THIS PROBLEM IS 5.60 PROCESS CHARGE UNITS

Figure C.8
50/50 Composition simulation result for vapor stream S02



S.E.S. 3/89

Figure C.9
50/50 Composition simulation result for liquid stream S03



APPENDIX D

ASTM standards

Pages 327-386 have been

redacted for online presentation

due to copyright concerns

Index