Spring 1989

Estimation of thermodynamic properties of petroleum fractions to supplement the ASPEN simulator

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

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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". 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 Simulator for Process Engineering) 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.

1 Joint MIT-ERDA news release on ASPEN project (Nov. 10, 1976)
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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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'.
Acknowledgments

The author acknowledges Dr. E. C. Roche Jr. for his suggestions, criticisms and encouragement throughout the course of this work.

Valuable assistance and constructive criticism were also provided by Todd Marut of Exxon Corporation.

Finally, I would like to thank Sheldon Eichenbaum and Daryl Boudreaux of Allied Signal Corporation for allowing me the use of the Corporate Technology Computational Facilities in the preparation of the program.
TABLE OF CONTENTS

Forward ........................................... ii

I. INTRODUCTION .................................. 1

II. THERMODYNAMIC MODELS OF ASPEN ............. 8
   A. Introduction .................................. 8
   B. Conventional Physical Properties .......... 9
   C. Conventional Option Sets .................. 10
   D. Universal and model specific parameters .. 12
   E. ASPEN Data banks ............................ 24

III. MODEL PARAMETER ESTIMATION ................. 27
   A. Introduction .................................. 27
   B. Molecular weight and critical properties .. 30
   B. Vapor Pressure ................................ 32
   C. Acentric Factor ............................... 36
   D. Rackett Saturated Liquid Molar Volume .... 37
   E. Solubility Parameter .......................... 38
   F. Ideal Gas Heat Capacity ..................... 40
   G. Enthalpy of Vaporization ..................... 41
   H. Cavett Enthalpy Parameter .................... 42
   I. Enthalpy and Gibbs free energy of Formation.. 44
   J. Characteristic molar volume .................. 47
   K. Normal boiling Point ......................... 48
   L. Liquid Molar volume at the normal boiling point ............. 48
   M. Radius of Gyration ............................ 49
   N. Dipole Moment ................................. 51
   O. Normal Freezing/Melting Point ............... 51
   P. Andrade Viscosity ............................. 53

IV. ESTPRO PROGRAM ............................... 56
   A. Introduction .................................. 56
   B. Basis and assumptions ....................... 56
   C. Main features ................................ 59
   D. Input ......................................... 61
   E. Program Execution ............................. 66

V. RESULTS AND DISCUSSION ....................... 67
   A. Introduction .................................. 67
   B. Simulation comparisons ....................... 67

VI. CONCLUSIONS .................................. 80

ENDNOTES ........................................ 82
# TABLE OF CONTENTS (CONT.)

**SELECTED BIBLIOGRAPHY**\[109\] 92  

**APPENDICES**\[109\] 104  
- **APPENDIX A**\[109\] 105  
- **APPENDIX B**\[109\] 135  
- **APPENDIX C**\[109\] 261  
- **APPENDIX D**\[109\] 326
LIST OF TABLES

Table 2.1  ASPEN pure component universal and unary parameters ........................................ 14
Table 2.2  Universal and unary parameters for Thermodynamic properties ............................. 15
Table 2.3  Cavett pure component vapor pressure constants .................................................. 18
Table 2.4  Cavett equation for enthalpy constants .................................................................. 22
Table 2.5  ASPEN pure component physical property data bank .............................................. 26
Table 3.1  Thermodynamic parameter summary ..................................................................... 28
Table 3.2  Riazi Daubert Correlation constants ..................................................................... 32
Table 3.3  Maxwell Bonnell Correlation constants .................................................................. 35
Table 3.4  Enthalpy and Gibbs free energy of formation constants ......................................... 46
Table 3.5  Freezing/Melting point Correlation constants .......................................................... 53
Table 3.6  Letsoo Steil model constants .................................................................................... 55
Table 4.1  ESTPRO range of application .................................................................................. 57
Table 5.1  Characterization parameters .................................................................................. 68
Table 5.2  Feed stream conditions ............................................................................................ 69
Table 5.3  Simulation temperature result summary .................................................................. 70
Table 5.4  50/50 Composition simulation result summary Ideal/LIBRARY for vapor Stream S02. ............. 71
Table 5.5  50/50 Composition simulation result summary Ideal/LIBRARY for liquid Stream S03. .......................................................... 71
Table 5.6  50/50 Composition simulation result summary SRK for vapor Stream S02. .................... 72
Table 5.7  50/50 Composition simulation result summary SRK for liquid Stream S03 ................. 72
Table 5.8  50/50 Composition simulation result summary PR for vapor Stream S02 ............... 73
Table 5.9  50/50 Composition simulation result summary PR for liquid Stream S03 .................. 73
Table 5.10 Comparison of pure pseudocomponent properties for Mole Weight. ....................... 77
Table 5.11 Comparison of pure pseudocomponent properties for Acentric factor. .................... 77
Table 5.12 Comparison of pure pseudocomponent properties for Critical pressure. ................. 78
Table 5.13 Comparison of pure pseudocomponent properties for Critical temperature .............. 78
<table>
<thead>
<tr>
<th>Table</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Table 5.14</td>
<td>Comparison of pure pseudocomponent properties for Critical volume</td>
<td>79</td>
</tr>
<tr>
<td>Table 5.15</td>
<td>Comparison of pure pseudocomponent properties for Critical compressibility factor</td>
<td>79</td>
</tr>
<tr>
<td>Table A.1</td>
<td>ASPEN pure component data bank summary for aromatic compounds</td>
<td>113</td>
</tr>
<tr>
<td>Table A.2</td>
<td>ASPEN pure component data bank summary for napthene compounds</td>
<td>114</td>
</tr>
<tr>
<td>Table A.3</td>
<td>ASPEN pure component data bank summary for paraffin compounds</td>
<td>115</td>
</tr>
<tr>
<td>Table A.4</td>
<td>Napthene pure compound properties obtained from ASPEN pure component data bank summary</td>
<td>117</td>
</tr>
<tr>
<td>Table A.5</td>
<td>Aromatic pure compound properties obtained from ASPEN pure component data bank summary</td>
<td>118</td>
</tr>
<tr>
<td>Table A.6</td>
<td>Paraffin pure compound properties obtained from ASPEN pure component data bank summary</td>
<td>119</td>
</tr>
<tr>
<td>Table A.7</td>
<td>Paraffin regression summary for enthalpy of formation constants</td>
<td>121</td>
</tr>
<tr>
<td>Table A.8</td>
<td>Napthene regression summary for enthalpy of formation constants</td>
<td>122</td>
</tr>
<tr>
<td>Table A.9</td>
<td>Aromatic regression summary for enthalpy of formation constants</td>
<td>123</td>
</tr>
<tr>
<td>Table A.10</td>
<td>Paraffin regression summary for Gibbs free energy of formation constants</td>
<td>124</td>
</tr>
<tr>
<td>Table A.11</td>
<td>Napthene regression summary for Gibbs free energy of formation constants</td>
<td>125</td>
</tr>
<tr>
<td>Table A.12</td>
<td>Aromatic regression summary for Gibbs free energy of formation constants</td>
<td>126</td>
</tr>
<tr>
<td>Table A.13</td>
<td>Paraffin regression summary for Radius of Gyration constants</td>
<td>127</td>
</tr>
<tr>
<td>Table A.14</td>
<td>Napthene regression summary for Radius of Gyration constants</td>
<td>128</td>
</tr>
<tr>
<td>Table A.15</td>
<td>Aromatic regression summary for Radius of Gyration constants</td>
<td>129</td>
</tr>
<tr>
<td>Table A.16</td>
<td>Paraffin regression summary for Freezing/Melting point constants</td>
<td>130</td>
</tr>
<tr>
<td>Table A.17</td>
<td>Napthene regression summary for Freezing/Melting point constants</td>
<td>131</td>
</tr>
<tr>
<td>Table A.18</td>
<td>Aromatic regression summary for Freezing/Melting point constants</td>
<td>132</td>
</tr>
<tr>
<td>Table A.19</td>
<td>Tia Juana Crude Assay characterization paraffin regression summary</td>
<td>133</td>
</tr>
<tr>
<td>Table A.20</td>
<td>Tia Juana Crude Assay characterization napthene regression summary</td>
<td>134</td>
</tr>
</tbody>
</table>
## LIST OF FIGURES

<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>A.1</td>
<td>Enthalpy of formation using ASPEN data bank</td>
<td>106</td>
</tr>
<tr>
<td>A.2</td>
<td>Gibbs free energy of formation using ASPEN data bank</td>
<td>107</td>
</tr>
<tr>
<td>A.3</td>
<td>Tia Juana Crude Assay % paraffins, napthenes, and aromatics</td>
<td>108</td>
</tr>
<tr>
<td>A.4</td>
<td>Correction of mean average boiling point based on TBP curve</td>
<td>109</td>
</tr>
<tr>
<td>A.5</td>
<td>Correction of cubic average boiling point based on TBP curve</td>
<td>110</td>
</tr>
<tr>
<td>A.6</td>
<td>Correction of mean average boiling point based on ASTM D86 curve</td>
<td>111</td>
</tr>
<tr>
<td>A.7</td>
<td>Correction of cubic average boiling point based on ASTM D86 curve</td>
<td>112</td>
</tr>
<tr>
<td>C.1</td>
<td>ESTPRO input data file</td>
<td>262</td>
</tr>
<tr>
<td>C.2</td>
<td>ESTPRO history output file</td>
<td>263</td>
</tr>
<tr>
<td>C.3</td>
<td>ESTPRO report output file</td>
<td>267</td>
</tr>
<tr>
<td>C.4</td>
<td>ASPEN SYSOP4 simulation input file</td>
<td>277</td>
</tr>
<tr>
<td>C.5</td>
<td>Process flow diagram</td>
<td>288</td>
</tr>
<tr>
<td>C.6</td>
<td>ASPEN report summary for 50/50 split simulation using SYSOP4</td>
<td>289</td>
</tr>
<tr>
<td>C.7</td>
<td>PROCESSTM listing for 50/50 split simulation using PR</td>
<td>310</td>
</tr>
<tr>
<td>C.8</td>
<td>50/50 composition simulation result for vapor stream S02</td>
<td>324</td>
</tr>
<tr>
<td>C.9</td>
<td>50/50 composition simulation result for liquid stream S03</td>
<td>325</td>
</tr>
</tbody>
</table>
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 as gas. Higher boiling mixtures consist of mixtures which at
normal temperatures and pressures exist largely as a liquid. 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. The higher boiling hydrocarbon mixtures consist of hundreds or possibly thousands of compounds 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, naphthene, aromatic, diolefin, and cyclic series. 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. 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.
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

\[
\text{VABP} = \sum X_{vi} T_{bi} \tag{1.1}
\]

\[
\text{MABP} = \sum X_i T_{bi} \tag{1.2}
\]

\[
\text{WABP} = \sum X_{wi} T_{bi} \tag{1.3}
\]

\[
\text{CABP} = \left( \sum X_{vi} T_{bi}^{1/3} \right)^3 \tag{1.4}
\]

\[
\text{MeABP} = \frac{\text{MABP} + \text{CABP}}{2} \tag{1.5}
\]

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.\textsuperscript{15}

Empirically determined charts have been prepared to convert from one boiling point to another.\textsuperscript{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.\textsuperscript{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

\[
\text{API} = \frac{141.5}{S_g} - 131.5
\]  \hspace{1cm} (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

\[
\text{UOPK} = \frac{T_b^{1/3}}{S_g}
\]  \hspace{1cm} (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.\textsuperscript{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.

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 phases23.
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\textsuperscript{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\textsuperscript{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\textsuperscript{26} (RK) equation of state, extended Scatchard-Hildebrand, and Chao-Seider\textsuperscript{27} models. SYSOP2 adds
the Redlich-Kwong equation of state, extended Scatchard-Hildebrand, and Grayson-Streed\textsuperscript{28} models. SYSOP3 adds the Soave modification to the Redlich-Kwong (SRK) equation of state\textsuperscript{26}. SYSOP4 adds the Peng-Robinson (PR) equation of state\textsuperscript{30}. SYSOP5 adds the Conformational Solution theory modification of the Benedict-Webb-Rubin (BWR) equation of state\textsuperscript{31}. SYSOP14 adds the ASPEN or Mathias modification of the Redlich-Kwong-Soave (ASRK) equation of state\textsuperscript{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\textsuperscript{33}, SYSOP9 the Van Laar equation\textsuperscript{34}, SYSOP10 the NRTL equation\textsuperscript{35}, and SYSOP12 the UNIQUAC equation\textsuperscript{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\textsuperscript{37} is used to model the mixture enthalpy and the Rackett equation\textsuperscript{38} is used to model the molar volume of the mixture.

The last option set, SYSOP12, adds the 1967 ASME water correlations\textsuperscript{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\textsuperscript{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.

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**

<table>
<thead>
<tr>
<th>Parameter name</th>
<th>Number Elements</th>
<th>Parameter Units</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>MW</td>
<td>1</td>
<td>Kg/Kmole</td>
<td>Molecular Wt.</td>
</tr>
<tr>
<td>TFP</td>
<td>1</td>
<td>°K</td>
<td>Normal freezing point</td>
</tr>
<tr>
<td>TB</td>
<td>1</td>
<td>°K</td>
<td>Normal Boiling point</td>
</tr>
<tr>
<td>TC</td>
<td>1</td>
<td>°K</td>
<td>Critical temperature</td>
</tr>
<tr>
<td>PC</td>
<td>1</td>
<td>Pascals</td>
<td>Critical Pressure</td>
</tr>
<tr>
<td>VC</td>
<td>1</td>
<td>M³/Kmole</td>
<td>Critical volume</td>
</tr>
<tr>
<td>ZC</td>
<td>1</td>
<td></td>
<td>Critical compressibility factor</td>
</tr>
<tr>
<td>OMEGA</td>
<td>1</td>
<td></td>
<td>Acentric Factor</td>
</tr>
<tr>
<td>RKTZRA</td>
<td>1</td>
<td>M³/Kmole</td>
<td>Rackett parameter</td>
</tr>
<tr>
<td>VB</td>
<td>1</td>
<td>M³/Kmole</td>
<td>Liquid molar volume at normal boiling point</td>
</tr>
<tr>
<td>CPIG</td>
<td>11</td>
<td>J/Kmole°K</td>
<td>Ideal gas heat capacity</td>
</tr>
<tr>
<td>DELTA</td>
<td>1</td>
<td>(J/M³)¹/²</td>
<td>Solubility parameter at T_{ref}</td>
</tr>
<tr>
<td>MUP</td>
<td>1</td>
<td>Coulomb*M</td>
<td>Dipole moment</td>
</tr>
<tr>
<td>PLXANT</td>
<td>9</td>
<td>Pascals</td>
<td>Extended Antoine vapor pressure</td>
</tr>
<tr>
<td>MULAND</td>
<td>5</td>
<td>N-Sec/M²</td>
<td>Modified Andrade model for liquid Viscosity</td>
</tr>
<tr>
<td>DHFORM</td>
<td>1</td>
<td>J/Kmole</td>
<td>Standard enthalpy of formation at T_{ref}</td>
</tr>
<tr>
<td>DGFORM</td>
<td>1</td>
<td>J/Kmole</td>
<td>Standard free energy of formation at T_{ref}</td>
</tr>
<tr>
<td>DHVLB</td>
<td>1</td>
<td>J/Kmole</td>
<td>Enthalpy of vapor-</td>
</tr>
<tr>
<td>DHVLWT</td>
<td>5</td>
<td>J/Kmole</td>
<td>Watson equation for Enthalpy of vaporization</td>
</tr>
<tr>
<td>PLCAVT</td>
<td>4</td>
<td>Pascals</td>
<td>Cavett pure component liquid vapor pressure</td>
</tr>
<tr>
<td>DHLCVT</td>
<td>1</td>
<td>J/Kmole</td>
<td>Cavett enthalpy parameter</td>
</tr>
<tr>
<td>VLCVT1</td>
<td>1</td>
<td>M³/Kmole</td>
<td>Scatchard Hildebrand Characteristic molar volume parameter</td>
</tr>
<tr>
<td>RGYR</td>
<td>1</td>
<td>M</td>
<td>Radius of gyration</td>
</tr>
</tbody>
</table>

* 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

<table>
<thead>
<tr>
<th>SYSOP name</th>
<th>Property</th>
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</thead>
<tbody>
<tr>
<td>SYSOP0</td>
<td>TC, PC, VC, ZC, DHFORM, DGFORM, PLXANT, CPIG, DHLWT, RKTZRA</td>
</tr>
<tr>
<td>SYSOP1</td>
<td>TC, PC, VC, ZC, DELTA, DHFORM, DGFORM, PLXANT, CPIG, VLCVT1, RKTZRA</td>
</tr>
<tr>
<td>SYSOP2</td>
<td>TC, PC, VC, ZC, DELTA, DHFORM, DGFORM, PLXANT, CPIG, DHLWT, RKTZRA</td>
</tr>
<tr>
<td>SYSOP3,4,5,14</td>
<td>TC, PC, OMEGA, DHFORM, DGFORM, PLXANT, CPIG</td>
</tr>
<tr>
<td>SYSOP8,9,10,11</td>
<td>TC, PC, VC, ZC, DHFORM, DGFORM, PLXANT, CPIG, RKTZRA, DHLCVT</td>
</tr>
<tr>
<td>SYSOP12</td>
<td>DHFORM, DGFORM, CPIG</td>
</tr>
</tbody>
</table>

Universal parameters are; molecular weight, critical properties, boiling points, Pitzer\textsuperscript{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 has nine available parameters (PLXANT) and is of the form

\[ \ln(P_{0L}) = C_1 + C_2 / (T + C_3) + C_4 \times T + C_5 \times \ln(T) + C_6 \times T^{C_7} \]  

(2.1)

where \( P_{0L} \) is liquid vapor pressure in Pascals and \( T \) is temperature in degrees Kelvin. Equation (2.1) is used for the range of temperatures of \( C_6 \) to \( C_9 \). Outside this range the vapor pressure is extrapolated as \( \ln(P_{0L}) \) 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 (\(P^0\)) has four available parameters (PLCAVT). The Cavett equation has two forms.

For \(T_r \geq 0.4\)

\[
\ln\left(\frac{P^0}{P_c}\right) = (1 - 1/T_r) \left[ A_1 + A_2/T_r + A_3/T_r^2 + A_4/T_r^3 \right. \\
\left. + AM \left( A_5 + A_6/T_r + A_7/T_r^2 + A_8/T_r^3 \right) \right] \\
+ \beta(A_{13} + A_{14} \times T_r) \left( T_r - 0.7 \right) \left( T_r - 1 \right) \tag{2.2}
\]

For \(T_r < 0.4\)

\[
\ln\left(\frac{P^0}{P_c}\right) = A_9 + AM \times A_{10} + (1/T_r - 2.5) \left[ A_{11} + AM \times A_{12} \right. \\
\left. + \beta(A_{13} + A_{14} \times T_r) \left( T_r - 0.7 \right) \left( T_r - 1 \right) \right] \tag{2.3}
\]

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, \(\alpha\) and \(\beta\), are the two characteristic parameters which are determined from vapor pressure data. A zero value is an acceptable default value for \(\beta\). 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 \(\ln(P^0)\) vs. \(1/T\).
Table 2.3

Cavett pure component vapor pressure constants

<table>
<thead>
<tr>
<th>Constant</th>
<th>Value</th>
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</thead>
<tbody>
<tr>
<td>$A_1$</td>
<td>8.6956145</td>
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<tr>
<td>$A_2$</td>
<td>-4.3610863</td>
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<tr>
<td>$A_3$</td>
<td>2.3312886</td>
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<tr>
<td>$A_4$</td>
<td>-0.37445964</td>
</tr>
<tr>
<td>$A_5$</td>
<td>0.41089072</td>
</tr>
<tr>
<td>$A_6$</td>
<td>-0.065391702</td>
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<tr>
<td>$A_7$</td>
<td>0.33193994</td>
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<tr>
<td>$A_8$</td>
<td>-0.080981301</td>
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<tr>
<td>$A_9$</td>
<td>-9.7687809</td>
</tr>
<tr>
<td>$A_{10}$</td>
<td>-1.5850550</td>
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<tr>
<td>$A_{11}$</td>
<td>-6.9238773</td>
</tr>
<tr>
<td>$A_{12}$</td>
<td>-1.1705661</td>
</tr>
<tr>
<td>$A_{13}$</td>
<td>4.7820604</td>
</tr>
<tr>
<td>$A_{14}$</td>
<td>-4.6670294</td>
</tr>
</tbody>
</table>

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

$$C_{p}^{IG} = C_1 + C_2 \times T + C_3 \times T^2 + C_4 \times T^3$$
$$+ C_5 \times T^4 + C_6 \times T^5$$  \hspace{1cm} (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:

$$C_{pIG} = C_9 + C_{10} \times T^{C_{11}}$$  \hspace{1cm} (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 has five parameters (DHVLWT). The five Watson parameters are: $\Delta h_{vap}^1$, $T_1$, $a$, $b$, and $T_{min}$. The Watson heat of vaporization equation is of the form:

$$\Delta h_{vap} = \Delta h_{vap}^1 \times \left( \frac{(1 - T/T_c)}{(1 - T_1/T_c)^a + b (1 - T/T_c)} \right)$$ \hspace{1cm} (2.6)$$

where $\Delta h_{vap}^1$ 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 $T_{\text{min}}$ default value is zero and the upper bound of the correlation is $T_c$.

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

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

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 equation for pure saturated liquid enthalpy departure, $\Delta h_{0L}$, has an enthalpy parameter, $Z_{\lambda}$, which is experimentally determined (DHLCVT). However, a reasonable estimate is the critical compressibility factor.
The equations used by the Cavett equation are,

for $T_r < 1$

$$\frac{\Delta h_{0L}}{T_c} = \max \left( \frac{\Delta h_{\text{sub}}}{T_c}, \frac{\Delta h_{\text{sup}}}{T_c} \right)$$ (2.8)

or for $T_r \geq 1$

$$\frac{\Delta h_{0L}}{T_c} = \Delta h_{\text{sub}} / T_c$$ (2.9)

where

$T_c$ is the critical temperature ($^\circ$K).

$T_r$ is the reduced temperature.

$$\frac{\Delta h_{\text{sub}}}{T_c} = a_1 + a_2 (1 - T_r)^{(1 - a_3 (T_r - 0.1))}$$

$$\frac{\Delta h_{\text{sup}}}{T_c} = \max (0.0, b_1 + b_2 t T_r^2 + b_3 t T_r^3 + b_4 t T_r^4 + b_5 P_r t T_r^2)$$

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

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

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

In the above equations $Z_\lambda$ is the Cavett equation enthalpy parameter and the universal parameters $B_1$ to $B_{12}$ and $b_1$ to $b_4$ are defined in Table 2.4.
Table 2.4
Cavett equation for enthalpy constants

<table>
<thead>
<tr>
<th>Constant</th>
<th>Value</th>
</tr>
</thead>
<tbody>
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<tr>
<td>$B_2$</td>
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<tr>
<td>$B_3$</td>
<td>-1613.1584</td>
</tr>
<tr>
<td>$B_4$</td>
<td>844.13728</td>
</tr>
<tr>
<td>$B_5$</td>
<td>-270.43935</td>
</tr>
<tr>
<td>$B_6$</td>
<td>4944.9795</td>
</tr>
<tr>
<td>$B_7$</td>
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</tr>
<tr>
<td>$B_8$</td>
<td>34152.878</td>
</tr>
<tr>
<td>$B_9$</td>
<td>8.9994977</td>
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<td>$B_{10}$</td>
<td>-78.472151</td>
</tr>
<tr>
<td>$B_{11}$</td>
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</tr>
<tr>
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</tr>
<tr>
<td>$b_3$</td>
<td>0.0193990</td>
</tr>
<tr>
<td>$b_4$</td>
<td>-0.0306083</td>
</tr>
<tr>
<td>$b_5$</td>
<td>-0.1688720</td>
</tr>
</tbody>
</table>
The extended Scatchard-Hildebrand model for liquid mixture activity coefficients uses one estimated parameter, the characteristic volume (VLCVT1). The extended Scatchard-Hildebrand model is given by:

\[
\ln(\gamma_i) = \frac{V_i}{RT} \sum_j \sum_k \phi_j \phi_k (A_{ji} - 0.5A_{jk}) + \Delta n(\gamma_i) \quad (2.10)
\]

where

- \(A_{ij} = (\delta_i - \delta_j)^2 + 2k_{ij} \delta_i \delta_j\)
- \(\gamma_i = \) activity coefficient of component i.
- \(V_i = \) liquid molar volume at 25 °C.
- \(\delta_i = \) solubility parameter at 25 °C.
- \(\ln(\gamma_i) = \ln(V_i/V_m) + 1 - V_i/V_m\)
- \(V_m = \) mole fraction averaged molar volume = \(\sum_j X_j V_j\)
- \(\phi_j = \) 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:

\[
V_i = V_i^* \times \left(5.7 + 3.0 \times \frac{298.15}{T_{ci}}\right) \quad (2.11)
\]

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:

\[
\ln(\eta_{0L}) = A + B/T + C \times \ln(T) \tag{2.12}
\]

where \(\eta_{0L}\) 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, \(T_1\) to \(T_h\), in which the model is applicable. There are no default values for any of the determined parameters but the \(T_{\text{min}}\) and \(T_{\text{max}}\) 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\textsuperscript{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 System (DFMS)\textsuperscript{53}. An example of the output obtained from DFMS for the ASPENPCD component water is shown in Table 2.5.
<table>
<thead>
<tr>
<th>NAME</th>
<th>SRCODE</th>
<th>REVDATE</th>
<th>NOE</th>
<th>VALUES</th>
</tr>
</thead>
<tbody>
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<td>1</td>
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<td>1</td>
<td>0.273200D+03</td>
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<td>TB</td>
<td>1</td>
<td>06/26/86</td>
<td>1</td>
<td>0.373200D+03</td>
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<tr>
<td>TC</td>
<td>1</td>
<td>06/26/86</td>
<td>1</td>
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<tr>
<td>PC</td>
<td>1</td>
<td>06/26/86</td>
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<tr>
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<td>0.558953D-01</td>
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<tr>
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<td>06/26/86</td>
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<tr>
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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

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<tr>
<th>Property Name</th>
<th>SYSOP 0</th>
<th>1</th>
<th>2</th>
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</table>

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, which is an explicit Jacobian method. It uses a term to combine the quadratic convergence of Newton Raphson near the solution and the robustness of the steepest descent method away from the solution. 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. Another use is in the calculation of model parameters such as the default Redlich-Kwong $A'$ and $B'$ mixture parameters.
The molecular weight and critical properties \( T_c \), \( P_c \), and \( V_c \) were estimated using the Riazi Daubert method. This method uses the specific gravity and boiling point of a petroleum fraction to estimate a property by

\[
\phi = A T_b^B S_g^C \tag{3.1}
\]

where \( \phi \) 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

\[
Z_c = \left( \frac{P_c \times V_c}{R \times T_c} \right) \tag{3.2}
\]

where \( R \) is the SI gas constant, which has a value of 8314.33 M³ 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°.
### Table 3.2

Riazi Daubert Correlation constants

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<th>physical property</th>
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<th>Constant B</th>
<th>Constant C</th>
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<td>0.3596</td>
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<td>$P_c$</td>
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<tr>
<td>$V_c$</td>
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<td>$\lambda$</td>
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<td>$C_p(0)$</td>
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<td>$C_p(600)$</td>
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<td>$C_p(1200)$</td>
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<td>$V$</td>
<td>7.6211E-5</td>
<td>2.1262</td>
<td>-1.8688</td>
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</table>

### B. Vapor Pressure

Various vapor pressure correlations have been proposed for use with petroleum fractions\textsuperscript{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\textsuperscript{66,67,68}. The base paraffin used is normal hexane. The Maxwell Bonnell correlation, as described in API
procedure 5A1.13, 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

$$X = \frac{T_b'/T - 0.0002867 \times T_b'}{(748.1 - 0.2145 \times T_b')}$$

(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)

$$\log(P^*) = \frac{(M_1 \times X - M_2)}{(M_3 \times X - M_4)}$$

(3.4)

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

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

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

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

(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

\[ T'_b = T_b - 2.5 \times f \times (UOPK - 12) \times \log(P^*/14.7) \]  \hspace{1cm} (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

\[ f = (T_b - 659.7)/200 \]  \hspace{1cm} (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).

\[ \ln(P^L) = C_1 + C_2 / (T + C_3) \]  \hspace{1cm} (3.8)
The Cavett vapor pressure parameters (PLCAVT) \(\alpha\) and \(\beta\) are fit to equations (2.2) and (2.3). The recommended value for \(\alpha\) is \(\omega/0.14123357\) and the recommended range for \(\beta\) is \(\pm 0.2\).

Table 3.3
Maxwell Bonell Correlation constants

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<th>Value</th>
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<td>(M_{10})</td>
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<td>36.0</td>
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<tr>
<td>(M_{12})</td>
<td>0.989679</td>
</tr>
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</table>
C. Acentric Factor

The acentric factor (OMEGA) is primarily used as a measure of complexity of a molecule. 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 as:

$$\omega = -\log(P_r) - 1.000$$  \hspace{1cm} (3.9)

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

It has been suggested that the method of Kesler Lee 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

$$\omega = -7.904 + 0.1352 \times \text{UOPK} - 0.007465 \times \text{UOPK}^2$$
$$+ 8.359 \times T_r + (1.408 - 0.01063 \times \text{UOPK}) / T_r$$  \hspace{1cm} (3.10)
For reduced temperature less than or equal to 0.8

\[
\omega = \frac{\ln(P_r) - 5.92714 + 6.09648/T_r}{15.2518 - 15.6875/T_r - 13.4721 \times \ln(T_r) + 0.43577 \times T_r^6} \tag{3.11}
\]

where

\[
UOPK = UOP \text{ characterization factor}
\]

\[
T_r = \text{reduced temperature}
\]

\[
P_r = \text{reduced vapor pressure at the boiling point}
\]

The suggested limits on the Kesler Lee correlation are that the value of \( \omega \) 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\textsuperscript{77,78,79,80,81,82,83}. The primary equation used by ASPEN is the Rackett saturated liquid molar volume model\textsuperscript{84}.

The Rackett parameter \( Z_{RA} \) is estimated by fitting data generated by the Gunn Yamada\textsuperscript{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:

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

where \( \omega \) 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 calculated 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:

\[
V_r^{(0)}(T_r) = 1.0 + 1.3(1 - T_r)^{\frac{1}{4}} \times \log(1-T_r) - 0.50879(1 - T_r) - 0.91534(1 - T_r)^2 \quad (3.14)
\]

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. Various methods have been proposed to estimate the solubility parameter.

The method selected to estimate the solubility parameter \( \delta \) is that suggested by API report 1-77 using the equation

\[
\delta = \left( \frac{E_{25}^v \rho}{\rho} \right)^{1/2}
\]

(3.15)

where

\( E_{25}^v \) = vaporization energy at 25 °C.

\( \rho \) = 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

\[
E_{25}^v = h_{25}^v - R \times T_{ref} / MW
\]

(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 and corrected to \( T_{ref} \) using the Gunn Yamada correlation. 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 \(C_p(T) = A T^B S^C\), 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).

\[
C_{p}^{IG} = C_1 + C_2 \times T + C_3 \times T^2
\]  

(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:

\[ C_{f}^{0IG} = C_{9} + C_{10} \times T \]  \hspace{1cm} (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\(^9\). 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\(^8\). 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:

\[ \frac{dP}{dT} = \frac{\Delta h_v}{(T \Delta V)} \]  \hspace{1cm} (3.19)

where \( \Delta h_v \) is the enthalpy of vaporization and \( \Delta V \) 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).

\[ \Delta h_{\text{vap}} = \Delta h_{\text{vap}}^1 \times \left( \frac{1 - T/T_c}{1 - T_1/T_c} \right)^a \]  

(3.20)

where \( \Delta h_{\text{vap}}^1 \) is the vaporization enthalpy at a the boiling point \( T_1 \), and the exponent 'a' is given the recommended value of 0.38. The value for \( T_{\text{min}} \) 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. The parameter (DHLCVT) is the Cavett equation enthalpy
parameter, $Z_\lambda$, 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\textsuperscript{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 using the appropriate polynomial form of $C_p^{0IG}$ and

\[
h^{0IG} = \Delta h_f^{0IG} + \int C_p^{0IG} \, dT
\]  
(3.21)

\[
s^{0IG} = \left( \frac{\Delta h_f^{0IG} - \Delta g_f^{0IG}}{T_{ref}} + \int \left( \frac{C_p^{0IG}}{T} \right) dT \right) \]  
(3.22)

\[
g^{0IG} = h^{0IG} - T \times s^{0IG}
\]  
(3.23)

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

$h^{0IG} =$ Ideal gas molar enthalpy

$\Delta h_f^{0IG} =$ Ideal gas standard enthalpy of formation

at $T_{ref}$ (DHFORM)

$s^{0IG} =$ Ideal gas molar entropy

$\Delta g_f^{0IG} =$ 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\textsuperscript{103,104,105,106,107} methods or correlations which are a function of reduced temperature or molecular weight\textsuperscript{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\textsuperscript{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:

$$\theta = A + B \times V_b + C \times V_b^2 + D \times V_b^3$$  \hspace{1cm} (3.24)

where $\theta$ is the property desired (DHFORM, DGFORM) and $A, B, C$ 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

<table>
<thead>
<tr>
<th>Type of Petroleum</th>
<th>Constant A</th>
<th>Constant B</th>
<th>Constant C</th>
<th>Constant D</th>
</tr>
</thead>
<tbody>
<tr>
<td>Paraffins</td>
<td>5.6803E8</td>
<td>-4.6027E6</td>
<td>9840.17</td>
<td>-8.2377</td>
</tr>
<tr>
<td>Napthenes</td>
<td>1.6169E9</td>
<td>-1.0641E7</td>
<td>21793.96</td>
<td>-15.8926</td>
</tr>
<tr>
<td>Aromatics</td>
<td>-1.1603E10</td>
<td>8.8977E9</td>
<td>-2.2301E5</td>
<td>183.32</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Type of Petroleum</th>
<th>Constant A</th>
<th>Constant B</th>
<th>Constant C</th>
<th>Constant D</th>
</tr>
</thead>
<tbody>
<tr>
<td>Paraffins</td>
<td>-3.0250E7</td>
<td>1.6932E6</td>
<td>-3258.3</td>
<td>2.619</td>
</tr>
<tr>
<td>Napthenes</td>
<td>-3.9762E9</td>
<td>-7.781E4</td>
<td>7933.6</td>
<td>-4.7579</td>
</tr>
<tr>
<td>Aromatics</td>
<td>-3.9760E9</td>
<td>3.101E7</td>
<td>-77805.4</td>
<td>64.835</td>
</tr>
</tbody>
</table>
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

\[
V_i^* = \frac{V_i}{(5.7 + 3.0 \times 298.15 / T_{ci})} \tag{3.25}
\]

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).
X. 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\textsuperscript{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\textsuperscript{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\textsuperscript{116}, the primary use is found in the characterization of the dimension, shape, and branching of a molecule. It has been shown\textsuperscript{117,118} that,

\[ RGYR \propto g \left( \frac{1^2}{6} \times n \right)^{\frac{1}{2}} \]  

(3.26)

or by collecting the constants,

\[ RGYR \propto C \times n^{p_1} \times l^{p_2} \]  

(3.27)

where \( g \) and \( C \) are constants, \( p_1 \) and \( p_2 \) 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:

\[ RGYR = A \ UOP^{B} \ MW^{C} \]  

(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

<table>
<thead>
<tr>
<th>Type of Petroleum</th>
<th>Constant A</th>
<th>Constant B</th>
<th>Constant C</th>
</tr>
</thead>
<tbody>
<tr>
<td>Paraffins</td>
<td>4.4908E-12</td>
<td>0.30375</td>
<td>0.80725</td>
</tr>
<tr>
<td>Napthenes</td>
<td>5.7662E-12</td>
<td>0.26866</td>
<td>0.76607</td>
</tr>
<tr>
<td>Aromatics</td>
<td>3.5630E-13</td>
<td>2.2211</td>
<td>0.38474</td>
</tr>
</tbody>
</table>

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, due to the lack of an adequate theory for predicting the melting point temperature or enthalpy of melting.

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 form was used to fit the freezing/melting point data found in Tables A.4 to A.6 for paraffins, napthenes, and aromatics by:

\[ \text{TFP} = A \, V_b^c \, S_g^c \]  \hspace{1cm} (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

<table>
<thead>
<tr>
<th>Type of Petroleum</th>
<th>Constant A</th>
<th>Constant B</th>
<th>Constant C</th>
</tr>
</thead>
<tbody>
<tr>
<td>Paraffins</td>
<td>3.6305E-2</td>
<td>1.4185</td>
<td>-8.5142E-2</td>
</tr>
<tr>
<td>Napthenes</td>
<td>32728.4497</td>
<td>-0.62428</td>
<td>6.6091</td>
</tr>
<tr>
<td>Aromatics</td>
<td>542.9949</td>
<td>-6.7363E-2</td>
<td>4.0803</td>
</tr>
</tbody>
</table>

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\textsuperscript{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\textsuperscript{125}. This model assumes that viscous forces are due to transfer of momentum\textsuperscript{126} and is the model most widely used to show the effect of temperature on liquid viscosity\textsuperscript{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
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:

\[ \eta^L \xi = (\eta^L \xi)^{(0)} + \omega (\eta^L \xi)^{(1)} \quad (3.30) \]

where

\[ \xi = 2.1735E6 \left( \frac{T_c^{1/5} \times P_c^{2/3}}{MW^{1/2}} \right) \]

\[ \omega = \text{Pitzer acentric factor (OMEGA)} \]

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

\[ (\eta^L \xi)^{(0)} = a_1 + a_2 \times T_r + a_3 \times T_r^2 \quad (3.31) \]
\[ (\eta^L \xi)^{(1)} = a_4 + a_5 \times T_r + a_6 \times T_r^2 \quad (3.32) \]

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

<table>
<thead>
<tr>
<th>Constant</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>a₁</td>
<td>0.015174</td>
</tr>
<tr>
<td>a₂</td>
<td>-0.02135</td>
</tr>
<tr>
<td>a₃</td>
<td>0.0075</td>
</tr>
<tr>
<td>a₄</td>
<td>0.042552</td>
</tr>
<tr>
<td>a₅</td>
<td>-0.07674</td>
</tr>
<tr>
<td>a₆</td>
<td>0.0340</td>
</tr>
</tbody>
</table>
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

<table>
<thead>
<tr>
<th>Parameter name</th>
<th>Range of application</th>
</tr>
</thead>
<tbody>
<tr>
<td>MW</td>
<td>70 to 295 °F, API 6.6 to 95</td>
</tr>
<tr>
<td>TB</td>
<td>input value</td>
</tr>
<tr>
<td>TC</td>
<td>70 to 295 °F, API 6.6 to 95</td>
</tr>
<tr>
<td>PC</td>
<td>70 to 295 °F, API 6.6 to 95</td>
</tr>
<tr>
<td>VC</td>
<td>70 to 295 °F, API 6.6 to 95</td>
</tr>
<tr>
<td>ZC</td>
<td>70 to 295 °F, API 6.6 to 95</td>
</tr>
<tr>
<td>OMEGA</td>
<td>0.4 to 1.4</td>
</tr>
<tr>
<td>RKTZRA</td>
<td>0.2 ≤ T_r ≤ 0.99</td>
</tr>
<tr>
<td>VB</td>
<td>70 to 295 °F, API 6.6 to 95</td>
</tr>
<tr>
<td>CPIG</td>
<td>70 to 295 °F, API 6.6 to 95</td>
</tr>
<tr>
<td>DELTA</td>
<td>70 to 295 °F, API 6.6 to 95</td>
</tr>
<tr>
<td>MUP</td>
<td>default value used</td>
</tr>
<tr>
<td>PLXANT</td>
<td>± 50 °R of boiling point</td>
</tr>
<tr>
<td>MULAND</td>
<td>0.76 ≤ T_r ≤ 0.98</td>
</tr>
<tr>
<td>DHVLB</td>
<td>70 to 295 °F, API 6.6 to 95</td>
</tr>
<tr>
<td>DHVLT</td>
<td>70 to 295 °F, API 6.6 to 95</td>
</tr>
<tr>
<td>PLCAT</td>
<td>± 50 °R of boiling point</td>
</tr>
<tr>
<td>DHCAT</td>
<td>default value used</td>
</tr>
<tr>
<td>VLCVT1</td>
<td>70 to 295 °F, API 6.6 to 95</td>
</tr>
<tr>
<td>RGYR</td>
<td>paraffins: 3.182-8.318 Å, napthenes: 2.850-4.367 Å, aromatics: 3.004-4.849 Å</td>
</tr>
</tbody>
</table>
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\textsuperscript{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\textsuperscript{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 SYSOPO.

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

\[
\begin{align*}
T-UNITS &= [ \text{cvalu1} ] \\
P-UNITS &= [ \text{cvalu2} ]
\end{align*}
\]

where:
- \text{cvalu1} is the temperature input unit, which must be a one character value from the set; F,R,C,K.
- \text{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\textsuperscript{131} using eight pseudocomponents. Table 5.1 summarizes the parameters used to characterize the eight pseudocomponents.

Table 5.1

<table>
<thead>
<tr>
<th>Pseudocomponent name</th>
<th>Boiling point °F</th>
<th>API gravity</th>
</tr>
</thead>
<tbody>
<tr>
<td>BP225</td>
<td>225.7</td>
<td>60.53</td>
</tr>
<tr>
<td>BP275</td>
<td>275.4</td>
<td>55.32</td>
</tr>
<tr>
<td>BP324</td>
<td>324.9</td>
<td>50.12</td>
</tr>
<tr>
<td>BP374</td>
<td>374.9</td>
<td>46.07</td>
</tr>
<tr>
<td>BP424</td>
<td>424.9</td>
<td>42.40</td>
</tr>
<tr>
<td>BP475</td>
<td>475.0</td>
<td>39.44</td>
</tr>
<tr>
<td>BP525</td>
<td>525.1</td>
<td>36.66</td>
</tr>
<tr>
<td>BP575</td>
<td>575.1</td>
<td>34.13</td>
</tr>
</tbody>
</table>

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 option 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\textsuperscript{132} and SYSOP4 uses the Peng Robinson EOS\textsuperscript{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

<table>
<thead>
<tr>
<th>Temperature: 400 °F</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure: 14.696 PSIA</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Pseudocomponent name</th>
<th>Compositions Lb. Moles/hr.</th>
</tr>
</thead>
<tbody>
<tr>
<td>BP225</td>
<td>22.6</td>
</tr>
<tr>
<td>BP275</td>
<td>23.5</td>
</tr>
<tr>
<td>BP324</td>
<td>22.4</td>
</tr>
<tr>
<td>BP374</td>
<td>20.0</td>
</tr>
<tr>
<td>BP424</td>
<td>17.4</td>
</tr>
<tr>
<td>BP475</td>
<td>15.8</td>
</tr>
<tr>
<td>BP525</td>
<td>14.7</td>
</tr>
<tr>
<td>BP575</td>
<td>13.8</td>
</tr>
<tr>
<td>Total</td>
<td>150.2</td>
</tr>
</tbody>
</table>

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 is the recommended method to obtain an ideal simulation. The SRK and PR methods 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>
<thead>
<tr>
<th>Case</th>
<th>ASPEN temp. °F</th>
<th>PROCESS™ temp. °F</th>
<th>Difference °F</th>
<th>Relative % Difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>50/50 Split</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>LIB-IDEAL</td>
<td>366.792</td>
<td>372.064</td>
<td>5.2710</td>
<td>1.417</td>
</tr>
<tr>
<td>SRK</td>
<td>375.587</td>
<td>373.953</td>
<td>1.6335</td>
<td>0.437</td>
</tr>
<tr>
<td>PR</td>
<td>375.190</td>
<td>373.918</td>
<td>1.2719</td>
<td>0.340</td>
</tr>
<tr>
<td>Bubble Pt.</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>LIB-IDEAL</td>
<td>283.721</td>
<td>307.761</td>
<td>24.0398</td>
<td>7.811</td>
</tr>
<tr>
<td>SRK</td>
<td>312.856</td>
<td>311.376</td>
<td>1.4797</td>
<td>0.475</td>
</tr>
<tr>
<td>PR</td>
<td>313.064</td>
<td>311.666</td>
<td>1.3977</td>
<td>0.448</td>
</tr>
<tr>
<td>Dew Pt.</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>LIB-IDEAL</td>
<td>452.650</td>
<td>450.262</td>
<td>-2.3885</td>
<td>-0.531</td>
</tr>
<tr>
<td>SRK</td>
<td>450.584</td>
<td>448.123</td>
<td>2.46100</td>
<td>0.549</td>
</tr>
<tr>
<td>PR</td>
<td>448.991</td>
<td>447.865</td>
<td>1.12630</td>
<td>0.251</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Name/ID</th>
<th>PROCESS™ Value</th>
<th>ASPEN Value</th>
<th>Difference</th>
<th>Relative % Difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>BP225</td>
<td>19.8596</td>
<td>20.0584</td>
<td>-0.1988</td>
<td>-1.0010</td>
</tr>
<tr>
<td>BP275</td>
<td>18.6927</td>
<td>19.4985</td>
<td>-0.8058</td>
<td>-4.3108</td>
</tr>
<tr>
<td>BP324</td>
<td>15.0166</td>
<td>15.2097</td>
<td>-0.1931</td>
<td>-1.2859</td>
</tr>
<tr>
<td>BP374</td>
<td>10.1569</td>
<td>9.9144</td>
<td>0.2425</td>
<td>2.3875</td>
</tr>
<tr>
<td>BP424</td>
<td>5.8989</td>
<td>5.5884</td>
<td>0.3105</td>
<td>5.2637</td>
</tr>
<tr>
<td>BP475</td>
<td>3.1604</td>
<td>2.8780</td>
<td>0.2824</td>
<td>8.9356</td>
</tr>
<tr>
<td>BP525</td>
<td>1.5739</td>
<td>1.3456</td>
<td>0.2283</td>
<td>14.054</td>
</tr>
<tr>
<td>BP575</td>
<td>0.7402</td>
<td>0.6067</td>
<td>0.1335</td>
<td>18.0357</td>
</tr>
<tr>
<td>TOTAL</td>
<td>75.0992</td>
<td>75.1000</td>
<td>0.0008</td>
<td>-0.0011</td>
</tr>
<tr>
<td>AVG MW</td>
<td>133.5917</td>
<td>139.8936</td>
<td>-6.3019</td>
<td>-4.7173</td>
</tr>
</tbody>
</table>

### Table 5.5

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

<table>
<thead>
<tr>
<th>Name/ID</th>
<th>PROCESS™ Value</th>
<th>ASPEN Value</th>
<th>Difference</th>
<th>Relative % Difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>BP225</td>
<td>2.7404</td>
<td>2.5415</td>
<td>0.1989</td>
<td>7.2581</td>
</tr>
<tr>
<td>BP275</td>
<td>4.8073</td>
<td>4.0014</td>
<td>0.8059</td>
<td>16.7641</td>
</tr>
<tr>
<td>BP324</td>
<td>7.3834</td>
<td>7.1902</td>
<td>0.1932</td>
<td>2.6167</td>
</tr>
<tr>
<td>BP374</td>
<td>9.8431</td>
<td>10.0855</td>
<td>-0.2424</td>
<td>-2.4626</td>
</tr>
<tr>
<td>BP424</td>
<td>11.5011</td>
<td>11.8115</td>
<td>-0.3104</td>
<td>-2.6989</td>
</tr>
<tr>
<td>BP475</td>
<td>12.6396</td>
<td>12.9220</td>
<td>-0.2824</td>
<td>-2.2342</td>
</tr>
<tr>
<td>BP525</td>
<td>13.1261</td>
<td>13.3544</td>
<td>-0.2283</td>
<td>-1.7393</td>
</tr>
<tr>
<td>BP575</td>
<td>13.0598</td>
<td>13.1932</td>
<td>-0.1334</td>
<td>-1.0215</td>
</tr>
<tr>
<td>TOTAL</td>
<td>75.1008</td>
<td>75.1000</td>
<td>0.0008</td>
<td>0.0011</td>
</tr>
<tr>
<td>AVG MW</td>
<td>185.1822</td>
<td>186.6313</td>
<td>-1.4491</td>
<td>-0.7825</td>
</tr>
</tbody>
</table>
### Table 5.6
50/50 Composition simulation result summary
SRK for vapor Stream S02

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

### Table 5.7
50/50 Composition simulation result summary
SRK for liquid Stream S03

<table>
<thead>
<tr>
<th>Name/ID</th>
<th>PROCESS™ value</th>
<th>ASPEN value</th>
<th>Difference</th>
<th>Relative % Difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>BP225</td>
<td>3.0913</td>
<td>3.2106</td>
<td>-0.1193</td>
<td>-3.8592</td>
</tr>
<tr>
<td>BP275</td>
<td>5.0721</td>
<td>5.1899</td>
<td>-0.1178</td>
<td>-2.3225</td>
</tr>
<tr>
<td>BP324</td>
<td>7.4359</td>
<td>7.4833</td>
<td>-0.0474</td>
<td>-0.6374</td>
</tr>
<tr>
<td>BP374</td>
<td>9.6783</td>
<td>9.6228</td>
<td>0.0555</td>
<td>0.5734</td>
</tr>
<tr>
<td>BP424</td>
<td>11.2693</td>
<td>11.1582</td>
<td>0.1111</td>
<td>0.9859</td>
</tr>
<tr>
<td>BP475</td>
<td>12.4682</td>
<td>12.3770</td>
<td>0.0912</td>
<td>0.7315</td>
</tr>
<tr>
<td>BP525</td>
<td>13.0457</td>
<td>13.0105</td>
<td>0.0352</td>
<td>0.2698</td>
</tr>
<tr>
<td>BP575</td>
<td>13.0391</td>
<td>13.0474</td>
<td>-0.0083</td>
<td>-0.0637</td>
</tr>
<tr>
<td>TOTAL</td>
<td>75.1000</td>
<td>75.1000</td>
<td>0.0000</td>
<td>0.0000</td>
</tr>
<tr>
<td>AVG MW</td>
<td>184.5679</td>
<td>184.8933</td>
<td>-0.3254</td>
<td>-0.1763</td>
</tr>
</tbody>
</table>
Table 5.8

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

<table>
<thead>
<tr>
<th>Name/ID</th>
<th>PROCESS Value</th>
<th>ASPEN Value</th>
<th>Difference</th>
<th>Relative % Difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>BP225</td>
<td>19.4716</td>
<td>19.3490</td>
<td>0.1226</td>
<td>0.6296</td>
</tr>
<tr>
<td>BP275</td>
<td>18.3864</td>
<td>18.2518</td>
<td>0.1348</td>
<td>0.7321</td>
</tr>
<tr>
<td>BP324</td>
<td>14.9332</td>
<td>14.8607</td>
<td>0.0725</td>
<td>0.4855</td>
</tr>
<tr>
<td>BP374</td>
<td>10.3155</td>
<td>10.3504</td>
<td>-0.0349</td>
<td>-0.3383</td>
</tr>
<tr>
<td>BP424</td>
<td>6.1513</td>
<td>6.2593</td>
<td>-0.1080</td>
<td>-1.7557</td>
</tr>
<tr>
<td>BP475</td>
<td>3.3664</td>
<td>3.4746</td>
<td>-0.1082</td>
<td>-3.2141</td>
</tr>
<tr>
<td>BP525</td>
<td>1.6887</td>
<td>1.7505</td>
<td>-0.0618</td>
<td>-3.6596</td>
</tr>
<tr>
<td>BP575</td>
<td>0.7869</td>
<td>0.8033</td>
<td>-0.0164</td>
<td>-2.0841</td>
</tr>
<tr>
<td>TOTAL</td>
<td>75.1000</td>
<td>75.1000</td>
<td>0.0000</td>
<td>0.0000</td>
</tr>
<tr>
<td>AVG MW</td>
<td>134.3444</td>
<td>141.8196</td>
<td>-7.4752</td>
<td>-5.5642</td>
</tr>
</tbody>
</table>

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\textsuperscript{136}. The dimensionless groups recommended for an equation of state are usually reduced temperature ($T/T_c$) and reduced pressure ($P/P_c$). Further semiempirical 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\textsuperscript{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)

<table>
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<th>PROCESS™ value</th>
<th>ASPEN value</th>
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<th>Relative % Difference</th>
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<td>103.976</td>
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<td>BP275</td>
<td>119.052</td>
<td>128.204</td>
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<tr>
<td>BP324</td>
<td>134.959</td>
<td>141.984</td>
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<td>-5.205</td>
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<tr>
<td>BP374</td>
<td>152.907</td>
<td>157.567</td>
<td>-4.660</td>
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<tr>
<td>BP424</td>
<td>172.682</td>
<td>174.749</td>
<td>-2.067</td>
<td>-1.197</td>
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<tr>
<td>BP475</td>
<td>194.969</td>
<td>194.045</td>
<td>0.924</td>
<td>0.474</td>
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<td>219.498</td>
<td>215.354</td>
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<td>246.330</td>
<td>238.929</td>
<td>7.401</td>
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Table 5.11
Comparison of pure pseudocomponent properties for Acentric factor

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<td>0.630</td>
<td>0.638</td>
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Table 5.12

Comparison of pure pseudocomponent properties for Critical pressure (PSIA)

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Table 5.13

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

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Table 5.14

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

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Table 5.15

Comparison of pure pseudocomponent properties for Critical compressibility factor

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<td>BP424</td>
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<td>BP475</td>
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<td>0.232</td>
<td>0.015</td>
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<td>0.244</td>
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<td>0.241</td>
<td>0.222</td>
<td>0.019</td>
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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.
ENDNOTES


74. Pedersen, K., P. Thomassen, A. Fredenslund, "Thermodynamics of Petroleum Mixtures Containing Heavy Hydrocarbons. 3. Efficient Flash Calculation Procedures"


Grayson, H.G., C. Streed, Proceedings of Sixth World


Thompson, W., Ph.D. Thesis, Department of Chemical Engineering, The Pennsylvania State University, University Park, 1966.


Willman, B., A.S. Teja, "Method for the Prediction of Pure-Component Vapor Pressures in the Range 1 kPa to
the Critical Pressure", Ind. Eng. Chem. Process

Willman, B.T., A.S. Teja, "Prediction of Dew Points of
Semicontinuous Natural Gas and Petroleum Mixtures.
1. Characterization by Use of an Effective Carbon
Number and Ideal Solution Predictions", Ind. Eng.

Willman, B., A.S. Teja, "Prediction of Dew Points of
Semicontinuous Natural Gas and Petroleum Mixtures.

Wilson, G., "Vapor-Liquid Equilibrium. XI. A New Expression
for the Excess Free Energy of Mixing", Journal of
127-130.

Wilson, G.M., R.H. Johnson, C.C. Hwang, C. Tsonopoulos,
"Volatile of Coal Liquids at High Temperatures and
1981, pp. 94-104.

Winkle, M.V., "Physical properties of Petroleum Fractions",

Winn, F.W., "Physical Properties by Nomogram", Petroleum

Woodle, R.A., "New ways to estimate characterization of lube

Yamada, T., R.D. Gunn, "Saturated liquid molar volumes, The
Rackett Equation", Journal of Chemical and engineering

Yarborough, L., "Application of a Generalized Equation of
State to Petroleum Reservoir Fluids", Paper presented
at 176th National meeting of the American Chemical

Zhou, P., "Correlation of average boiling points of
petroleum fractions with pseudocritical constants",
International Chemical Engineering, vol. 24, 1984,
pp. 731-741.

Zudkevitch, D., P.D. Krautheim, D. Gayos, "Vapor pressure of
Coal-Liquid Fractions - Data and Correlation", Fluid
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

![Graph showing Gibbs free energy of formation against boiling point for different types of hydrocarbons. The graph includes data points and trend lines for paraffin, naphthene, and aromatic compounds.](image)

**Figure Legend**
- **TYPE**
  - Paraffin
  - Naphthene
  - Aromatic
- **Trend Lines**
  - Paraffin
  - Naphthene
  - Aromatic

S.E.S. 3/89
Figure A.5
Tia Juana Crude Assay % paraffins, napthenes, & aromatics

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</table>

S.E.S. 3/89

Percent Napthene/Paraffin

Boiling point (Deg. F)

TYPE: Paraffin - Napthene
Fit Paraffin - Fit Napthene
Figure A.4
Correction of mean average boiling point
based on TBP curve

Slope of TBP curve

TYPE

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

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S.E.S. 3/89
Figure A.6
Correction of mean average boiling point based on ASTM D86 curve

Slope of ASTM D86 curve

TYPE

+ + + 200 Deg. F
*** 600 Deg. F
----- 800 Deg. F

-- 200 F fit
----- 400 F fit
----- 600 F fit
----- 800 F fit

S.E.S. 3/89
Figure A.7
Correction of cubic average boiling point based on ASTM D86 curve

S.E.S. 3/89
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*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

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Note: See Table 2.1 for definition of ASPEN pure component parameter names and units.

114
### Table A.3
ASPIN pure component data bank summary
For paraffin compounds

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<th>Component name</th>
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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

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<th>Component name</th>
<th>Alias</th>
<th>TFP</th>
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<th>DGFORM</th>
<th>RGYR</th>
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**Note:**  
TFP = normal freezing point, (deg. E)  
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**

<table>
<thead>
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<th>Component name</th>
<th>Alias</th>
<th>TFP</th>
<th>DHFORM</th>
<th>DGFORM</th>
<th>RGYR</th>
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**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)
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Note: TFP = normal freezing point, (deg. K)
DHFORM = standard Enthalpy of formation at 25 deg. C, (J/mole)
DGFORM = standard Gibbs free energy of formation at 25 deg. C, (J/mole)
RGYR = Radius of gyration (Å)
## 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) = -1460700.36.**

**A(3) = 9840.17072.**

**A(4) = -8.23774867.**

**DEG. OF FREEDOM = 47.00000.**

**R-SQUARE = 0.9798177.**

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<th>Y-CALC (DGINFORM J/KMOLE)</th>
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**AVERAGE ABSOLUTE PERCENT DEVIATION = 3.6160**

**MAXIMUM ABSOLUTE PERCENT DEVIATION = 11.8798**

**SUM OF RESIDUALS = -0.259783E-04**
Table A.8
Naphthene regression summary for enthalpy of formation constants

**TYPE OF FIT DESIRED IS Y VS X**

**FORM:** 

\[ Y = A(1) + A(2) \cdot X + A(3) \cdot X^2 + \ldots \]

A(1) = 0.16168948E+10
A(2) = -10611113.5
A(3) = 21793.9633
A(4) = -15.892512

**DEG. OF FREEDOM = 21.00000**  
**R-SQUARE = 0.9754591**

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<th>Y-CALC (DGFORM J/KMOLE)</th>
<th>% DEVIATION</th>
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**AVERAGE ABSOLUTE PERCENT DEVIATION = 5.9035**

**MAXIMUM ABSOLUTE PERCENT DEVIATION = 11.562**

**SUM OF RESIDUALS = -1.01122790E-04**
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**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) = 169327722.
A(3) = -325830675.
A(4) = 2.6193545

DEG. OF FREEDOM = 47.00000 R-SQUARE = 0.9783215

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<td>4672215.00</td>
<td>37.42161</td>
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<td>0.10056700 + 0.099592 + 0.0207</td>
<td>0.643125</td>
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<td>373.2000</td>
<td>1231840.00</td>
<td>8149523.00</td>
<td>-153.000</td>
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<tr>
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<td>0.41418500 + 0.3517802 + 0.0207</td>
<td>-8.559177</td>
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</tr>
<tr>
<td>351.4000</td>
<td>0.19292600 + 0.181332 + 0.0207</td>
<td>9.011590</td>
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</tr>
<tr>
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<td>-7.21770</td>
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</tr>
<tr>
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<td>0.50071100 + 0.528315 + 0.0207</td>
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<td>-4800000.00</td>
<td>-2761701.00</td>
<td>-2.11597</td>
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<tr>
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<tr>
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<td>314.7000</td>
<td>0.31121000 + 0.261390 + 0.0207</td>
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<td>492.1000</td>
<td>0.13732000 + 0.163756 + 0.0207</td>
<td>33.50970</td>
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<tr>
<td>413.4000</td>
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<tr>
<td>397.3000</td>
<td>0.13439600 + 0.2071147 + 0.0207</td>
<td>-50.63978</td>
<td></td>
</tr>
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</table>

AVERAGE ABSOLUTE PERCENT DEVIATION = 129.52
MAXIMUM ABSOLUTE PERCENT DEVIATION = 490.22
SUM OF RESIDUALS = -321865000E-05
Table A.11
Naphthene regression summary for Gibbs free energy of formation constants

**TYPE OF FIT DESIRED IS** Y VS X

**FORM:**
\[ Y = A(1) + A(2)X + A(3)X^2 + ... \]

\[ A(1) = 607352828. \]
\[ A(2) = -3824503.65 \]
\[ A(3) = 7933.60033 \]
\[ A(4) = -1.75792750 \]

**DEG. OF FREEDOM = 24.00000**
**R-SQUARE = 0.9748015**

<table>
<thead>
<tr>
<th>X-INPUT (TEMPERATURE K)</th>
<th>Y-INPUT (DGFORM J/KMOLE)</th>
<th>Y-CALC (DGFORM J/KMOLE)</th>
<th>% DEVIATION</th>
</tr>
</thead>
<tbody>
<tr>
<td>598.6000</td>
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<td>-2.317732</td>
</tr>
<tr>
<td>584.1000</td>
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</tr>
<tr>
<td>476.3000</td>
<td>0.7825130E+08</td>
<td>0.7145757E+08</td>
<td>0.681928</td>
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</table>

**DEVIATION**

-2.317732
-4.769577
8.661938
-10.11350
-12.62139
-10.11350
-10.11350
-10.11350
-10.11350
-10.11350
-10.11350

**AVERAGE ABSOLUTE PERCENT DEVIATION = 10.318**
**MAXIMUM ABSOLUTE PERCENT DEVIATION = 38.529**
**SUM OF RESIDUALS = 0.31292139E-05**
### Table A.12

Aromatic regression summary for Gibbs free energy of formation constants

Type of fit desired is \( Y \ versus \ X \)

**Form:** \( Y = A(1) + A(2)X + A(3)X^2 + \ldots \)

<table>
<thead>
<tr>
<th>( A(1) )</th>
<th>(-0.39761537 \times 10^{10})</th>
</tr>
</thead>
<tbody>
<tr>
<td>( A(2) )</td>
<td>31010830.9</td>
</tr>
<tr>
<td>( A(3) )</td>
<td>-77805.3565</td>
</tr>
<tr>
<td>( A(4) )</td>
<td>64.8352936</td>
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</tbody>
</table>

**Deg. of freedom = 15.00000 \quad R-square = 0.9028633**

<table>
<thead>
<tr>
<th>X-Input (Temperature K)</th>
<th>Y-Input (DGFORM J/KMOLE)</th>
<th>Y-Calc (DGFORM J/KMOLE)</th>
<th>% Deviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>449.2000</td>
<td>0.1246441E+09</td>
<td>0.1273374E+09</td>
<td>-5.069214</td>
</tr>
<tr>
<td>432.4000</td>
<td>0.1373270E+09</td>
<td>0.1373374E+09</td>
<td>0.000000</td>
</tr>
<tr>
<td>353.3000</td>
<td>0.1297490E+09</td>
<td>0.1273374E+09</td>
<td>1.791028</td>
</tr>
<tr>
<td>432.5000</td>
<td>0.1170210E+09</td>
<td>0.1289705E+09</td>
<td>-10.21144</td>
</tr>
<tr>
<td>450.3000</td>
<td>0.1329660E+09</td>
<td>0.1313648E+09</td>
<td>1.204216</td>
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<tr>
<td>425.6000</td>
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<tr>
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<td>0.2211706E+09</td>
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<tr>
<td>456.4000</td>
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<tr>
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<tr>
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<td>0.1211285E+09</td>
<td>19.73971</td>
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<tr>
<td>347.9000</td>
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<tr>
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<td>0.1220670E+09</td>
<td>0.1303269E+09</td>
<td>-6.749231</td>
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</tbody>
</table>

**Average absolute percent deviation = 5.1843**

**Maximum absolute percent deviation = 19.719**

**Sum of residuals = -1.123703E-03**
### Paraffin Regression Summary for Radius of Gyration Constants

*Form:* $\text{RGPR} = \exp(B(1)) \cdot \text{UOPK}^{B(2)} \cdot \text{MW}^{B(3)}$

<table>
<thead>
<tr>
<th>Iteration</th>
<th>Sum of Squares</th>
<th>Angle (Degrees)</th>
<th>Number of Times Ysolve Called</th>
<th>Number of Functional Evaluations</th>
<th>Lambda</th>
<th>R-Square</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>0.13963532</td>
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<td>31.0</td>
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<td>0.10000000E-07</td>
<td>0.91456633</td>
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<table>
<thead>
<tr>
<th>$B(1)$</th>
<th>$B(2)$</th>
<th>$B(3)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>-26.129</td>
<td>0.30375</td>
<td>0.80725</td>
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</table>

<table>
<thead>
<tr>
<th>Obs.</th>
<th>Y-Calc</th>
<th>Y-Actual</th>
<th>Difference</th>
<th>% Deviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.30990E-09</td>
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<td>-0.2890E-10</td>
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<tr>
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<td>6.4585</td>
</tr>
<tr>
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<tr>
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<tr>
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</tbody>
</table>

Average Absolute Percent Deviation = 1.7985
Maximum Absolute Percent Deviation = 22.795

---

**Table A.13**

Paraffin regression summary for radius of gyration constants.
Table A.14
Naphthene regression summary for
Radius of Gyration constants

Form: $\text{RGYR} = \text{EXP}(B(1)) \cdot UOPK^* \cdot B(2) \cdot MW^{B(3)}$

| 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 |

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

<table>
<thead>
<tr>
<th>Obs.</th>
<th>Y-Calc</th>
<th>Y-Actual</th>
<th>Difference</th>
<th>% Deviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.28584E-09</td>
<td>0.28500E-09</td>
<td>0.84359E-12</td>
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<tr>
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<tr>
<td>4</td>
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</tr>
<tr>
<td>5</td>
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<tr>
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<td>1.1423</td>
</tr>
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</tr>
<tr>
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</tr>
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<td>10</td>
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</tr>
<tr>
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</tr>
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</tr>
</tbody>
</table>

Average Absolute Percent Deviation = 0.7040
Maximum Absolute Percent Deviation = 2.1272
Table A.15
Aromatic regression summary for
Radius of Gyration constants

**FORM:**  
\[ \text{RGYR} = \exp(B(1)) \cdot \text{UOPK}^B(2) \cdot \text{MW}^B(3) \]

**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** = \[0.97478680\]

\[B(1) = -28.663\]

\[B(2) = 2.2211\]

\[B(3) = 0.38475\]

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**MAXIMUM ABSOLUTE PERCENT DEVIATION** = 3.7075
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

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**AVERAGE ABSOLUTE PERCENT DEVIATION** = 10.667

**MAXIMUM ABSOLUTE PERCENT DEVIATION** = 37.744
Table A.17
Naphthene regression summary for Freezing/Melting point constants

FORM: $TFP = \exp(B(1)) \cdot TBK^{B(2)} \cdot SG^{B(3)}$

| 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 | $0.21622014$ |

$B(1) = 10.396$

$B(2) = -0.63421$

$B(3) = 5.6091$

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AVERAGE ABSOLUTE PERCENT DEVIATION = 11.878
MAXIMUM ABSOLUTE PERCENT DEVIATION = 32.265
### Table A.18
Aromatic regression summary for freezing/melting point constants

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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) =  | -0.192727115E-05 |

| DEG. OF FREEDOM = 19.00000 | R-SQUARE = 0.9677219 |

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<th>X-INPUT (TEMPERATURE °F)</th>
<th>Y-INPUT (% PARAFFINS)</th>
<th>Y-CALC (% PARAFFINS)</th>
<th>% DEVIATION</th>
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| AVERAGE ABSOLUTE PERCENT DEVIATION = 2.7349 |
| MAXIMUM ABSOLUTE PERCENT DEVIATION = 8.8802 |
| SUM OF RESIDUALS = 0.1334501E-11 |
### Table A.20

Tia Juana Crude Assay characterization
regression summary for napthenes

**TYPE OF FIT DESIRED IS Y VS X**

**FORM:** \( Y = A(1) + A(2)X + A(3)X^2 + \ldots \)

| \( A(1) \) | \(-135.918371\) |
| \( A(2) \) | \( 2.11056119\) |
| \( A(3) \) | \(-0.100266584E-01\) |
| \( A(4) \) | \( 0.196502211E-04\) |
| \( A(5) \) | \(-0.139185252E-07\) |

**DEG. OF FREEDOM = 18.00000**  
**R-SQUARE = 0.9472170**

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<th>X-INPUT (TEMPERATURE °F)</th>
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<th>Y-CALC (%) NAPTHENES</th>
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**AVERAGE ABSOLUTE PERCENT DEVIATION = 6.0125**

**MAXIMUM ABSOLUTE PERCENT DEVIATION = 7.1156**

**SUM OF RESIDUALS = -7.6793906E-11**
APPENDIX B

ESTPRO program listing
PROGRAM ESTPRO

NAME OF MODULE - ESTPRO
MODULE TITLE - MAIN PROGRAM TO CALC ASPEN PROPERTIES FOR HYDROCARBON PSEUDOCOMPONENTS
PURPOSE - TO CONTROL THE CALCULATION PROCEDURE AND OBTAIN PROPERTIES OF HYDROCARBON PSEUDOCOMPONENTS
MODIFIED - 12-20-88
COPYWRITE 1989 STEVEN E. SUND

'WARNING' POSSIBLE PROBLEM
'ERROR' CONTINUE ON ERROR
'**SEVERE ERROR**' STOP ON ERROR

INTERNAL UNITS = SI

ROUTINE NAME|TYPE| DESCRIPTION
---|---|---
ANDRA(S) MOD. ANDRADE MODEL LIQ VISC
ASTMCF(S) CHARA. OF PET. FRAC BOIL PTS (ASTM)
CAP(S) CONVERT INPUT TO CAPITALS
CAYENT(S) CAVENT ENTHALPY VALUE
CAYVP(S) CAVENT VAPOR PRESSURE
CHKSOP(S) CHECK SYSSOP NUMBER AND SET CALC VECTOR
CONV(S) CONVERSION CHAR TO REAL OR INTEGER
DGFRM(S) GIBBS ENERGY OF FORMATION
DHFRM(S) ENTHALPY OF FORMATION
DIPOL(S) DIPOLE MOMENT
ESTFRA(S) ESTIMATE PAR, MAP, AND AROMATIC FRACS
EXTOK(S) EXTRACT TOKEN
FIND(S) FIND NON BLANK END OF 80 CHAR RECORD
GNYAR(S) LIQUID DENSITY CALC
GYKL(S) ACENTRIC FACTOR CALC
HVABP(S) HEAT OF VAPORIZATION AT THE BOILING POINT
INEP(F) LINEAR INTERPOLATION-EXTRAPOLATION
INIT(S) INITIALIZATION ROUTINE
INPT(S) INPUT TRANSLATOR
LMVABP(S) LIQUID MOLAR VOLUME AT BOILING PT
MAHNR(S) MAXWELL BORDELL FIT TO ANTOINE
RABG(S) MAXWELL BORDELL FIT (ONE PT)
NEED(S) CALC NEEDED VALUES FROM INPUT
NFMP(S) NORMAL FREEZING/MELTING POINT
OPENF(S) OPEN FILES
OUTF(S) OUTPUT RESULTS
PCOM(S) PRESSURE CONVERSION
PROP(S) DRIVER FOR CALCULATION OF PURE COMP PROPS
RADDYR(S) RADIUS OF GYRATION
RBCHECK(S) CHECK OF RIAZI AND DAUBERT ROUTINES
RDCPS(S) RIAZI AND DAUBERT SPEC HEAT
RIAN(S) RIAZI AND DAUBERT MOL WT
RIABP(S) RIAZI AND DAUBERT CRIT PRES
Rtoc(S) RIAZI AND DAUBERT CRIT TEMP
RIAT(S) RIAZI AND DAUBERT CRIT VOLUME
REFLV(S) BACKET LIQUID VOLUME PARAMETER CALC
SECOND(S) CALCS CPU TIME IN SECONDS (VAX DEPENDENT)
SOLPAR(S) SOLUBILITY PARAMETER
STRIP(S) RECORD TRAILING BLANK STRIPPER
TBCALC(S) NORMAL BOILING POINT CALC
TPC(S) CHARA. OF PET. FRAC. BOIL PTS (TB)
IMPLICIT REAL*8 (A-H,O-Z)
IMPLICIT INTEGER (I-N)

REAL*8 MULAND, MULREG, MABP, MEABP, MUP

PARAMETER (MNC=25)

CHARACTER*32 CNAME, FILE

MIN = INPUT LOGICAL UNIT
NOUT = OUTPUT LOGICAL UNIT (NOT USED)
NHSTRY = HISTORY LOGICAL UNIT
NREPT = REPORT LOGICAL UNIT

COMMON /10 / NIN, NOUT, NHSTRY, NREPT

COMMON /ERRC / IWARN, INERR, ISERR

FILE = FILE NAME (IE FILE.INP, FILE.REP, FILE.HIS, FILE.MIC)

COMMON /FILES / FILE

RMISS = MISSING VALUE FOR PARAMETERS

COMMON /SYS1 / RMISS

NSYSOP = DESIRED SYSOP NUMBER
NPCVEC = VECTOR OF PROPERTIES REQUIRED FOR NSYSOP

COMMON /SYS2 / NSYSOP, NPCVEC (22)

IERCAL = ERROR IN PROPS SAVE

COMMON /SYS3 / IERCAL (22)

LDBUG = CALCULATION DEBUG LEVEL (0-8)
LDBUG = REPORT DEBUG LEVEL (0-8)

COMMON /DEBUG / LDBUG, LDBUG

TREF = ASPEN REFERENCE TEMP (DEG K)
PRE = ASPEN REFERENCE PRES (PASCALS)
RGAS = GAS CONSTANT (M**3*PA/K MOLE K)

COMMON /REFS / LDBUG, LDBUG

NCOMP = NUMBER OF COMPOUNDS
CNAME = NAMES OF COMPOUNDS
ICF = CHARACTERIZE FRACTION FLAG

COMMON /NPROP1/ NCOMP, CNAME (MNC), ICF

VABP = VOLUME AVERAGE BOILING POINT (DEG K)
SLOP = SLOPE OF CHAR CURVE
CABP = CUBIC AVERAGE BOILING POINT (DEG K)
MABP = MOLAL AVERAGE BOILING POINT (DEG K)
MEABP = MEAN AVERAGE BOILING POINT (DEG K)

COMMON /NPROP2/ VARP(MNC), SLOP(MNC), CABP(MNC), MABP(MNC), MEABP(MNC)

UOPK = UOP CHARACTERIZATION FACTOR (WATSON K) MEABP'1/3 / SG
API = API GRAVITY
SG = SPECIFIC GRAVITY (60/60F)
AMW = AVERAGE MOLE WT.

COMMON /NPROP3/ UOPK(MNC), API(MNC), SG(MNC), AMW(MNC)

PP = PERCENT PARAFFINS
PM = PERCENT NAPTHENES
PA = PERCENT AROMATICS
IPF = PERCENT FLAG

COMMON /NPROP4/ PA(MNC), PM(MNC), PA(MNC), IPF

XPAR = FRACTION PARAFFINS
XNAP = FRACTION NAPTHENES
XARO = FRACTION AROMATICS

COMMON /EPROP1/ XPAR(MNC), XNAP(MNC), XARO(MNC)

NDAT = NUMBER OF DATA POINTS FOR MAXWELL BONEL
ST = LOWER TEMP FOR MAX BON.
HT = UPPER TEMP FOR MAX BON.

COMMON /EPROP2/ NDAT(MNC), ST(MNC), HT(MNC)

TC = CRITICAL TEMP (DEG K)

COMMON /CPPRO1/ TC(MNC)

PC = CRITICAL PRESSURE (PA)

COMMON /CPPRO2/ PC(MNC)

VC = CRITICAL VOLUME (M**3/KG-MOLE)

COMMON /CPPRO3/ VC(MNC)

ZC = CRITICAL COMPRESSIBILITY FACTOR

COMMON /CPPRO4/ ZC(MNC)

OMEGA = ACENTRIC FACTOR

COMMON /CPPRO5/ OMEGA(MNC)

PLXANT = EXTENDED ANTOINE VAPOR PRESSURE CONSTS. (LN(PA) VS. 0.3 K)
PLXREG = SUMMARY OF VALUES FOR REGRESSION OF PLXANT

COMMON /CPPRO6/ PLXANT(MNC), PLXREG(MNC)

CPFG = IDEAL GAS HEAT CAPACITY (J/KMOLE DEG K)

COMMON /CPPRO7/ CPFG(MNC), CPREG(MNC)

DHVLWT = WATSON EQUATION FOR HEAT OF VAPORIZATION

COMMON /CPPRO8/ DHVLWT(MNC)

MULAND = VISCOSITY BY MODIFIED ANDRADE MODEL (LOG(NOL) = A + B/T + C'LOG(T))

COMMON /CPPRO9/ MULAND(MNC), MULREG(MNC)
DHFORM = STANDARD HEAT OF FORMATION (J/KMOL)

COMMON /CPRP10/ DHFORM(MNC)

DGFORM = STANDARD FREE ENERGY OF FORMATION (J/KMOL)

COMMON /CPRP11/ DGFORM(MNC)

RKTZRA = RACKET EQUATION FOR LIQUID VOLUME

COMMON /CPRP12/ RKTZRA(MNC), RKTREG(3,MNC)

DHLCVT = CAUSETT EQUATION FOR ENTHALPY

COMMON /CPRP13/ DHLCVT(MNC)

TB = ATMOSPHERIC BOILING POINT (DEG K)

COMMON /CPRP14/ TB(MNC)

VB = LIQUID MOLAR VOLUME AT TB (M**3/KMOL)

COMMON /CPRP15/ VB(MNC)

DHVLB = HEAT OF VAPORIZATION AT TB (J/KMOL)

COMMON /CPRP16/ DHVLB(MNC)

TFP = NORMAL FREEZING/MELTING POINT (DEG K)

COMMON /CPRP17/ TFP(MNC)

DELTA = SOLUBILITY PARAM AT 25 DEG C (J/M**3)**1/2

COMMON /CPRP18/ DELTA(MNC)

MUP = DIPOLE MOMENT (COULOMB'M)

COMMON /CPRP19/ MUP(MNC)

RGYR = RADIUS OF GYRATION (M)

COMMON /CPRP20/ RGYR(MNC)

PLCAVT = CAUSETT EQUATION PARAMS

PLCREG = SUMMARY OF VALUES FOR REGRESSION OF PLCAVT

COMMON /CPRP21/ PLCAVT(MNC), PLCREG(3,MNC)

VLCVT = CHARACTERISTIC MOLAR VOLUME PARAMETER

COMMON /CPRP22/ VLCVT(MNC)

IWARN=0
INERR=0
ISERR=0

NIN= 2
NOUT= 3
NHSTRY=4
NREPT= 5

REFERENCE CONDITIONS
CPU TIME SUMMARY INFORMATION

SECO=0.0
CALL SECOND(SECO)
TSTART=SECONDS(0.0)

ASK FOR INPUT DATA FILE NAME

WRITE(*,100)
READ(*,200)FILE

CALL OPENF(1,IER1)
IF (IER1.GT.0) GOTO 5593
WRITE(*,350)
WRITE(*,360)

CALL OPENF(2,IER2)
IF(IER2.GT.0)GOTO 9999
WRITE(*,400)

CALL INPUT TRANSLATOR

CALL INPT(IER3)

WRITE(*,500)
IF(IER3.LT.0)THEN
WRITE(*,510)
ELSE IF(IER3.GT.0)THEN
WRITE(*,520)
ENDIF

OPEN PEP FILE

CALL OPENF(3,IER4)
IF(IER4.GT.0)GOTO 9999

INITIALIZE

CALL INIT(IER5)
WRITE(*,700)
IF(IER5.LT.0)THEN
WRITE(*,710)
ENDIF

BEGIN CALCULATIONS

CALL NEED(IER6)
WRITE(*,800)
IF(IER6.LT.0)THEN
WRITE(*,810)
ENDIF
WRITE(*,906)
WRITE(*,250)
WRITE(*,210)

CALC PROPS

CALL PROPS(IER7)
IF(IER7.GT.0)THEN
WRITE(*,1000)
ELSE
WRITE(*,250)
ENDIF
ENDIF
C WRITE FINAL FLAG
C CALL SECOND(TIME)
C WRITE(HISTORY,2000) NCMP,TIME,INAMP,INERR,ISERR
C FORMATS
C
100 FORMAT(2X,'Enter input data file name $ ',A15)
200 FORMAT(A15)
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,'** WARNING 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 **)
590 FORMAT(5X,'** CALCULATE NEEDED VALUES COMPLETE **)
610 FORMAT(5X,'** WARNING/ERROR IN NEEDED ROUTINE (SEE .HIS FILE) **)
900 FORMAT(5X,'** ERROR/WARNING COUNT IN ROUTINE PRODS = ',I6, '**)
1100 FORMAT(5X,'** ERROR IN ROUTINE = ',I6, ' ERROR NUMBER = ',I6, '**)
1200 FORMAT(5X,'** ALLOCATION ON VARIABLES COMPLETE **)
1300 FORMAT(5X,'** WARNING ERROR IN INIT ROUTINE (SEE .HIS FILE) **)
800 FORMAT(5X,'** CALCULATE NEEDED VALUES COMPLETE **)
900 FORMAT(5X,'** ERROR/WARNING COUNT IN ROUTINE PRODS = ',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..............................,110, **
6 T5 , ** CPU TIME ....................................... ,2X,912.6, **
7 T5 , ** NUMBER OF WARNINGS PRINTED...................... ,110, **
8 T5 , ** NUMBER OF ERRORS PRINTED ..................... ,110, **
9 T5 , ** NUMBER OF SEVERE ERRORS PRINTED............ ,110, **
T T5 , **
3 T5 , **
1 T5 , '----------------------------------------------------------
C 9999 STOP
END
C SUBROUTINE ANDRA(JC, IERR)
C
NAME OF MODULE - ANDRA
MODULE TITLE - CALCULATE MODIFIED ANDRADE MODEL PARAMETERS
PURPOSE - TO CALC PARAMETERS FOR MODIFIED ANDRADE MODEL
FOR LIQ VISCOSITY FROM
MATHEMATICAL MODIFIED - 10-19-88
VARIABLE USED-

C VARIABLE I/O TYPE SPEC DIMENSION DESCRIPTION AND RANGE
C JC I 1 - COMPONENT ARRAY ID
C IERR 0 1 - ERROR CODE
C -1 = NO IMPROVEMENT POSSIBLE IN
C THE VALUE OF PB EVEN THOUGH
C CONVERGENCE HAS NOT BEEN REACHED
C -2 = MORE UNKNOWNS THAN FUNCTIONS AND
UNIQUE SOLUTION GENERALLY IS IMPOSSIBLE.
-3 = TOTAL NUMBER OF VARIABLES TO BE
VARIED IS ZERO
-4 = CONVERGENCE CRITERION NOT BUT FLA
STILL LARGE
-5 = IC NOT A VALID NUMBER ON ENTRY
-6 = X(I) IS NOT WITHIN XMIN(I) TO
XMAX(I)
-7 = ZERO DIAGONAL ELEMENT IN EQUATION
SOLVE
-10 = TRY TO CALC. DERIVATIVE
ANALITCALLY
-11 = RUN EXCEEDED MAXIT SPECIFIED

IMPLICIT REAL*8 (A-H,O-Z)
IMPLICIT INTEGER (I-N)

REAL*8 MULAND, MULREG

PARAMETER (MNC=25)

COMMON /IO/ NIN,NOUT,NHSTRY,NREFT

COMMON /NPROP3/ UOPK(MNC),API(MNC),SG(MNC),AMW(MNC)

COMMON /CPPP02/ PC(NNC)

COMMON /CPRP02/ PC(MNC)

COMMON /CPRP05/ OMEGA(MNC)

COMMON /CPRP09/ MULAND(5,MNC), MULREG(3,MNC)

DIMENSION NDATA(26), DATA(16), OUTPUT(6)

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), BMJN(3)

CONSTANTS
OS=1.D0/6.D0
OH=1.D0/2.D0
TT=2.D0/3.D0

XI=2.17356*TC(JC)**OS / AMW(JC)**OH* PC(JC)**TT

SET UP RANGE FOR LETSOU-STEIL

TRL=0.76D0
TRH=0.98D0
TRD=(TRH-TRL)/50.D0 TR=TRL-TRD

MARQUARDT SET DEFAULTS
NUMBER OF UNKNOWNS DATA POINTS     K=3
NUMBER OF DATA POINTS
N=50

IF(LDBUG.GE.3)THEN
BEGIN=FLOAT(K-K)
ENDIF

ITER = 0
IF(MAXIT.LE.0)MAXIT=10000

SET EQUAL TO 1 FOR INITAL CALL
NOATS(1)=1
SET INPUT PARAMETER DATA

DATA(1) - FNU, FACTOR USED TO CHANGE FLA. SET INTERNALLY TO 10.0 IF ZERO ON INITIAL CALL.
DATA(2) - FLA, FACTOR USED TO COMBINE GRADIENT AND NEWTON-RAPHSON METHODS. SET INTERNALLY TO 0.01 IF ZERO ON INITIAL CALL.
DATA(3) - TAU, USED IN CONVERGENCE TEST. SET INTERNALLY TO 0.001 IF ZERO ON INITIAL CALL.
DATA(4) - EPS, USED IN CONVERGENCE TEST. SET INTERNALLY TO 0.00002 IF ZERO ON INITIAL CALL.
DATA(5) - PHMIN, WHEN PH .LT. PHMIN, PARTIAL DERIVATIVES FROM THE PREVIOUS ITERATION ARE USED INSTEAD OF COMPUTING THEM AGAIN.
DATA(6) THRU DATA(16) - VARIABLES USED INTERNALLY

DO 10 I=1,5
  DATA(I)=0.0D0
10 CONTINUE

BV = VARY VECTOR (0=HOLD PARAMETER CONST,1=ALLOW TO VARY)

DO 20 I=1,K
  BV(I)=1.0D0
20 CONTINUE

INITIAL VALUES OF PARMS

B(1)=1.0D0 B(2)=1.0D0 B(3)=0.0D0

BMIN AND MAX VALUES

BMAX(1)=2000.0D0 BMIN(1)=-2000.0D0
BMAX(2)=20000.00 BMIN(2)=-900000.D0
BMAX(3)=20000.00 BMIN(3)=-20000.D0

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

BEGIN CALC (CALC 50 POINTS TO BE FIT)

LOG(ETA)=A+B/TEMP(K) + C*LOG(TEMP(K))

UNIVERSAL FUNCTIONS FOR LETSOO-STEEL MODEL

UFO = (N XI) UFI = (N XI)

DO 40 1=1,50
  TR=TR+TRD
  UF0=0.015174D0-0.0214SDO TR+0.0075D0 TR TR
  UF1=0.042552D0-0.076743D0 TR+0.0340D0 TR TR
  Y11=LOG(UF0+UF1*OMEGA(JC))/XI
  X11=TR*TC(JC)
40 CONTINUE

IF (LDBUG.GE.7) THEN
WRITE(NHSTRY,1020)X(I),Y(I)
YSUM=YSUM+X(I)
YSUM2=YSUM2+X(I)**2
XSUM=XSUM+X(I)
YSUM=YSUM2+Y(I)
YSUM2=YSUM2+Y(I)**2
ENDIF
CONTINUE

MEANS, VARIANCES AND STANDARD DEV.

IF(LDBUG.GE.7)THEN
XMEAN=XSUM/FLOAT(N) XVAR=(FLOAT(N)*XSUM2-XSUM*XSUM)/FLOAT(N)/FLOAT(N-1)
YMEAN=YSUM/FLOAT(N) YVAR=FLOAT(N)*YSUM2-YSUM*YSUM)/FLOAT(N)/FLOAT(N-1)
ENDIF

BEGIN REGRESSION

50 ITER=ITER+1
IF(ITER.GT.MAXIT)THEN
IERR=-1
WRITE(NHSTRY,1000)ITER,NDATA,OUTPUT,J=1,5
ENDIF

EVALUATE Z VECTOR (FUNCTION VALUE)

DO 60 I=1,N
Z(I)=B(1)+B(2)/X(I)+B(3)*LOG(X(I))
CONTINUE

CALC ANALYTICAL DERIVATIVES (PI Vector)

CONTINUE

CALC DERIVATIVE

IF(NDATA.2).GT.0)THEN
IERR=-10
WRITE(NHSTRY,1090)IERR
GOTO 9000
ENDIF

CALC R-SQUARE(SAS VERSION) AND ADJ R-SQUARE

IF(NSSAS.2).EQ.0)DO THEN
RSQU=SQU/(SQU+YMEC)
ENDIF
ELSE
RSQUSAS=0.0D0
ENDIF
IF(DEGFR.EQ.0.0D0)THEN
ADJRSQU=0.0D0
ELSE
ADJRSQU=1.0D0-(1.0D0-RSQU)*(FLOAT(N)-1.0D0)/DEGFR
ENDIF
IF(ABS(RSQU-RSQUSAS).GT.1.0D8)THEN
WRITE(NHSTHY,1112)RSQU,ADJRSQU,RSQUSAS,ADJRSQUSAS
ELSE
WRITE(NHSTHY,1110)RSQU,ADJRSQU
ENDIF
C
DO 100 J=1,K
WRITE(NHSTHY,1030)J,B(J)
100 CONTINUE
C
IF(LDBUG.EQ.0)THEN
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))*100.0D0
WRITE(NHSTHY,1095)I,Z(I),Z(I)-Y(I),PERERR
110         CONTINUE
ENDIF
C  120 CALL YSOLVE (K, N, NDATA, DATA, H, BV, BMX, Y, Z, PJ, OUTPUT, P, A, AC)
C
NDATA(2) - NERST, USED FOR CONTROL IN CALLING PROG
C
IF = 0, CALCULATE FUNCTION
IF = 1, CALCULATE DERIVATIVE
IF = -1, EXAMINE HELP FOR WHAT TO DO NEXT
C
IF(NDATA(2)).EQ.0,50,10
C
NDATA(3) - LDM, MAY TAKE ON VARIOUS VALUES
C
IF POSITIVE, CONTAINS THE NUMBER OF VARIABLES DO
SATISFYING CONVERGENCE CRITERION
C
IF = 0, CONVERGENCE SATISFIED AND SOLUTION IS
IF = -1, NO UPHOLM PROGRESS POSSIBLE IN THE VALUE AT
EVEN THROUGH CONVERGENCE HAS NOT BEEN
REACHED.
C
IF = -2, MORE DISCONTINUOUS THAN FUNCTIONS AND UNIQUE
SOLUTION GENERALLY IS IMPOSSIBLE.
IF = -3, TOTAL NUMBER OF VARIABLES TO BE VARIED
IS ZERO
C
IF = -4, CONVERGENCE CRITERION NOT MET BUT STILL
C
IF = -5, IF NOT A VALID NUMBER ON ENTRY
C
IF = -6, B(I) IS NOT WITHIN BMX(I) TO BMX(I)
C
IF = -7, ZERO DIAGONAL ELEMENT IN EQUATION SOLVE
130 IF(NDATA(3)).EQ.140,110
C
FINAL STATISTICAL RESULTS
C
CONTINUE
IF(LDBUG.GE.6)THEN
WRITE(NHSTHY,1000)ITER,NDATA(3),OUTPUT(J1,J=1,5)
YMYC =0.0D0
SS =0.0D0
SSSSAS =0.0D0
DO 150 I=1,N
YMYC=YMYC+(Y(I)+Z(I)-YMEAN)**2
150        CONTINUE
$$SS = SS + (Z(I) - Y_{mean})^2$$

$$SSSAS = SSSAS + (Y(I)^2 - Y_{mean}^2)$$

CONTINUE

CALC R-SQUARE (SAS VERSION) AND ADJ R-SQUARE

RSQUAS = 1 - VARIANCE (FULL MODEL) / VARIANCE (MEAN MODEL)

RSQU = SS / (SS + YMCC)

RSQUSAS = 1 - (1 - RSQU) * (FLOAT(N) - 1) / DEGFR

ADJRSQUAS = 1 - RSQUSAS * FLOAT(N) - 1 / DEGFR

IF (ABS(RSQU - RSQUSAS) > 1.0D0) THEN

WRITE(NHSTRY, 1112) RSQU, ADJRSQU, RSQUSAS, ADJRSQUSAS

ENDIF

FINAL PARAMETERS

DO 160 J = 1, K

WRITE(NHSTRY, 1030) J, B(J)

160 CONTINUE

FINAL SUMMARY

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

LOAD DATA INTO MULAND ARRAY

IERR = NDATA(3)

DO 900 JJ = 1, 5

MULAND(JJ, JC) = 0.0D0

900 CONTINUE

IF (IERR = 0) THEN

MULAND(1, JC) = B(1)

MULAND(2, JC) = B(2)

MULAND(3, JC) = TRL * TC(JC)

WRITE(NHSTRY, 1001)

ELSE

MULAND(1, JC) = B(1)

MULAND(2, JC) = B(2)

MULAND(3, JC) = B(3)

ENDIF

ENDIF
MULAND(4,JC) = TRL * TC(JC)
MULAND(5,JC) = TRL * 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) = TRL * 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 FORMATS
1000 FORMAT(/, 1X, 'IN MODULE ANDRA', /)
   1 IX, 'ITERATION', '19, /
   2 IX, 'IERR' = ', I15,
   3 IX, 'SUM OF SQUARES' = ', G15.8,
   4 IX, 'NUMBER OF TIMES VALMOL CALLED' = ', F15.1,
   5 IX, 'NUMBER OF FUNCTIONAL EVALUATIONS' = ', F15.1,
   6 IX, 'NUMBER OF ANALYTICAL DERIVATIVE EVALUATIONS' = ', F15.1,
1001 FORMAT(/, 1X, 'NO IMPROVEMENT POSSIBLE IN THE VALUE OF', /)
1002 FORMAT(/, 1X, 'PREVIOUS TOLERANCE HAS BEEN REACHED', /)
1003 FORMAT(/, 1X, 'FALSE'. (N)'.0', 1X, 'NUMBER OF VARIABLES TO BE VALMED = ', 0, /)
1004 FORMAT(/, 1X, 'CONVERGENCE CRITERION NOT MET BUT IT IS STILL LARGE', /)
1005 FORMAT(/, 1X, 'IC NOT A VALID NUMBER ON ENTRY', /)
1006 FORMAT(/, 1X, 'X(j) IS NOT WITHIN SUBSET TO VALMOL', /)
1007 FORMAT(/, 5X, 'ZERO DIAGNOSTIC ELEMENT IN EQUATION SOLVER', /)
1008 FORMAT(/, 5X, 'X(j) * X(j) .NE. 0', 1X, 'MARQUARDT METHOD REJECTED', /)
1009 FORMAT(/, 5X, 'NUMBER OF PARAMETERS TO BE VALMED = ', I14,
   2 5X, 'NUMBER OF DATA POINTS' = ', I14,
   3 5X, 'INITIAL V-MATRIX B-NAK', 1VARY FLAG = ', I)
1010 FORMAT(/, 5X, 'VARY FLAG', /)
1011 FORMAT(/, 5X, 'VARY FLAG', /)
1012 FORMAT(/, 5X, 'VARY FLAG', /)
1013 FORMAT(/, 5X, 'VARY FLAG', /)
1014 FORMAT(/, 5X, 'VARY FLAG', /)
1015 FORMAT(/, 5X, 'VARY FLAG', /)
1016 FORMAT(/, 5X, 'VARY FLAG', /)
1017 FORMAT(/, 5X, 'VARY FLAG', /)
1018 FORMAT(/, 5X, 'VARY FLAG', /)
1019 FORMAT(/, 5X, 'VARY FLAG', /)
1020 FORMAT(/, 5X, 'VARY FLAG', /)
1021 FORMAT(/, 5X, 'VARY FLAG', /)
1022 FORMAT(/, 5X, 'VARY FLAG', /)
1023 FORMAT(/, 5X, 'VARY FLAG', /)
1024 FORMAT(/, 5X, 'VARY FLAG', /)
1025 FORMAT(/, 5X, 'VARY FLAG', /)
1026 FORMAT(/, 5X, 'VARY FLAG', /)
1027 FORMAT(/, 5X, 'VARY FLAG', /)
1028 FORMAT(/, 5X, 'VARY FLAG', /)
1029 FORMAT(/, 5X, 'VARY FLAG', /)
1030 FORMAT(/, 5X, 'VARY FLAG', /)
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1078 FORMAT(/, 5X, 'VARY FLAG', /)
1079 FORMAT(/, 5X, 'VARY FLAG', /)
1080 FORMAT(/, 5X, 'VARY FLAG', /)
1081 FORMAT(/, 5X, 'VARY FLAG', /)
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1089 FORMAT(/, 5X, 'VARY FLAG', /)
1090 FORMAT(/, 5X, 'VARY FLAG', /)
1091 FORMAT(/, 5X, 'VARY FLAG', /)
1092 FORMAT(/, 5X, 'VARY FLAG', /)
1093 FORMAT(/, 5X, 'VARY FLAG', /)
1094 FORMAT(/, 5X, 'VARY FLAG', /)
1095 FORMAT(/, 5X, 'VARY FLAG', /)
1096 FORMAT(/, 5X, 'VARY FLAG', /)
1097 FORMAT(/, 5X, 'VARY FLAG', /)
1098 FORMAT(/, 5X, 'VARY FLAG', /)
1099 FORMAT(/, 5X, 'VARY FLAG', /)
1100 FORMAT(/, 5X, 'VARY FLAG', /)
1101 FORMAT(/, 5X, 'VARY FLAG', /)
1102 FORMAT(/, 5X, 'VARY FLAG', /)
1103 FORMAT(/, 5X, 'VARY FLAG', /)
1104 FORMAT(/, 5X, 'VARY FLAG', /)
1105 FORMAT(/, 5X, 'VARY FLAG', /)
1106 FORMAT(/, 5X, 'VARY FLAG', /)
1107 FORMAT(/, 5X, 'VARY FLAG', /)
1108 FORMAT(/, 5X, 'VARY FLAG', /)
1109 FORMAT(/, 5X, 'VARY FLAG', /)
1110 FORMAT(/, 5X, 'VARY FLAG', /)

1 IX, 'R-SQUARE', 1F15.8
2 IX, 'R-SQUARE', 1F15.8
1112 FORMAT(
  1 IX, 'R-SQUARE' = ',F15.8/, \\n  2 IX, 'ADJ R-SQUARE' = ',F15.8/, \\n  3 IX, 'R-SQUARE(1-VAR.FM.MM)' = ',F15.8/, \\n  4 IX, 'ADJ R-SQUARE(1-FR2 R-SQUARE)' = ',F15.8/)
1120 FORMAT(//,10X,'STATISTICS',//, \\n  1 5X,'X-VALUES',26X,'Y-VALUES',/,, \\n  2 5X,'-------------',26X,'-----------',/,, \\n  3 5X,'MEAN = ',G15.5,8X,'MEAN', \\n  4 5X,'VARIANCE = ',G15.5,8X,'VARIANCE = ',G15.5,/, \\n  5 5X,'STD. DEV. = ',G15.5,8X,'STD. DEV. = ',G15.5,/) 
1045 FORMAT(/,1X,'IN ANDRA',/,, \\n  1 IX, 'RUN EXCEEDED MAX IT OF ',I5,' ITER = ',I5,'*********//') 
1090 FORMAT(I, 'IN MODULE ANDRA IERR = ',I5,' TRY TO CALC.'., \\n  1 I 'DERIVATIVE ANALYTICALLY, CALC. ABORTED') 
9000 CONTINUE RETURN END 
C********************************************************************************* 
C SUBROUTINE ASTMCF(VABB, SASTM, CABP, IERR) 
C********************************************************************************* 
C NAME OF MODULE - ASTMCF 
C PURPOSE - METHOD FOR CHARACTERIZE PETROLEUM FRACTION BOILING 
C POINTS OF ASTND 1 
C MODIFIED - 1-6-88 
C LIMITATIONS: 
C 
C ASTNM SLOPE 0-9.0 
C CABP 200-400 
C VARIABLES USED: 
C VARIOUS I/O TYPE SPECIFICATION DESCRIPTION AND RANGE 
C VABB 1 R - VOLUME AVERAGE BOILING POINT (DEG F) 
C SASTM 1 R - ASTM 86 10% TO 90% SLOPE (DEG F %OFF) 
C CABP 0 R - CUBIC AVERAGE BOILING POINT (DEG F) 
C MABB 0 R - BOLAL AVERAGE BOILING POINT (DEG F) 
C IERR 0 I - ERROR CODE 
C 0 = 0b 
C 1 = ASTNM NOT IN RANGE ABOVE 
C 2 = CABP NOT IN RANGE ABOVE 
C 
C IMPLICIT REAL*8(A-H, O-Z) IMPLICIT INTEGER(I-N) 
C REAL*8 MABP, MABPC 
C COMMON /IO/ ... 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 
C C CHECK IF IN RANGE 
C IF SASTM.GT.9.0.OR.SASTM.GT.0.0 THEN IERR=-1 CALL MESS(1) WRITE(NHSTRY,900) WRITE(NHSTRY,1000)SASTM 
C IF (SASTM.LT.0.0) THEN IERR=-1 CALL MESS(1) WRITE(NHSTRY,900) WRITE(NHSTRY,1000)SASTM
IF (VABP .LT. 200.00 .OR. VABP .GT. 800.00) THEN
   IERR=-2
   CALL MESS(1)
   WRITE(NHSTRY,900)
   WRITE(NHSTRY,2000)VABP
ENDIF

C CUBIC AVERAGE BOILING PT (F)
C
IF (SASTM .GT. 0.00) THEN
   CC(1)=-0.50618D0
   CC(2)=-2.9959D0
   CC(3)=0.47688D-2
   CC(4)=0.24128D-2
   CC(5)=-0.15742D0
   CC(6)=-0.4914D-5
   CC(7)=0.16337D-6
   CC(8)=-0.24640D-1

   CABPC=CC(1)
   1 + CC(2)*SASTM + CC(3)*VABP + CC(4)*SASTM**2 + 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 MOLAL AVERAGE BOILING POINT (F)
C
IF (SASTM .GT. 0.00) 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)=-0.15915D-5
   CM(7)=0.68208D-6
   CM(8)=-0.15537D0

   WABPC=CM(1)
   1 + CM(2)*SASTM + CM(3)*VABP + CM(4)*SASTM**2*VABP
   2 + CM(5)*SASTM**2 + CM(6)*VABP**2 + CM(7)*SASTM**2*VABP**2
   3 + CM(8)*SASTM**3

   WABP=VABP+WABPC
ELSE
   WABP=VABP
ENDIF

C WEIGHT AVERAGE BOILING POINT (F)
C
IF (SASTM .GT. 0.00) THEN
   CW(1)=0.21102D6
   CW(2)=2.83016D0
   CW(3)=0.11291D-2
   CW(4)=0.24739D-2
   CW(5)=0.42851D-1
   CW(6)=0.1497D-5
   CW(7)=0.63621D-7
   CW(8)=0.22497D-1

   WABPC=CW(1)
   1 + CW(2)*SASTM + CW(3)*VABP + CW(4)*SASTM**2 + 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
  WARP=WARP
ENDIF

* FORMATS *

900 FORMAT('IN MODULE ASTMCF')
1000 FORMAT('ASTM SLOPE VALUE IS NOT IN RANGE 0-9.0',/,
  1 IX,'ASTM SLOPE-VALUE = ',G12.6,',' CALC. CONTINUES')
2000 FORMAT('VABP VALUE IS NOT IN RANGE 200-800',/,
  1 IX,'VABP-VALUE = ',G12.6,',' CALC. CONTINUES')

RETURN

END

SUBROUTINE CAPS(INCASE,UPCASE)

NAME OF MODULE - CAPS
MODULE TITLE - INPUT TRANSLATOR FILTER
PURPOSE - TO CONVERT ONE INPUT CHARACTER TO VALID OUTPUT CHARACTER
MODIFIED - 3-25-88

VARIABLES USED -

VARIABLE I/O TYPE SPEC DIMENSION DESCRIPTION AND RANGE
INCASE I  C  -  INPUT CHARACTER
UPCASE O  C  -  OUTPUT CHARACTER

CHARACTER*1 INCASE,UPCASE,ABLANK
PARAMETER (ABLANK = ' ')

CONVERT LOWERCASE LETTERS TO UPPERCASE LETTERS

IF(ICHAR(INCASE).GE.97.AND.
  1 ICHAR(INCASE).LE.122)THEN
  UPCASE=CHAR(ICHAR(INCASE)-32)

CHECK FOR UPPERCASE LETTERS

ELSE IF(ICHAR(INCASE).GE.65.AND.
  1 ICHAR(INCASE).LE.90)THEN
  UPCASE=INCASE

CHECK FOR NUMBERS

ELSE IF(ICHAR(INCASE).GE.48 .AND.
  1 ICHAR(INCASE).LE.57 )THEN
  UPCASE=INCASE

CHECK FOR $, @, - , _ , & , ; , , 

ELSE IF(ICHAR(INCASE).EQ.64) .OR.
  1 ICHAR(INCASE).EQ.44 .OR.
  2 ICHAR(INCASE).EQ.45 .OR.
  3 ICHAR(INCASE).EQ.36 .OR.
  3 ICHAR(INCASE).EQ.46 .OR.
  4 ICHAR(INCASE).EQ.99 )THEN
  UPCASE=INCASE

ELSE
  UPCASE=A BLANK
ENDIF
SUBROUTINE CAVENT(JC, IERR)

NAME OF MODULE - CAVENT

MODULE TITLE - CAVENT EQUATION FOR ENTHALPY

PURPOSE - TO SUPPLY DEFAULT VALUE FOR CAVENT ENTHALPY PARAMETER

MODIFIED - 16-5-88

METHOD - DEFAULT VALUE

VARIABLES USED-

J C 1 1  - COMPONENT ARRAY ID
I ERR 0 1  - ERROR CODE

IMPLICIT REAL*8 (A-H, O-Z)
IMPLICIT INTEGER (I-N)

PARAMETER (MHC=25)

COMMON /IO/ MIN, MOUT, MTHY, MHEPT
COMMON /DEBUG/ LDEBUG, LDEBUG

COMMON /CPP104/ ZC(MHC)
COMMON /CPP111/ DHLCVT(MHC)

I ERR=0

USES DEFAULT SUGGESTED IN ASPEN

DHLCVT(JC)=ZC(JC)

FORMATS

RETURN

END

SUBROUTINE CAVP(JC, ICALC, IERR)

NAME OF MODULE - CAVP

MODULE TITLE - CAVENT EQUATION FOR VAPOR PRESSURE

PURPOSE - TO CALCULATE CHARACTERISTIC PARAMETERS AND TEMP RANGE

FOR CAVENT EQUATION FREE COMP. LIQ VAPOR PRESSURE

MODIFIED - 16-27-88

METHOD - UNIQUAT REGRESSION

VARIABLES USED-

J C 1 1  - COMPONENT ARRAY ID
ICALC 1 1  - CALC TYPE
0 = FIT 1 CONST
1 = FIT 2 CONST.
I ERR 0 1  - ERROR CODE
0 = OK
-1 = NO IMPROVEMENT POSSIBLE IN THE VALUE OF PH EVEN THOUGH
CONVERGENCE HAS NOT BEEN REACHED.
-2 = MORE UNKNOWNS THAN FUNCTIONS AND
UNIQUE SOLUTION GENERALLY IS
IMPOSSIBLE.
-3 = TOTAL NUMBER OF VARIABLES TO BE
VARIED IS ZERO
-4 = CONVERGENCE CRITERION NOT BUT PLA
STILL LARGE
-5 = IC NOT A VALID NUMBER ON ENTRY
-6 = XI1 IS NOT WITHIN XMIN(I1) TO
XMAX(I1)
-7 = ZERO DIAGONAL ELEMENT IN EQUATION
SOLVE
-10 = TRY TO CALC. DERIVATIVE
ANALYTICALLY
-11 = RUN EXCEEDED MAXIT SPECIFIED

IMPLICIT REAL*8 (A-H,O-Z)
IMPLICIT INTEGER (I-N)

PARAMETER (MNC=25)

COMMON /IO / NIN,NOUT,HISTORY,NREPT
COMMON /DEBUG / LDBG,LDBGH

COMMON /CPRD01/ TC(MNC)
COMMON /CPRD02/ PC(MNC)
COMMON /CPRD05/ OMEGA(MNC)
COMMON /CPRD06/ PLXANT(0,MNC),PLXREG(3,MNC)
COMMON /CPRD21/ PLCAVT1,MNC,PLCREG(3,MNC)

DIMENSION NDATA(261),DATA(16),OUTPUT(6)

DIMENSION X(50),Y(50),XMAX(50),XMIN(50),Y(50),
Z(100),V(50),P(120),A(15),AT(15)

DIMENSION RL(1),Ri(1),RMAX(2),RMIN(2)

DIMENSION AS(111)

DATA AS / 8.695x1500.1341088320.231288400.1341088320.2312884000.
-0.1745156440.0110820720.0.0651917200.0.0651917200.0.
0.3333333330.0.0309850100.0.76870900.0.
1.585655000.0.923877300.0.1130556100.0.
4.782064100.0.1867329400.0 /

ITER=0

IF (LDBG.GT.0) WRITE(HISTORY,900)

MARQUARDT SET DEFAULTS

NUMBER OF VARIABLES
K=2

NUMBER OF DATA POINTS
N=50

IF (LDBG.GE.5) THEN
DGOF=FLOAT(N-K)
ENDIF

ITER = 0
IF (MAXIT.LE.0) MAXIT=10000

SET EQUAL TO 1 FOR INITIAL CALL
NDATA(1)=1

SET INPUT PARAMETER DATA
DATA(1) - FNU, FACTOR USED TO CHANGE FLA. SET INTERNALLY TO 10.0 IF ZERO ON INITIAL CALL.

DATA(2) - FLA, FACTOR USED TO COMBINE GRADIENT AND NEWTON-RAPHSON METHODS. SET INTERNALLY TO .01 IF ZERO ON INITIAL CALL.

DATA(3) - TAU, USED IN CONVERGENCE TEST. SET INTERNALLY TO 0.0001 IF ZERO ON INITIAL CALL.

DATA(4) - EPS, USED IN CONVERGENCE TEST. SET INTERNALLY TO 0.00002 IF ZERO ON INITIAL CALL.

DATA(5) - PMIN, WHEN PH .LT. PMIN, PARTIAL DERIVATIVES FROM THE PREVIOUS ITERATION ARE USED INSTEAD OF COMPUTING THEM AGAIN.

DATA(6) THRU DATA(16) - VARIABLES USED INTERNALLY

DO 10 I=1,5
  DATA(I)=0.0D0
10 CONTINUE

BV = VARY VECTOR ( 0=HOLD PARAMETER CONST, 1=ALLOW TO VARY)

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

INITIAL VALUES OF PARS

B(1)=OMEGA(JC)/0.1442357DO
B(2)=0.0D0

MIN AND MAX VALUES

BMIN(I)=2000.0D0
BMAX(I)=200000.0D0
BMIN(I)=200000.0D0
BMAX(I)=200000.0D0

IF (LDBUG.EQ.7) THEN
  WRITE(NBSTRY,1068)K,N
  DO 30 I=1,K
    WRITE(NBSTRY,1069)BMIN(I),BMAX(I),BMIN(I),BV(I)
 30 CONTINUE
ENDIF

BEGIN CALC [CALC 50 POINTS TO BE FIT]

CAVEYTT EQUATION

CALC 50 DATA POINTS BY EXTENDED ANTON'S EQUATION

TD=(PLXANT(5,JC)-PLXANT(0,JC)) 50.0D0
TT=PLXANT(8,JC)-TD

DO 40 I=1,50
  TT=TT+TD
  X(I)=TT
  Y(I)=PLXANT(1,JC)+1.0D0
  X(I)=PLXANT(2,JC)/(TT+PLXANT(3,JC))
  X(I)=PLXANT(4,JC)**TT
C         3       + PLXANT(5,JC)*LOG(TT)
C         4       + PLXANT(6,JC)*TT**PLXANT(7,JC)
C IF(LDBG.GE.7)THEN
WRITE(NHSTRY,1020)Y(I)
XSUM=XSUM+X(I)
XSUM2=XSUM2+X(I)**2
YSUM=YSUM+Y(I)
YSUM2=YSUM2+Y(I)**2
ENDIF
CONTINUE
C MEANS, VARIANCES AND STANDARD DEVIATION
C IF(LDBG.GE.7)THEN
XMEAN=XSUM/FLOAT(N)
XVAR=(FLOAT(N)**2-(XSUM2-XSUM**2)/FLOAT(N))/FLOAT(N-1)
XS=SQRT(XVAR)
YMEAN=YSUM/FLOAT(N)
YVAR=(FLOAT(N)**2-(YSUM2-YSUM**2)/FLOAT(N))/FLOAT(N-1)
YS=SRT(YVAR)
WRITE(NHSTRY,1120)XMEAN,YMEAN,XVAR,YVAR,XS,YS
ENDIF
C BEGIN REGRESSION
C I=ITER+1
IF(ITER.GT.MAXIT)THEN
IER=1
WRITE(NHSTRY,1645)MAXIT,ITER
GOTO 9000
ENDIF
C EVALUATE 2 VECTOR FUNCTION VALUE
C REGRESS TO MODIFIED CAVETT EQUATION
DO 60 I=1,N
THR=X(I)/FC(JC)
RTHR=1./THR
IF(RTHR.LT.0.000001)THEN
Z(I)=AS(9)+I*AS(I)*AS(I)
1 + (I/THR-2.500)*AS(I)+(I*1.00)*AS(I)
2 + (I*2)*AS(I)+AS(I)+THR+(THR-0.750)*(THR-1.00)
3 + LOG(FC(JC))
ELSE IF(RTHR.GE.0.4000)THEN
Z(I)=(1.00-1.00/THR) + I*AS(1)+AS(2)/THR+AS(3)/THR
1 + AS(3)/THR+AS(4)*THR+AS(5)+AS(6)/THR
2 + AS(7)/THR+AS(8)/THR
3 + AS(9)+AS(10)+AS(11)*THR+(THR-0.750)*(THR-1.00)
4 + LOG(FC(JC))
ENDIF
CONTINUE
C CALC ANALYTICAL DERIVATIVES 2D VECTOR
C CONTINUE
C CALC DERIVATIVE
C IF(NDATA(2).GE.2)THEN
IER=-10
WRITE(NHSTRY,1090)IER
GOTO 9000
ENDIF
WRITE (NHSTY, 1000) ITER, NDATA, 1, OUTPUT(J), J=1, 5
YMVC = 0.0D0
SS  = 0.0D0
SSAS = 0.0D0
DO 20 I = 1, N
YMVC = YMVC + (Y(I) - Z(I))**2
SS  = SS  + (Z(I) - YMVC)**2
SSAS = SSAS + (Y(I))**2 - YMVC**2
CONTINUE

C CALC R-SQUARE (SAS VERSION) AND ADJ R-SQUARE
C 1-VARIANCE OF FULL MODEL/VARIANCE OF MEAN MODEL
C
RSQU = SS / (SS + YMVC)
IF (SSAS .NE. 0.0D0) THEN
RSQUSAS = 1.0D0 - YMVC / SSAS
ELSE
RSQUSAS = 0.0D0
ENDIF
IF (DEGFR .EQ. 0.0D0) THEN
ADJRSQU = 0.0D0
ELSE
ADJRSQU = 1.0D0 - (1.0D0 - RSQU) * (FLOAT(N) - 1.0D0) / DEGFR
ENDIF
IF (ABS(RSQU - RSQUSAS) .GT. 1.0D0) THEN
WRITE (NHSTY, 1112) RSQU, ADJRSQU, RSQUSAS, ADJRSQUSAS
ELSE
WRITE (NHSTY, 1114) RSQU, ADJRSQU
ENDIF

DO 100 J = 1, K
WRITE (NHSTY, 1030) J, B(J)
CONTINUE

C IF (LOGUS .EQ. 8) THEN
WRITE (NHSTY, 1040)
DO 116 I = 1, N
YMVC = YMVC + (Y(I) - Z(I))**2
SS  = SS  + (Z(I) - YMVC)**2
PERER = ABS(Y(I) - Z(I)) / ABS(Y(I))**2 + 0.0D0
WRITE (NHSTY, 1695) I, 201, Y(I), Z(I) - Y(I), PERER
CONTINUE
ENDIF
ENDIF

120 CALL YSOLVE (G, N, HDATA, DATA, B, BY, BMAX, BMWIN, Y, Z, P, D)
1
HDATA(2) - NTERK, USED FOR CONTROL IN CALLING PROG
IF = 0, CALCULATE FUNCTION
IF = 1, CALCULATE DERIVATIVE
IF = -1, EXTERNAL ERR FOR WHAT TO DO NEXT
C HDATA(3) - HNL, MAY TAKE ON VARIOUS VALUES
C IF POSITIVE, CONTAINS THE NUMBER OF VARIABLES NO SATISFYING CONVERGENCE CRITERION
C IF = 0, CONVERGENCE SATISFIED AND SOLUTION REACH
C IF = -1, NO IMPROVEMENT POSSIBLE IN THE VALUE OF FH EVEN THOUGH CONVERGENCE HAS NOT BEEN REACHED.
C IF = -2, MORE UNKNOWNS THAN FUNCTIONS AND UNIQUE SOLUTION GENERALLY IS IMPOSSIBLE.
C IF = -3, TOTAL NUMBER OF VARIABLES TO BE VARIED IS ZERO
C IF = -4, CONVERGENCE CRITERION MET BUT FLA STILL 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                                  ENDIF
C            FINAL PARAMETERS
C DO 160 J=1, K
       WRITE(NHSTRY, 1030) J, B(J)
160       CONTINUE
C            FINAL SUMMARY
C       WRITE(NHSTRY,1040) DO 170 I=1,N
IERR=NDATA(3)
   DO 800 JJ=1,4
      PLCAVT(JJ,JC)=0.0D0
800       CONTINUE
C IF(IERR.EQ.0)THEN
C            CONVERGED
C        PLCAVT(1,JC)=B(1) PLCAVT(2,JC)=B(2) PLCAVT(3,JC)=B(8,JC)
C ELSE
C            NONCONVERGED
C        ENDIF
C            FINAL PARAMETERS
C DO 160 J=1, K
       WRITE(NHSTRY,1030) J, B(J)
160       CONTINUE
C            FINAL SUMMARY
C       WRITE(NHSTRY,1040) DO 170 I=1,N
IERR=NDATA(1)
   DO 800 II=1,N
      PERERR=ABS(Z(II)-Y(II))/ABS(Y(II))*100.0D0
     WRITE(NHSTRY,1095) Z(II), Y(II), Z(II)-Y(II), PERERR
800       CONTINUE
C ENDIF
C LOAD DATA INTO PLCAVT ARRAY
C IERR=NDATA(1)
   DO 800 II=1,N
      PLCAVT(II,JC)=0.0D0
800       CONTINUE
C IF(IERR.EQ.0)THEN
C            CONVERGED
C        PLCAVT(1,JC)=B(1) PLCAVT(2,JC)=B(2) PLCAVT(3,JC)=PLXANT(B,JC)
PLCAVT(4,JC)=PLXANT(9,JC)

C IF(NDER.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(NDER.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,1001)
ELSE IF(NDER.EQ.-3) THEN
    WRITE(NHSTRY,1000) ITER,NDATA(3),(OUTPUT(J),J=1,5)
    WRITE(NHSTRY,1003)
ELSE IF(NDER.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(NDER.EQ.-5) THEN
    WRITE(NHSTRY,1000) ITER,NDATA(3),(OUTPUT(J),J=1,5)
    WRITE(NHSTRY,1005)
ELSE IF(NDER.EQ.-6) THEN
    WRITE(NHSTRY,1000) ITER,NDATA(3),(OUTPUT(J),J=1,5)
    WRITE(NHSTRY,1006)
ELSE IF(NDER.EQ.-7) THEN
    WRITE(NHSTRY,1000) ITER,NDATA(3),(OUTPUT(J),J=1,5)
    WRITE(NHSTRY,1007)
ENDIF

PLCHEG(1,JC)=FLOAT(ITER)
PLCHEG(2,JC)=FLOAT(NDATA(3))
PLCHEG(3,JC)=OUTPUT(1)

C CHECK AGAINST FLOWTRAN ESTIMATES
C
IF(PLANS(PLCAVT(1,JC)-OMEGA(1JC)/0.141233570D0.GT.0.1000) THEN
    CALL HESS()
    WRITE(NHSTRY,900)
    WRITE(NHSTRY,1130) PLCAVT(1,JC),OMEGA(1JC)/0.141233570D0
ENDIF

IF(PLCAVT(2,JC).GT.0.200.OR.PLCAVT(2,JC).LT.-0.200) THEN
    CALL HESS()
    WRITE(NHSTRY,900)
    WRITE(NHSTRY,1130) PLCAVT(2,JC)
ENDIF

C FORMATS
C
900 FORMAT(IX,' IN MODULE CAWP')
1000 FORMAT(/,
      1 IX,'ITERATION:',',15,/,
      2 IX,'ID=',',15,/,
      3 IX,'SUM OF SQUARES=',',15.8/,
      4 IX,'ANGLE (DEGREES)=','.15.2/,
      5 IX,'NUMBER OF TIMES TSOLVE CALLED=','.15.1/,
      6 IX,'NUMBER OF FUNCTIONAL EVALUATIONS=','.15.1/,
      7 IX,'NUMBER OF ANALYTICAL DERIVATIVE EVALUATIONS=','.15.1/,
      8 IX,'PH EVEN THOUGH CONVERGENCE HAS NOT BEEN REACHED.',/)
1001 FORMAT(IX,'MORE UNKNOWNS THAN FUNCTIONS AND UNIQUE'',/)
TOTAL NUMBER OF VARIABLES TO BE VARIED = 0,

CONVERGENCE CRITERION MET BUT FLA STILL LARGE,

IC NOT A VALID NUMBER ON ENTRY,

XI NOT WITHIN XMIN(I) TO XMAX(I),

ZERO DIAGONAL ELEMENT IN EQUATION SOLVE,

PARQUARD METHOD REGRESSION,

NUMBER OF PARAMETERS TO BE VARIED = 14,

NUMBER OF DATA POINTS = 14,

INITIAL B, B-MIN, B-MAX,

VARY FLAG,

FORMAT(12X,4(G15.5,1X))

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:',/

FORMAT(1X,3G15.6)

FORMAT(1X,'B1',12,'I1') = ',G13.5)

FORMAT(/,1X,'OBS. Y-CALC

Y-ACTUAL

DIFF.

ERROR',/)

1X,'ERROR',/)

IN ANDRA',/)

1X,'**MAX EXCEEDED MAXIT OF ',15,' ITER = ',15,

2**',/)

IN MODULE ANDRA IERR = ',15,' TRY TO CALC.',/

DERIVATIVE ANALYTICALLY. CALC. ABORTED!

FORMAT(/,10X,'INPUT DATA',/)

5X,'X-VALUE

Y-VALUE',/)

2X,'--------

--------',/)

FORMAT(1X,9R-SQUARE

ADJ R-SQUARE

VAR FN/VAR.HU)

ADJ R-SQUARE (FOR 2ND R-SQUARE)

FORMAT(/,10X,'STATISTICS',/)

5X,'X-VALUES, 26X,Y-VALUES',/)

5X,'-------,26X,--------',/)

5X,'MEAN', 'G15.5,8X', 'MEAN', 'G13.5,

5X,'VARIANCE', 'G15.5,8X', 'VARIANCE', 'G15.5,

5X,'STD. DEV.', 'G15.5,8X', 'STD. DEV.', 'G15.5,

1ST VALUE FOR PLCAVT = ',G13.6,

NOT CLOSE TO OMEGA/0.1412357 = ',G13.6,

CALC CONTINUES!

2X,'CALC CONTINUES!

CONTINUE

END

SUBROUTINE CHEGOF(IERR)

NAME OF MODULE - CHEGOF

MODULE TITLE - CHECK SYSP NUMBER AND SET CALC VECTOR

PURPOSE - TO SET UP NPCVEC VECTOR OF SIZE 22 WHICH SPECIFIES

WHAT PROPERTIES MUST BE CALCULATED FOR EACH SYSP

IN SUBROUTINE PROPS(IF NPCVEC=1 CALC PROP)

VARIABLES USED:

VARIABLE I/O TYPE SPEC DIMENSION DESCRIPTION AND RANGE
C IERR = 0 I ERROR FLAG
  0 = OK
  -1 = INVALID SYSOP

IMPLICIT REAL*8 (A-H,O-Z)
IMPLICIT INTEGER(I-N)

PARAMETER (MN=15)

COMMON /10/ NNS,NOUT,NHSTY,NEPRT
COMMON /DEBUG/ LDBG,LDBGRT

COMMON /SYS2/ NNSOP,HPCVEC(22)

DEFAULT PROPERTY CALC BASED ON SYSOP0

DIMENSION MPDEF(22)

CALC ORDER

1 2 3 4 5
TC , VC , VC , ZC , OMEGA ,
6 7 8 9 10
PSLANT , CP1G , DLFORM , DGFORM , DLHCT ,
11 12 13 14 15
TH , BH , DHUVRT , NTHRA , DHVR ,
16 17 18 19 20
TFP , DELTA , HIF , HULAND , RGBY ,
21 22
PLCAVT , VLCT1

DATA MPDEF /
  1 1  1  1  1  1
  2 1  1  1  1  0
  3 1  1  1  1  0
  4 0  0  0  0  0
  5 0  0  0 /

IF (LDBG.GT.7) WRITE (NHSTY, 900)

IERR = 0

PROPERTIES WHICH ARE CONSIDERED EXTRA PROPERTIES:

ARRAY ELEMENT 1 2 3 4 5 6 7
TFP, DELTA, DHVR, PLCAVT, DLHCT, VLCT1, RGBY

FOR SYSOP6, SYSOP3, SYSOP4, SYSOP5, SYSOP9, SYSOP10, SYSOP11,
SYSOP12, SYSOP14 DO NOT CALC ALL 7 EXTRA PROPS
FOR SYSOP1, SYSOP2 DO NOT CALC NUMBERS 1, 2, 4, 7

LOAD HPCVEC VECTOR WITH DEFAULT VALUES (SYSOP0)

DO 10 RS = 1, 22
  HPCVEC(RS) = HRPLF(RS)
  CONTINUE

CHANGE DEFAULT VALUES FOR SYSOP1 AND SYSOP12

IF (NSYSOP.EQ.1.OR.NSYSOP.EQ.11).THEN
  HPCVEC(16) = 1
  HPCVEC(17) = 1
  HPCVEC(22) = 1
ELSE IF (NSYSOP.EQ.6.OR.NSYSOP.EQ.7.OR.
  1  NSYSOP.EQ.13.OR.NSYSOP.EQ.14) THEN

NONEXISTANT SYSOPS

IERR=-1
CALL MESS(2)
WRITE(NHSTRY,900)
WRITE(NHSTRY,1000) NSYSOP
NSYSOP=0
ELSE IF(NSYSOP.LT.0) THEN
    TO FORCE CALC OF ALL PROPS
    NPCVEC(10)=1
    NPCVEC(15)=1
    NPCVEC(16)=1
    NPCVEC(17)=1
    NPCVEC(20)=1
    NPCVEC(21)=1
    NPCVEC(22)=1
ENDIF

FORMATS
900 FORMAT(I9,'IN MODULE CHESOP: ')
1000 FORMAT(I9,'ASPN SYSOP SELECTED IS INVALID: ',I2,'/',I9,'SYSOP IS SET TO SYSOP0')

RETURN
END

SUBROUTINE CONV(IFLAG,RECORD,IS,IE,IVAL,IVAL,IEHR)

NAME OF MODULE - CONV
MODULE TITLE - EXTRACT NUMBER FROM STRING
PURPOSE - TO EXTRACT NUMBER TOKEN VALUE FROM INPUT RECORD
MODIFIED - 10-1-88

VARIABLES USED-

IFLAG I I - INTEGER-REAL FLAG 0 = INTEGER 1=REAL
RECORD I/O C - INPUT RECORD
IS I I - START BYTE OF TOKEN
IE I I - END BYTE OF TOKEN
IVAL Q I - OUTPUT INTEGER NUMBER
IEHR Q I - ERROR CODE
0=OK
1=ERROR ON CONVERT TO REAL
2=ERROR ON CONVERT TO INTEGER

IMPLICIT REAL(A-H,O-Z)
IMPLICIT INTEGER(I-H)

COMMON /10/ NH,NGT,NHSTRY,REPT

IF=0
IDEL-IE-15+1
IF(IFLAG.EQ.0) THEN
    DECODE(IDEL,1000,RECORD(IS:IE),ERR=10)IVAL
ELSE
    DECODE(IDEL,2000,RECORD(IS:IE),ERR=20)IVAL
ENDIF
GOTO 9990
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,1000) RECORD(IS:IE)
   IERR=1
   GOTO 9990
C
   FORMATS
C
500 FORMAT(IX,'IN MODULE CONV')
1000 FORMAT(I6)
2000 FORMAT(F6.0)
3000 FORMAT(IX,'ERROR ON CONVERT TO INTEGER FROM',/,'A')
4000 FORMAT(IX,'ERROR ON CONVERT TO REAL FROM',/,'A')
9990 RETURN
END

SUBROUTINE DGFRM(TB,XP,XN,XA,DGF,IERR)
C*********************************************************************************************
C NAME OF MODULE - DGFRM
C MODULE TITLE - ESTIMATION OF GIBBS ENERGY OF FORMATION
C PURPOSE - EST OF GIBBS ENERGY OF FORMATION (J/KMOL)
C MODIFIED - 11-23-88
C METHOD - REGRESSION OF ASPEN DATA BANK FOR PARAFFINS, NAPHTHENES, AND AROMATICS
C
C VARIABLES USED-
C
C VARIABLE I/O TYPE SPEC DIMENSION DESCRIPTION AND RANGE
C TB  R   -   BOTTLE POINT (DEG K)
C XP  R   -   MOL FRACTION PARAFFINS
C XN  R   -   MOL FRACTION NAPHTHENES
C XA  R   -   MOL FRACTION AROMATICS
C DGF  R   -   GIBBS ENERGY OF FORMATION
C IERR  I   -   ERROR CODE
C
C = OK
C -1 = TB OUT OF RANGE FOR PARA.
C -2 = TB OUT OF RANGE FOR NAPT.
C -3 = TB OUT OF RANGE FOR ARON.
C
C IMPLICIT REAL*8 (A-H,O-Z)
C IMPLICIT INTEGER(I-N)
C
C COMMON /10 / NTH, NMOH, NHSTRY, NHMPT
C
C CHECK IF TB IS OUT OF RANGE
C PARAFFINS
C
IF(TB.GT.301.00)THEN
   IF(TB.LT.301.00)THEN
      IERR=-1
      CALL MESS(1)
      WRITE(NHSTRY,900)
      WRITE(NHSTRY,1000)TB
      TB=301.00
ENDIF
IF(TB.GT.617.00)THEN
   IERR=-1
CALL MESS(1)
WRITE(NHSTRY, 900)
WRITE(NHSTRY, 1000)
TB = 617.0D0
ENDIF
ENDIF

MAPTHEMES

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 = 322.4D0
 ENDIF
 IF(TB.GT.637.0D0) THEN
  IERR = -2
  CALL MESS(1)
  WRITE(NHSTRY, 900)
  WRITE(NHSTRY, 2000)
  TB = 637.0D0
 ENDIF
ENDIF

AROMATICS

IF(XA.GT.0.D0) THEN
 IF(TB.LT.353.3D0) THEN
  IERR = -3
  CALL MESS(1)
  WRITE(NHSTRY, 900)
  WRITE(NHSTRY, 3000)
  TB = 353.3D0
 ENDIF
 IF(TB.GT.517.8D0) THEN
  IERR = -3
  CALL MESS(1)
  WRITE(NHSTRY, 900)
  WRITE(NHSTRY, 3000)
  TB = 517.8D0
 ENDIF
ENDIF

DATA REGRESSED FOR PARAFFINS

AA = -0.392503521D0
BD = 1.68331721D0
CI = -0.325405675D0
DP = 2.619350545D0

DGFIN = AA + BD*TB + CI*TB*TB + DP*TB*TB*TB

DATA REGRESSED FOR MAPTHEMES

AN = 0.123522681D0
UM = -3.241503650D0
CN = 1.63340381D0
DN = -1.75792750D0

DGFIN = AN + UM*TB + CN*TB*TB + DN*TB*TB*TB

DATA REGRESSED FOR AROMATICS

AA = -0.397615347D10
BA = 3.10108309D0
CA = -7.78053565D0
`DA=64.8352936D0

DGFIA=AA + BA*TB + CA*TB*TB + DA*TB^2*TB

EST. FOR FRACTION

DGF=DGFIP*XP + DGFIM*XN + DGFIA*XA

FORMATS

900 FORMAT(IX,'IN MODULE DGFHM')
1000 FORMAT(IX,'TB(K) VALUE OF ',G13.6,/,1)
   2 2X,'IS NOT IN PARAFFIN CORRELATION RANGE 301-617'/,,
2X,'CORRECTIVE ACTION TAKEN AND CALC. CONTINUES')
2000 FORMAT(IX,'TB(K) VALUE OF ',G13.6,/,1)
   2 2X,'IS NOT IN NAPHTHA CORRELATION RANGE 322.4-637'/,,
2X,'CORRECTIVE ACTION TAKEN AND CALC. CONTINUES')
3000 FORMAT(IX,'TB(K) VALUE OF ',G13.6,/,1)
   2 2X,'IS NOT IN AROMATIC CORRELATION RANGE 353.3-519.8'/,,
2X,'CORRECTIVE ACTION TAKEN AND CALC. CONTINUES')
RETURN
END

SUBROUTINE DHRMTHB, XP, XN, XA, DHR, IERR)

NAME OF MODULE - DHRMTHB
MODULE TITLE - ESTIMATES OF ENTHALPY OF FORMATION
PURPOSE - EST OF ENTHALPY OF FORMATION (H/KJ/MOL)
MODIFIED - 11-23-86
METHOD - REGRESSION OF ASIAN DATA BANK FOR PARAFFINS, NAPHTHA,
AND AROMATICS TO FORM: H1 + H2*TH + H3*TH^2 + H4*TH^3

VARIABLES USED-

VAR. I/O TYPE SPEC DIMENSION DESCRIPTION AND RANGE
TH I R  - Boiling point (deg K)
XP I R  - Mole fraction paraffins
XN I R  - Mole fraction naphthenes
XA I R  - Mole fraction aromatics
DHR G R  - Enthalpy of formation
IERR G I  - ERROR CODE
   0 = OK
   -1 = TH OUT OF RANGE FOR PARA.
   -2 = TH OUT OF RANGE FOR NAP.
   -3 = TH OUT OF RANGE FOR AROM.

IMPLICIT REAL*8 (A-H,O-Z)
IMPLICIT INTEGER(1-H)

COMMON /DHRMTH/ DHR, H, NAPHTHY, AROMAT

CHECK IF TH IS OUT OF RANGE
PARAFFINS

IF (XP.GT.0.D0) THEN
IF (TH.LT.301.D0) THEN
   IERR=-1
   CALL MESS(1)
   WRITE(H,900)
   WRITE(NAPHTHY,1000)
   TH=301.D0
ENDIF
IF (TH.GT.617.D0) THEN
IERR=-1
CALL MESS(1)
WRITE(NHSTRY,900)
WRITE(NHSTRY,1000)TB
TB=617.D0
ENDIF
ENDIF

NAPHTHENES

IF(INX.N.GT.0.DD)THEN
IF(TB.LT.322.400)THEN
IERR=-2
CALL MESS(1)
WRITE(NHSTRY,900)
WRITE(NHSTRY,2000)TB
TB=322.400
ENDIF
ENDIF

IF(INX.GT.637.50)THEN
IERR=-2
CALL MESS(1)
WRITE(NHSTRY,900)
WRITE(NHSTRY,2000)TB
TB=637.50
ENDIF
ENDIF

AROMATIC

IF(INX.A.GT.0.DD)THEN
IF(TB.LT.353.100)THEN
IERR=-3
CALL MESS(1)
WRITE(NHSTRY,900)
WRITE(NHSTRY,3000)TB
TB=353.100
ENDIF
ENDIF

DATA REGRESSED FOR PARAFFINS

AF=56003154.56, D0
BF=-3662760 3600
CF=9840.1797200
DF=8.23774867,DD

DHIFIF=AF + BF TB + CF TH' TH + DF TH' TH

DATA REGRESSED FOR NAPHTHENES

AN=0.16168440E10
HN=-16441.1141560
CN=24153.961150
DN=15.892571250

DHFIN=AN + HN TB + CN TH' TH + DN TH' TH

DATA REGRESSED FOR AROMATICS

AA=-0.116028149D11
BA=88976967.9D0
CA=-223012.655D0 DA=183.320881D0

DHFIAA = AA + BA*TB + CA*TB*TB + DA*TB*TB*TB

EST. FOR FRACTION

DHF=DHFIAA*XA+DHFIN*XN+DHFIP*XPI

FORMATS

900 FORMAT(1X,'IN MODULE DHFRM')
1000 FORMAT(1X,'TM(X) 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

SUBROUTINE DIPOLE(JC, IERR)

NAME OF MODULE - DIPOLE

MODULE TITLE - ESTIMATION OF DIPOLE MOMENT

PURPOSE - EST OF DIPOLE MOMENT (COULOMB'S)

MODIFIED - 1-22-88

VARIABLES USED-

VARIABLE I/O TYPE SPEC DIMENSION DESCRIPTION AND RANGE

JC  I  1 - COMPONENT ATOM ID
IERR  O  1 - ERROR CODE

IMPLICIT REAL*8 (A-H,O-Z)
IMPLICIT INTEGER(I-N)

REAL*8 MUP

PARAMETER (MNC=25)

COMMON /CPRP19/ MUP(MNC)

IERR=0

SET TO DEFAULT SUGGESTED BY ASPEN AND DIPPR

MUP(JC)=0.0D0

FORMATS

RETURN
END

SUBROUTINE ESTFRA(TB,JC,IERR)

NAME OF MODULE - ESTFRA
MODULE TITLE - ESTIMATE PERCENT PARAFFINS, NAPTHENES, AND AROMATICS

PURPOSE - TO ESTIMATE PERCENT PARAFFINS, NAPTHENES, AND AROMATICS FOR A GIVEN TEMPERATURE BASED ON TIA JUANA LIGHT (VENEZUELA)

VARIABLES USED:

VARIABLE I/O TYPE SPEC DIMENSION DESCRIPTION AND RANGE
TH I R - BOILING POINT (DEG F)
JC I I - COMPONENT ARRAY ID
IERR O I - ERROR CODE
0 = OK
-1 = TH OUT OF RANGE

IMPLICIT REAL*8 (A-H,O-Z)
IMPLICIT INTEGER(I-N)

PARAMETER (MNC=25)

COMMON /IO / NIN, NOUT, NHSTRY, NREPT
COMMON /DBUG / LDLUG, LDLUGH
COMMON /NPROP4/ PA(MNC), PN(MNC), PP(MNC), LPP
COMMON /EPROP1/ XPAR(MNC), XPARP(MNC), XARO(MNC)

IF(LDBGUG.GT.7) WRITE(NHSTRY,900)
IERR=0

CHECK TH

IF(TH.LE.113.D0) THEN
  IERR=-1
  CALL MESS(1)
  WRITE(NHSTRY,900)
  WRITE(NHSTRY,1060) TH
  TH=113.D0
ENDIF

IF(TH.GE.549.D0) THEN
  IERR=-1
  CALL MESS(1)
  WRITE(NHSTRY,900)
  WRITE(NHSTRY,1600) TH
  TH=549.D0
ENDIF

EST. PERCENT PARAFFINS, NAPTHENES, AND AROMATICS
REGRESSION OF PARAFFINS VOL% VS TEMP (F)
ADJ. R-SQUARE = 0.9511488

AP = 161.361491
BP = -0.83552267
CP = 0.216785193E-02
DP = -0.181295241E-05

VP=AP*HP*TH+BP+CP*TH+DP*TH^2
TH(TH)=VP

REGRESSION OF NAPTHAS VOL% VS TEMP (F)
ADJ. R-SQUARE = 0.8799234

AN = -134.126283
BN = 2.15899658
CN = -0.996716079E-02
DN = 0.1966709815E-04
EN = -0.140405351E-07
VN=AN+BN*TB+CN*TB^2+DN*TB^3+EN*TB^4
PN(JC)=VN

AROMATICS BY DIFFERENCE

PA(JC)=100.DO0-PP(JC)-PN(JC)

CORRECT FOR IMPOSSIBLE CASE

IF(PA(JC).LE.0.DO0) THEN
  PA(JC)=0.DO00
  PSUM=PN(JC)+PP(JC)
  PN(JC)=PN(JC)/PSUM*100.DO0
  PP(JC)=PP(JC)/PSUM*100.DO0
ENDIF

CALC MOLE FRACTION PARAFFINS, NAPHTHALES, AND AROMATICS

XARO(JC)=PA(JC)/100.DO0
XNAP(JC)=PN(JC)/100.DO0
XPAR(JC)=PP(JC)/100.DO0

FORMATS
900 FORMAT(IX,'IN MODULE ESTBRA')
1000 FORMAT(IX,'TH(F) VALUE OF ',/G13.6,' IS NOT IN CORRELATION'
  \RANGE 113-549'/,/
  IX,'CORRECTIVE ACTION TAKEN AND CALC. CONTINUES')
RETURN
END

SUBROUTINE EXTN(ISTART, IEND, RECORD, ICNT)

NAME OF MODULE - EXTN
MODULE TITLE - EXTRACT TOKEN BETWEEN DELIMS
PURPOSE - TO EXTRACT TOKEN VALUES FROM INPUT RECORD
MODIFIED - 12-15-80

VARIABLES USED-

VARIABLE I/O TYPE-SPEC DIMENSION DESCRIPTION AND RANGE
ISTART I 1 10 START BYTE OF TOKEN
IEND I 1 10 END BYTE OF TOKEN
RECORD I/O C - INPUT RECORD
ICNT I 1 - COUNT OF TOKENS FOUND

CHARACTER*1 DELMS(2)
CHARACTER*80 RECORD
INTEGER ISTART(10), IEND(10)
DATA DELMS/*,'~',*/
INITIALIZE
K=1
INDE=80
DO 10 JJ=1,10
  ISTART(JJ)=0
  IEND(JJ)=0
10 CONTINUE
20 CONTINUE
C BEGIN COUNT OF TOKENS
C ICNT=ICNT+1
C FIND BEGIN OF TOKEN
C DO 10 IS=K,IWIDE
    IF(RECORD(IS:IS).NE.DELMS(1)) AND.
         1 RECORD(IS:IS).NE.DELMS(2)  IGOTO 40
10 CONTINUE
   ICNT=ICNT-1
   RETURN
C FIND END OF TOKEN
C CONTINUE
C DO 50 IE=IS,IWIDE
    IF(RECORD(IE:IE).EQ.DELMS(1)) OR.
         1 RECORD(IE:IE).EQ.DELMS(2)  IGOTO 50
50 CONTINUE
   RETURN
C FOUND START AND END OF TOKEN
C CONTINUE
C IES=IE-1
C IDELT=IES-1S
   IF(IDEL.T.LT.0)THEN
   ICNT=ICNT-1
   GOTO 80
ENDIF
C LOAD START AND END OF TOKENS
C ISTART(ICNT)=IS
TEND(ICNT)=IES
80 CONTINUE
K=IES+1
GOTO 20
C 9999 RETURN
END
C SUBROUTINE GUNYAM(VR,OMEGA,TRD,ICALC,VD,INH)
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 - 11-16-85
C METHOD - REF: ALCHE 17:1 111 (1971)
C GUNN & YAMADA
C 1 CHEM ENG. DATA 18: 594 (1971)
C YAMADA & GUNN
C VARIABLES USED-
C VARIABLE I/O  TYPE-SPEC  DIMENSION DESCRIPTION AND RANGE
C VR  I  H   -  REFERENCE VOLUME(M**3/KG MOLE)
C TR  I  H   -  REFERENCE TEMP REDUCED
C OMEGA I  H   -  ACENTRIC FACTOR
C TRD I  H   -  REDUCED TEMP OF VOL DESIRED
C I CALC I  I   -  CALC TYPE
0 = GUNN YAMADA
1 = YAMADA GUNN
VOLUME AT DESIRED TEMP(M^3/KNOLE)
ERROR CODE
0 = OK
-1 = REDUCED TEMP > 0.99
-2 = REDUCED TEMP < 0.2

IMPLICIT REAL*8 (A-H,O-Z)
IMPLICIT INTEGER(I-N)

COMMON /IO / NIN,NOUT,NHSTRY,NKLYT
COMMON /DEBUG / LDBUG,LDBUG

IERR=0
IF(LDBUG.GT.7)WRITE(NHSTRY,900)

IF(ICALC.LE.0)ICALC=0
IF(ICALC.GT.1)ICALC=1

WHITE WARNINGS

IF(TR.GT.0.99D0)THEN
CALL MESS(1)
WRITE(NHSTRY,900)
WRITE(NHSTRY,1600)TR
TH=39D0
IERR=-1
ENDIF
IF(TR.GT.0.99D0)THEN
CALL MESS(1)
WRITE(NHSTRY,900)
WRITE(NHSTRY,1600)TR
TH=39D0
IERR=-1
ENDIF

IF(TR.LT.0.2D0)THEN
CALL MESS(1)
WRITE(NHSTRY,900)
WRITE(NHSTRY,1020)TH
THD=0.2D0
IERR=-2
ENDIF

IF(TRD.LE.0.8D0)THEN
VHADT=0.33953D0-0.33953D0*TR+1.51941D0*TRD
ELSE
VHADT=0.60695D0*TRD-0.5D0*LOG10(1.0D0-TR)
ENDIF

IF(TRD.LE.0.8D0)THEN
VHGAT=0.33953D0-0.33953D0*TRD+1.51941D0*TRD*TRD
ELSE
VHGAT=0.60695D0*TRD-0.5D0*LOG10(1.0D0-TR)
ENDIF

1 ENDIF
C
GAMATR = 0.290405 - 0.04842 * TR + 0.09045 * TR**2
GAMADT = 0.290405 - 0.04842 * TR - 0.09045 * TR**2

C
VD = VR * (VRADT + (1.0D0 - GAMATR))
C
ELSE
TS = 2.0D0 / 7.0D0
ZC = 0.290405 + 0.09045 * (1.0D0 - TR)**2
PHI = 1.0D0 - TR**3
TS = (1.0D0 - TR)**3

C
ENDIF
C
FORMATS
C
306 FORMAT(1X, 'IN MODULE CYKL')
1060 FORMAT(1X, 'TR VALUE IS GREATER THAN 0.99', /)
1     IX, 'TR-VALUE OF 'G15.6', SET TO 0.99 CALC. CONTINUES'
1010 FORMAT(1X, 'TR VALUE IS GREATER THAN 0.99', /)
1     IX, 'TR-VALUE OF 'G15.6', SET TO 0.99 CALC. CONTINUES'
1020 FORMAT(1X, 'TR VALUE IS LESS THAN 0.2', /)
1     IX, 'TR-VALUE OF 'G15.6', SET TO 0.2 CALC. CONTINUES'
1030 FORMAT(1X, 'TR VALUE IS LESS THAN 0.2', /)
1     IX, 'TR-VALUE OF 'G15.6', SET TO 0.2 CALC. CONTINUES'
C
RETURN
END
C
SUBROUTINE CYKL(TR, TC, PC, WEP, API, OMEGA, TERR)
C
C
NAME OF MODULE - CYKL
C
MODULE TITLE - LOSSY/SCATTERED SELECT LEE CALC OF ACETRIC FACTOR
C
PURPOSE - TO CALC ACETRIC FACTOR USING SELECT LEE METHOD
C
MODIFIED - 11-10-88
C
METHOD - HEP: HYDROCARBON PROCESSING VOL. 15 NO 3 PP 153
C
"IMPROVED PREDICTION OF ENTHALPY OF FRACTIONS"
C
H. J. LESLIE AND R. L. LESLIE (PAPER 211)
C
VARIABLES USED:
C
C
VARIABLE
i/o     TYPE   SIZE    DESCRIPTION AND RANGE
C
TR     i     R     -     NORMAL AVERAGE POINT TEMP (DEG R)
TC     i     R     -     CRITICAL TEMP (DEG R)
PC     i     R     -     CRITICAL PRESS (PSI)
WEP    i     R     -     WATER/EOS CHIP FACTOR
API    i     R     -     API VALUE
OMEGA o     R     -     ACETRIC FACTOR
TERR   o     I     -     ERROR CODE
C
implicit real(a-h,o-z)
implicit integer(i-n)
C
COMPIE / 10 , 99, NOHT, MENTY, UNL, UN
COMMON / DEBUG / LDBG, LDBG, TERR
C
TERR = 0
IF (LDBG .GT. 1) WRITE (INDUSTRY, 900)
C
CHECK IF WORK IN RANGE(10-13) WARNING
C
IF (WORK .LT. 10.0D0 .OR. WORK .GT. 13.0D0) THEN
IERR=1
CALL MESS(1)
WRITE(NHSTRY,500)
WRITE(NHSTRY,1000)UOPK
ENDIF

C API (0-80)
C
IF(API.LT.0.0D0.OR.API.GT.80.0D0)THEN
IERR=2
CALL MESS(1)
WRITE(NHSTRY,900)
WRITE(NHSTRY,1000)API
ENDIF

C REDUCED PROPERTIES
C
REDT=(TSR/TC)
BOILP=1.896D0
REDF=BOILP/VC
C
IF(REDT.LE.0.0D0)THEN
OMEGA=(LOG(REDP)-5.92714D0+6.09648D0/REDT+
1.28862D0*LOG(REDT)-0.169347D0*REDT**6)
3.7518D0-15.6875D0/REDT-
13.4721D0*LOG(REDT)+0.33577D0*REDT**6)
ELSE
OMEGA=7.3946D0+0.1352D0*UOPK-0.0073465D0*UOPK**2+0.3550D0/REDT+
1.1060D0-0.60163D0*UOPK/REDT
ENDIF
C OMEGA
C
IF(OMEGA.LT.0.2D0.OR.OMEGA.GT.1.4D0)THEN
IERR=3
CALL MESS(1)
WRITE(NHSTRY,900)
WRITE(NHSTRY,1000)OMEGA
ENDIF
C FOMATS
C
900 FORMAT('IN MODULE GYKL')
1000 FORMAT('API VALUE NOT IN OPTIMAL RANGE (10-13)',/,
1.4D6,'CALC. CONTINUES')
2000 FORMAT('API GRAVITYVALUE NOT IN OPTIMAL RANGE (6-8)',/,
1.4D6,'CALC. CONTINUES')
3000 FORMAT('OMEGA VALUE NOT IN OPTIMAL RANGE (0.2-1.4)',/,
1.4D6,'CALC. CONTINUES')
RETURN
END
C******************************************************************************
C SUBROUTINE HVRP(XC,IERR)
C******************************************************************************
C NAME OF MODULE - HVRP
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 - 12/15/88
C METHOD - ASPEN'S WATSON HEAT OF VAPORIZATION EQUATION
C VARIABLES USED -
C VARIABLE I/O TYPE SPEC DIMENSION DESCRIPTION AND RANGE
COMPONENT ARRAY ID

ERROR CODE

0 = OK

PARAMETER

COMMON /IO / NIN, NOUT, NISTRY, NREPT
COMMON /DEBUG / LDEBUG, LDEBUGR

COMMON /CPRP01/ TC(MNC)
COMMON /CPRP08/ DHVLWT(5, MNC)
COMMON /CPRP14/ TB(MNC)
COMMON /CPRP16/ DHVLB(MNC)

IERR=0
IF (LDEBUG .GT. 7) WRITE (NHSTRY, 900)

TBUSE = TB(JC)

CHECK LIMITS OF EQUATION

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

IF (TB(JC) .GE. TC(JC)) THEN
  IERR = 2
  CALL MESS(2)
  WRITE (NHSTRY, 900)
  WRITE (NHSTRY, 1000) TC(JC), TB(JC)
  TBUSE = TC(JC)
ENDIF

CALC HEAT OF VAPORIZATION AT BOILING POINT USING ASPEN'S

WATSON EQUATION

DHVLB(JC) = DHVLWT(1, JC) + (1.0 - TBUSE/TC(JC)) / (1.0 - DHVLWT(3, JC)/TC(JC))

FORMATS

900 FORMAT(1X, 'IN MODULE HVARP')
1000 FORMAT(1X, 'TB VALUE LESS THAN LOWER LIMIT OF ', G13.6, ', ')
       (1X, 'TB VALUE OF ', G13.6, ' SET TO LOWER LIMIT ',
       'CALC. CONTINUES')

RETURN
END

SUBROUTINE INIT_IERR

NAME OF MODULE - INIT

MODULE TITLE - INITILIZE TO DEFAULT VALUE FOR PROPERTIES

PURPOSE - TO INITILIZE ALL PROPERTIES

VARIABLES USED--

VARIABLE I/O TYPE SPEC DIMENSION DESCRIPTION AND RANGE
IMPLICIT REAL*8 (A-H,O-Z)
IMPLICIT INTEGER(1-N)

REAL*8       MULAND,MULREG,MUP
CHARACTER(12) CNAME

PARAMETER    (MNC=25)

COMMON /IO / MIN,NOUT,NHSTHY,NREPT
COMMON /DEBUG / LDBG,LDBGUR
COMMON /SYS1 / RMISS

COMMON /MPROP1/ MCOMP,CNAME(MNC),ICF

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(1,MNC),CPIREG(3,MNC)
COMMON /CPRP08/ DHVLT(5,MNC)
COMMON /CPRP09/ MULAND(5,MNC),MULREG(3,MNC)
COMMON /CPRP10/ DHFORM(MNC)
COMMON /CPRP11/ DGFORM(MNC)
COMMON /CPRP12/ KBETA(MNC),KBTRG(3,MNC)
COMMON /CPRP13/ DLCEVT(MNC)
COMMON /CPRP14/ TB(MNC)
COMMON /CPRP15/ VB(MNC)
COMMON /CPRP16/ DHVLT(MNC)
COMMON /CPRP17/ TFF(MNC)
COMMON /CPRP18/ DELTA(MNC)
COMMON /CPRP19/ MUL(MNC)
COMMON /CPRP20/ RGYR(MNC)
COMMON /CPRP21/ PLCAVDT(4,MNC),PLCRTG(3,MNC)
COMMON /CPRP22/ VLCVT1(MNC)

IF(LDBG.GT.7.0WHITE(NHSTHY,900))

IERR=0

DO 50 JC=1,NCOMP

TC(JC)=RMISS
PC(JC)=RMISS
VC(JC)=RMISS
ZC(JC)=RMISS

DO 10 IN=1,5

10

DO 20 IN=1,11

20

CPIG(JC)=RMISS

DO 30 IN=1,5

30 CONTINUE

OMEGA(JC)=RMISS
DHFORM(JC)=RMISS
DGFORM(JC)=RMISS
KBETA(JC)=RMISS
KBTRG(JC)=RMISS
DLCEVT(JC)=RMISS
TB(JC)=RMISS
VB(JC)=RMISS
DHVLT(JC)=RMISS
TFF(JC)=RMISS
DELTA(JC)=RMISS
MUL(JC)=RMISS
RGYR(JC)=RMISS
PLCAVDT(JC)=RMISS
PLCRTG(JC)=RMISS
VLCVT1(JC)=RMISS

...
DO 40 IN=1,
   PLSREG(IN,JC)=RMISS
   CPREG(IN,JC)=RMISS
   MULREG(IN,JC)=RMISS
   FLCHEG(IN,JC)=RMISS
   RKREG(IN,JC)=RMISS
10 CONTINUE
50 CONTINUE

FORMAT

500 FORMAT(1X,'IN MODULE INIT')

RETURN
END

SUBROUTINE INIT(IO)

NAME OF MODULE - INIT
MODULE TITLE - INPUT TRANSLATOR
PURPOSE - TO READ INPUT FILE AND OBTAIN INPUT VALUES
MODIFIED - 12-20-68

VARIABLES USED-

C VARIABLE I/O TYPE SPEC DIMENSION | DESCRIPTION AND RANGE
C TERR I/O 1  1 -  ERROR CODE
C C 0 = OK
C C -1 = EXTOK ERROR
C C 1 = TEMP INPUT WARNING
C C 2 = PREQ INPUT WARNING
C C 3 = TOO MANY DESCRIPTION LINES
C C 4 = SYSPRINT WARNING
C C 5 = ASPNOUT WARNING
C C 6 = PC WARNING
C C 7 = TC WARNING
C C 8 = CAL-DRUG WARNING
C C 9 = REP-DRUG WARNING

C INPUT COMMANDS

ALL INPUT MUST BE IN CAPS
; FOR COMMENT CARDS

PKW  SKW  TKW
C C (UP TO 62 CHARACTERS)
C C (UP TO 25 LINES)
C C F K C R
C C PA MMHG PSIA PSIG ATM
C C COMP-LIST
C C CVAL
IMPLICIT REAL*8 (A-H, O-Z)
IMPLICIT INTEGER(I-N)

REAL*8   PABP, MEABP

PARAMETER ( MNC = 25 )
PARAMETER ( MFODESC = 25 )

CHARACTER*1 INPUTCH, OUTCH
CHARACTER*32 TITLE, CHNAME
CHARACTER*60 TITLE2, DESC ( MDESC, 1, CVAL )

INTEGER ( NSYS ) 15(10), 16(10)

COMMON / IO / MINT, MINT, MUNIT, MREPT
COMMON / IFILE / FILE
COMMON / IDESC / IFLAG, IDESC
COMMON / IPRINT / IUNIT
COMMON / ISYS1 / RSYS
COMMON / ISYS2 / MYSYS, MDESC, I2
COMMON / IINFO / TITLE, DESC, IDESC
COMMON / NPROP / MCOM, CNAME ( MNC, 1, 1 )
COMMON / NPROP / VARNAME, IUNIT, CNAME, NAME ( MNC, 1, MEAB ( MNC )
COMMON / NPROP / VARNAME, IUNIT, CNAME, NAME ( MNC, 1, 1, MOD ( MNC )
COMMON / NPROP / TITLE, DESC, IDESC

COMMON / CPARM1 / TC1, MNC
COMMON / CPARM2 / TC1, MNC

SET DEFAULTS

IERR = 0
ICT = 0
IDESC = 0
IFICT = 0
NCOMP = 0
NSYS = 0
NPRINT = 0
ICLASS = 1
IUNIT = 1
ICT = 0
IMOD = 0
IFP = 0
CALL IDATE(IM, ID, IY)
WRITE(NHSTRY, 900)IM, ID, IY
BEGIN INPUT TRANSLATION
READMIN, 1000, END=9600|REC1
CONTINUE
FILTER OUT BAD CHARACTERS AND CAPITALIZE IF NECESSARY
DO 200 IC=1, 80
INCHA=REC1(IC:IC)
CALL CAPS(INCHA, OUTCHA)
REC1(IC:IC)=OUTCHA
CONTINUE
ECHO INPUT
CALL STRIP(REC1, [NUM, NHSTRY, IENS])
LOOK FOR :
IF(REC1(1:1).EQ.';')GOTO 100
FOUND TITLE PW
IF(REC1(1:5).EQ.'TITLE')THEN
TITLE=REC1(6:80)
ENDIF
FOUND DESC PW
IF(REC1(1:1).EQ.'DESC')THEN
IDESC=IDESC+1
IF(IDESC.GT.MXDESC)THEN
CALL MESS(1)
WRITE(NHSTRY, 5000)
TERR=3
GOTO 100
ENDIF
DESC(IDESC)=REC1(5:80)
ENDIF
FOUND T-UNITS PW
IVAL1=INDEX(REC1, 'T-UNITS=')
IF(IVAL1.EQ.1)THEN
REC2=REC1(IWALL+6:80)
IF(INDEX(REC2, 'F').NE.0)THEN
ITUNIT=1
ELSE IF(INDEX(REC2, 'T').NE.0)THEN
ITUNIT=2
ELSE IF(INDEX(REC2, 'P').NE.0)THEN
ITUNIT=4
ELSE IF(INDEX(REC2, 'E').IE.0)THEN
ITUNIT=6
ELSE
ITUNIT=1
REC2=REC2
CALL MESS(1)
WRITE(NHSTRY, 5010)
TERR=1
GOTO 100
ENDIF
ENDIF
FOUND V-UNITS PW
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 HE55(2)
    WRITE(NHSTRY,5620)
    TERR = 2
    GOTO 100
  ENDIF
ENDIF
ENDIF

FOUND PROP-DATA PEW

IVAL1 = INDEX(REC1, 'PROP-DATA')

IF(IVAL1.EQ.1) THEN
  ICNT = 0
  READ(NIN,1000,END=9000|REC2
  FILTER OUT BAD CHARACTERS AND CAPITALIZE IF NECESSARY
  DO 500 IC=1,80
    INCHA = REC2(IC:IC)
    CALL CAPS(INCHA,OUTCHA)
    REC2(IC:IC) = OUTCHA
  CONTINUE
  ECHO INPUT
  CALL STRIP(REC2,1NOM,NHSTRY,TERR)
  LOOK FOR :
  IF(REC2(1:1).EQ.':') GOTO 100
  CHECK IF FIRST CHAR IS NON BLANK
  IF(REC2(1:1).NE.' ') THEN
    REC1 = REC2
    GOTO 101
  ENDIF

  FOUND COMP-LIST SW

  IVAL2 = INDEX(REC2, 'COMP-LIST')
  IF(IVAL2.NE.0) THEN
    NCOMP = NCOMP + 1
    CHNAME(NCOMP) = REC2(IVAL2+10:IVAL2+10+32)
  GOTO 400
  ENDIF

  FOUND CVAL TRM

  IVAL2 = INDEX(REC2, 'CVAL')
  IF(IVAL2.NE.0) THEN
CVALU=REC2(IVAL2+5:80)

FIND TOKENS

CALL EXTNK(IS, IE, CVALU, ICNT)
IF (ICNT.LE.0) THEN
  IEREC=-1
GOTO 400
ENDIF

FOUND MW

IF (CVALU(IS(1):IE(1)).EQ. 'MW') THEN
  IFLAG=1
  CALL CONV(IFLAG, CVALU, IS(2), IE(2), AMM(NCOMP), IDUM, IERC)
  GOTO 400
ENDIF

FOUND VARP

IF (CVALU(IS(1):IE(1)).EQ. 'VARP') THEN
  IFLAG=1
  CALL CONV(IFLAG, CVALU, IS(2), IE(2), VARP, IDUM, IERC)
  IF (ITUNIT.EQ.1) THEN
    CALL TCON(VARP, VARP(NCOMP), 14, IERT)
  ELSE IF (ITUNIT.EQ.2) THEN
    CALL TCON(VARP, VARP(NCOMP), 24, IERT)
  ELSE IF (ITUNIT.EQ.3) THEN
    CALL TCON(VARP, VARP(NCOMP), 34, IERT)
  ELSE
    VARP(NCOMP)=VARP
  ENDIF
  GOTO 400
ENDIF

FOUND STOP

IF (CVALU(IS(1):IE(1)).EQ. 'STOP') THEN
  ICF=0
  IFLAG=1
  CALL CONV(IFLAG, CVALU, IS(2), IE(2), SLOP(NCOMP), IDUM, IERC)
  GOTO 400
ENDIF

FOUND SASTMB86

IF (CVALU(IS(1):IE(1)).EQ. 'SASTMB86') THEN
  IFLAG=1
  ICF=1
  CALL CONV(IFLAG, CVALU, IS(2), IE(2), SLOP(NCOMP), IDUM, IERC)
  GOTO 400
ENDIF

FOUND API

IF (CVALU(IS(1):IE(1)).EQ. 'API') THEN
  IFLAG=1
  CALL CONV(IFLAG, CVALU, IS(2), IE(2), API(NCOMP), IDUM, IERC)
  GOTO 400
ENDIF
FOUND SG

IF (CVALU(IS(1):IE(1)).EQ.'SG') THEN

IFLAG = 1
CALL CONV(IFLAG, CVALU, IS(2), IE(2), SG(NCOMP), IDUM, IERC)
GOTO 400
ENDIF

FOUND UOPK

IF (CVALU(IS(1):IE(1)).EQ.'UOPK') THEN

IFLAG = 1
CALL CONV(IFLAG, CVALU, IS(2), IE(2), UOPK(NCOMP), IDUM, IERC)
GOTO 400
ENDIF

FOUND WK

IF (CVALU(IS(1):IE(1)).EQ.'WK') THEN

IFLAG = 1
CALL CONV(IFLAG, CVALU, IS(2), IE(2), WK(NCOMP), IDUM, IERC)
GOTO 400
ENDIF

FOUND TC

IF (CVALU(IS(1):IE(1)).EQ.'TC') THEN

IFLAG = 1
CALL CONV(IFLAG, CVALU, IS(2), IE(2), TC1, IDUM, IERC)
IF (IERC.GT.0) THEN
CALL MESS(1)
WRITE(HISTORY, 5040)
IERR = 7
TC(NCOMP) = RMISS
GOTO 100
ENDIF

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
GOTO 400
ENDIF

FOUND FC

IF (CVALU(IS(1):IE(1)).EQ.'FC') THEN

IFLAG = 1
CALL CONV(IFLAG, CVALU, IS(2), IE(2), FC1, IDUM, IERC)
IF (IERC.GT.0) THEN
CALL MESS(1)
WRITE(HISTORY, 5050)
PC(NCOMP) = RMISS
IERR = 6
GOTO 100
ENDIF
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 (ITUNIT.EQ.4) THEN
    CALL PCON (PCI, PC(NCOMP), 45, IERP)
ELSE
    PC(NCOMP) = PCI
ENDIF
GOTO 400
ENDIF

C
FOUND PER-PAR
C
IF (CVALU(IS11): IE(11), .EQ. 'PER-PAR') THEN
C
    IFLAG = 1
    CALL CONV( IFLAG, CVALU, IS(1), IE(1), PN(NCOMP), IDUM, IERC)
GOTO 400
ENDIF
C
FOUND PER-ARO
C
IF (CVALU(IS11): IE(11), .EQ. 'PER-ARO') THEN
C
    IFLAG = 1
    CALL CONV( IFLAG, CVALU, IS(1), IE(2), PN(NCOMP), IDUM, IERC)
GOTO 400
ENDIF
C
FOUND PER-NAP
C
IF (CVALU(IS11): IE(11), .EQ. 'PER-NAP') THEN
C
    IFLAG = 1
    CALL CONV( IFLAG, CVALU, IS(1), IE(1), PN(NCOMP), IDUM, IERC)
GOTO 400
ENDIF
C
FOUND PRINT-OPT PW
C
IVAL1 = INDEX(HEC1,'PRINT-OPT')
IF (IVAL1, .EQ. 1) THEN
C
700
TCNT = 0
READININ, 1000, END = 9000, IREC
C
FILTER OUT BAD CHARACTERS AND CAPITALIZE IF NECESSARY
C
DO 650 IC = 1, IC
    INCHA = REC2(1:IC, IC)
    CALL CAPSINCHA, OUTCHA
    REC2(1:IC, IC) = OUTCHA
    CONTINUE
C
ECHO INPUT
C
CALL STRIP(REC2, INUM, HISTRY, IERS)
C
LOOK FOR :
C
IF (REC2(1:1), .EQ. ':') GOTO 600
C
CHECK IF FIRST CHAR IS NON-BLANK
C           IF(REC2(1:1).NE.,',') THEN
RECI=REC2
GOTO 101
ENDIF

C           FOUND CAL-DBG SKW

IVAL2=INDEX(REC2,'CAL-DBG')
IF(IVAL2.NE.0) THEN
CVALU=REC2(IVAL2+8:80)
CALL EXTOK(IS,IE,CVALU,ICNT)
IF(IE(1).LE.0) THEN
IERR=-1
GOTO 600
ENDIF
IFLAG=0
CALL CONV(IFLAG,CVALU,IS(1),IE(1),RDUM,LDBG,LERC)
IF(IERC.GT.0) THEN
CALL MESS(1)
WRITE(*,5060)
ISRN=8
LDBG=0
ENDIF
IF(LDBG.LT.0)LDBG=0
IF(LDBG.GT.8)LDBG=8
GOTO 600
ENDIF

C           FOUND REP-DBG SKW

IVAL2=INDEX(REC2,'REP-DBG')
IF(IVAL2.NE.0) THEN
CVALU=REC2(IVAL2+8:80)
CALL EXTOK(IS,IE,CVALU,ICNT)
IF(IE(1).LE.0) THEN
IERR=-1
GOTO 600
ENDIF
IFLAG=0
CALL CONV(IFLAG,CVALU,IS(1),IE(1),RDUM,LDBG,LERC)
IF(IERC.GT.0) THEN
CALL MESS(1)
WRITE(*,5070)
IERR=9
LDBG=0
ENDIF
IF(LDBG.LT.0)LDBG=0
IF(LDBG.GT.8)LDBG=8
GOTO 600
ENDIF

C           FOUND PROP-OPT= SKW

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'.FL.0) THEN
MSYSOP=-1
ELSE
  IS(1)=IVAL3
  IE(2)=IE(1)+4
  IS(2)=ival3+5
  IE(2)=IVAL3+5
ENDIF
ENDIF
IFLAG=0
CALL CONV(IFLAG,CVALU,IS(2),IE(2),RDUM,MSYSOP,IERC)
ENDIF GOTO 600
ELSE
    REC1=REC2
    ISYSOP=0
    CALL MESS(2)
    WRITE(NHSTRY,5030)
    TERR=4
    GOTO 100
ENDIF
ENDIF

C
FOUND ASPENOUT SW

IVAL2=INDEX(REC2,'ASPENOUT')
IF (IVAL2.NE.0) THEN
    CVALU=REC2(IVAL2+6:80)
    IF (INDEX(CVALU,'DFMS').NE.0) THEN
        IPTYPE=1
    ELSE IF (INDEX(CVALU,'INF').NE.0) THEN
        IPTYPE=0
    ELSE
        CALL MESS(1)
        WRITE(NHSTRY,5080)
        IPTYPE=0
        TERR=5
    ENDFI
    GOTO 600
ENDIF

C
FOUND REP-FILE SW

IVAL2=INDEX(REC2,'REP-FILE')
IF (IVAL2.NE.0) THEN
    CVALU=REC2(IVAL2+6:80)
    CALL EXTKIT(15,15,CVALU,ICNT)
    IF (ICNT.NE.0) THEN
        EERR=-1
        GOTO 600
    ENDFI
    FILE=CVALU(15:15111)
    IFF=1
    GOTO 600
ENDIF
    REC1=REC2
    GOTO 100
ENDIF

C
FOUND END-INPUT IFN

IVAL1=INDEX(REC1,'END-INPUT')
IF (IVAL1.NE.0) THEN
    GOTO 9100
ENDIF
GOTO 100

9000 WRITE(NHSTRY,5200)
C
WRITE SUMMARY TO HIS FILE

9100 WRITE(NHSTRY,6000)NCOMP, INUN, LDBUG, LDBGUN, 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

IF (ICF.EQ.1) THEN
WRITE(NHSTRY,6060)
ELSE
WRITE(NHSTRY,6070)
ENDIF

WRITE(NHSTRY,6030)
WRITE(NHSTRY,6100)
WRITE(NHSTRY,5100)

FORMATS

900 FORMAT(IHI,/,5X,'ESTPHO BEGINS EXECUTION','.//,
     1  5X,'RUN MADE ON ',12,':/','12,':/','12,//,
     2  5X,'INPUT ECHO FOR PROGRAM COMPET','.//,
     3  1X,----',1X,621'='1)
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 P-UNITS, DEFAULT P-UNITS=PSIA 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 FC, FC WILL BE ESTIMATED')
5060 FORMAT(2X,'IN READ OF CAL-DRUG, CAL-DRUG SET TO 0')
5070 FORMAT(2X,'IN READ OF HAY-DRUG, HAY-DRUG SET TO 0')
5080 FORMAT(2X,'IN READ OF ASPENOUT TYPE (DFHS,INPUT, INPUT ASSUMED')
5100 FORMAT(IHI,/,5X,'COMPONENT ESTIMATION SUMMARY',/)
5200 FORMAT(2X,'END-INPUT NOT FOUND, END-INPUT IS ASSUMED')

FORMAT(IHI,/,)
1 T5,**INPUT SUMMARY**
2 T5,**
3 T5,**
4 T5,**
5 T5,**NUMBER OF COMPOUNDS
6 T5,**NUMBER OF INPUT LINES
7 T5,**SIMULATION DEBUG NUMBER
8 T5,**REPORT DEBUG NUMBER
9 T5,**NUMBER OF DESC. STORED

6010 FORMAT(T5,',''ASOPEN PRINT TYPE''
6020 FORMAT(T5,',''ASOPEN PRINT TYPE''
6030 FORMAT(T5,',''REP FILE NAME''
6040 FORMAT(T5,',''SYSP NUMBER''
6050 FORMAT(T5,',''SYSP NUMBER''
6060 FORMAT(T5,',''BOILING POINT CONV TYPE''
6070 FORMAT(T5,',''BOILING POINT CONV TYPE''

6100 FORMAT(1 T5,**
2 T5,**
3 */)

RETURN
END

*******************************
SUBROUTINE STRIP(REC,INUM,IOLOG,IERR)

NAME OF MODULE - STRIP
MODULE TITLE - RECORD TRAILING STRIPPER
PURPOSE - TO STRIP OFF TRAILING BLANKS FROM A RECORD AND WRITE
OUT (UTILITY FOR IMPT)
MODIFIED - 12-16-88

VARIABLES USED-

VARIABLE I/O TYPE SPEC DIMENSION DESCRIPTION AND RANGE
REC I/O C 80 RECORD TO BE WRITTEN
INUM I I - INTEGER NUMBER OF RECORD
IOLOG I I - I/O LOGICAL NUMBER
IERR O I - ERROR FLAG
0 = OK
1 = NO CHARACTERS IN RECORD

IMPLICIT INTEGER(-N)
CHARACTER*AD REC

IERR=0
INUM=INUM+1

CALL FEND(REC,IE,IERR)
IF(IERR.GT.0)GOTO 9990
WRITE(IOLOG,1000)INUM,REC(1:IE)

FORMAT
1000 FORMAT(IX,14,IX,A)
9990 RETURN
END

SUBROUTINE LHVAP(JC,IERR)

NAME OF MODULE - LHVAP
MODULE TITLE - LIQUID MOLAR VOLUME AT BOILING POINT
PURPOSE - TO CALC LIQUID MOLAR VOLUME AT THE NORMAL BOILING
POINT
MODIFIED - 11-15-88
METHOD - ESTIMATE LHV AT 20 C AND 1 ATM BY DAUBERT METHOD
AND CONNECT TO BOILING POINT BY GUNN & TAYLOR METHOD

VARIABLES USED-

VARIABLE I/O TYPE SPEC DIMENSION DESCRIPTION AND RANGE
JC I I - COMPONENT ARRAY ID
IERR O I - ERROR CODE
0 = OK
-1 = REDUCED TEMP > 0.99
-2 = REDUCED TEMP < 0.1

IMPLICIT REAL'S (A-H,O-Z)
IMPLICIT INTEGER(-N)

PARAMETER (MNC=25)

COMMON /IO / NIN,NOUT,NHSTRY,NHRT
COMMON /DEBUG/ LDBUG,LDBUGR
COMMON /NPROP3/ VOPK(INNC1,API(MNC),SG(MNC),AMW(MNC))
COMMON /CPROP3/ TC(MNC)
COMMON /CPROP5/ OMEGA(MNC)
COMMON /CPROP4/ TB(MNC)
COMMON /CPROP5/ VB(MNC)

IERR=0
IF(LDBUG.GT.1)WRITE(99999,900)

LIQUID MOLAR VOLUME AT 20 DEG C AND 1 ATM (CM**3/KG-MOLE)
CALL TCON(TB(JC),T1,42,IERR)
S1=SG(JC)

CHECK LIMITS ON VOL CALC
IF(T1.LT.569.67D0.OR.T1.GT.1369.67D0)THEN
   CALL MESS(1)
   WRITE(HISTORY,900)
   WRITE(HISTORY,1000)T1
ENDIF

IF(S1.GT.6247D0.OR.S1.GT.1.0244D0)THEN
   CALL MESS(1)
   WRITE(HISTORY,900)
   WRITE(HISTORY,1000)SIG
ENDIF

V=7.6211D-5*T1**2/(2.1262D0+SG**1.8600D0)

LIQUID MOLAR VOLUME AT 20 DEG C AND 1 ATM (M**3/KG-MOLE)
VR=V/1.0D6*1000.00

CORRECT TO BOILING POINT TEMPERATURE TB
TB=(20.0D+77.15D0)/TC(JC)
TB=TB(JC)/TC(JC)
TCALC=0
OMEGA=OMEGA(JC)

CALL GUNYAM(VR,TR,SGHEAT,THEN,TCALC,VO1,IERR)
IERR=IERR

VB(JC)=VO1

FORMAT
500 FORMAT(X,' IN MODULE LNVAPP')
1000 FORMAT(X,'THDUG R) VALUE IS NOT IN RANGE 569.67-1369.67',/, 
   ' IX,'TH-VALUE = ',G12.6,'CALC. CONTINUES')
2000 FORMAT(X,'SG VALUE IS NOT IN RANGE 0.6247-1.0244',/, 
   ' IX,'SG VALUE = ',G12.6,'CALC. CONTINUES')
RETURN

END

SUBROUTINE MAXBNI(HAMPF,VOPK,SG,MAXIT,NDAT,ST,BT,JC,IERR)

NAME OF MODULE - MAXBNI

MODULE TITLE - VAPOR PRESSURES USING MAXWELL-BONELL

PURPOSE - TO CALCULATE VAPOR PRESSURES USING MAXWELL-BONELL
METHOD OF TRIAL AND ERROR FOR THE ESTIMATION OF PRESSURES BASED
UPON BENZENE AS A STANDARD. REFERENCE: I+EC, VOL. 49, 1107, JULY 1957
MODIFIED - 11-3-88 AND COMPLETED

VARIABLES USED:

<table>
<thead>
<tr>
<th>VARIABLE</th>
<th>I/O TYPE SPEC</th>
<th>DIMENSION</th>
<th>DESCRIPTION AND RANGE</th>
</tr>
</thead>
<tbody>
<tr>
<td>MBPF</td>
<td>I</td>
<td>R</td>
<td>MEAN AVG BOILING POINT DEG F</td>
</tr>
<tr>
<td>UCPK</td>
<td>I</td>
<td>R</td>
<td>UOF K OR WATSON K</td>
</tr>
<tr>
<td>SG</td>
<td>I</td>
<td>R</td>
<td>SPECIFIC GRAVITY (60/60F)</td>
</tr>
<tr>
<td>MAXIT</td>
<td>I</td>
<td>I</td>
<td>MAXIMUM ITERATIONS ON CALC</td>
</tr>
<tr>
<td>NDAT</td>
<td>I</td>
<td>I</td>
<td>NUMBER OF DATA POINTS (DEF=50)</td>
</tr>
<tr>
<td>BT</td>
<td>I</td>
<td>R</td>
<td>SMALL TEMP (F) (DEF=-50F FROM VAPF)</td>
</tr>
<tr>
<td>HT</td>
<td>I</td>
<td>R</td>
<td>BIG TEMP (F) (DEF=+50F FROM VAPF)</td>
</tr>
<tr>
<td>JC</td>
<td>I</td>
<td>I</td>
<td>COMPONENT ARRAY ID</td>
</tr>
<tr>
<td>IERR</td>
<td>O</td>
<td>I</td>
<td>ERROR CODE</td>
</tr>
</tbody>
</table>

0 = OK
-1 = NO IMPROVEMENT POSSIBLE IN THE VALUE OF PH EVEN THOUGH CONVERGENCE HAS NOT BEEN REACHED.
-2 = MORE UNKNOWNS THAN FUNCTIONS AND UNIQUE SOLUTION GENERALLY IS IMPOSSIBLE.
-3 = TOTAL NUMBER OF VARIABLES TO BE VARIED IS ZERO
-4 = CONVERGENCE CRITERION NOT BUT FTA STILL LARGE
-5 = IC NOT A VALID NUMBER ON ENTRY
-6 = X(I) IS NOT WITHIN XMIN(I) TO XMAX(I)
-7 = ZERO DIAGONAL ELEMENT IN EQUATION SOLVE
-10 = TRY TO CALC. DERIVATIVE ANALYTICALLY
-11 = RUN EXCEEDED MAXIT SPECIFIED

IMPLICIT REAL*8 (A-H,O-Z)
IMPLICIT INTEGER(I-H)

REAL*8
MBPF

PARAMETER
MIN=N25)

COMMON /IO / NMIN,NOUT,NRSTY,NKPT
COMMON /DEBUG / LDHUG,LD Hugh

COMMON /CPRPG/ PI, XANT(5,NHC), FLXREG(3,NHC)

DIMENSION NDATA(261), DATA(16), OUTPUT(6)

DIMENSION X(501), Y(501), Z(501), A(501), A1(501), A2(501)

DIMENSION R(61), R1(61), R2(61)

IF (LDBG.GT.7) WRITE(*,100)

SET DEFAULTS

NUMBER OF UNKNOWNS
K=3

NUMBER OF DATA POINTS

IF (NDAT.GT.50.AND.NDAT.LE.50) THEN
N=NDAT
ELSE
DEFAULT
NDAT=50
ENDAT
ENDIF
C
IF (ST.LE.0.0D0) ST=MABPF-40.0D0
IF (BT.LE.0.0D0) BT=MABPF+40.0D0
C
IF (LDBUG.GE.5) THEN
DEGFDE=FLOAT(I-I)
ENDIF
C
ITER = 0
IF<IMAXIT.LE.DIMAXIT=10000
C
SET EQUAL TO 1 FOR INITIAL CALL
NDATA(1)=1
C
SET INPUT PARAMETER DATA
DATA(1) - FNU, FACTOR USED TO CHANGE FUA. SET INTERNALLY TO 10.0 IF ZERO ON INITIAL CALL.
DATA(2) - FUA, FACTOR USED TO COMBINE GRADIENT AND NEWTON-RAPHSON METHODS. SET INTERNALLY TO .01 IF ZERO ON INITIAL CALL.
DATA(3) - TAU, USED IN CONVERGENCE TEST. SET INTERNALLY TO 0.001 IF ZERO ON INITIAL CALL.
DATA(4) - EPS, USED IN CONVERGENCE TEST. SET INTERNALLY TO 0.00002 IF ZERO ON INITIAL CALL.
DATA(5) - PHMIN, WHEN PH .LT. PHMIN, PARTIAL DERIVATIVES FROM THE PREVIOUS ITERATION ARE USED INSTEAD OF COMPUTING THEM AGAIN.
DATA(6) THRU DATA(16) - VARIABLES USED INTERNALLY
C
GO TO 10
10 I=1,5
DATA(I)=0.0D0
CONTINUE
C
BV = VARY VECTOR (0=HOLD PARAMETER CONST, 1=ALLOW TO VARY)
C
DO 20 I=1,K
BV(I)=1.0D0
CONTINUE
C
INITIAL VALUES OF BAMS
C
B(1)=10.0D0
B(2)=-1000.0D0
B(3)=1.0D0
C
MIN AND MAX VALUES
C
BMAX(1)=2600.0D0
BMIN(1)=-2600.0D0
BMAX(2)=200000.0D0
BMIN(2)=-500000.0D0
BMAX(3)=20000.0D0
BMIN(3)=-20000.0D0
C
IF (LDBUG.GE.1) THEN
WRITE(NHSTY,1008) K
DO 30 I=1,K
WRITE(NHSTY,1009) B(I), BMIN(I), BMAX(I), BV(I)
CONTINUE
WRITE(NHSTY,1010)
WRITE(NHSTY,1100)
XSUM=0.0D0
XSUM2=0.0D0
YSUM=0.0D0
YSUM2=0.0D0
ENDIF

BEGIN CALC (CALC 5 POINTS TO BE FIT)

\[ \log(PA) = A + \frac{B}{C + \text{TEMP}(K)} \]

\[ \text{DEL} = \frac{\text{BT} - \text{ST}}{\text{FLOAT(NDAT)}} \]

\[ T = \text{ST} - \text{DEL} \]

DO 40 I=1, NDAT

\[ T = T + \text{DEL} \]

CALL MAXBN2(MAIRPF, Dopk, SG, T, MAXIT, PA, IERR2)

CHECK ERR

IF(IERR2 .EQ. 0) THEN
CALL TCON(T, X(I), I4, IERT)
Y(I) = LOG(PA)
ELSE
CALL TCON(MAIRPF, X(I), I1, IERT)
Y(I) = LOG(1.01325D5)
ENDIF

IF(LDBG .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
CONTINUE

MEANS, VARIANCES AND STANDARD DEVS.

IF(LDBG .GE. 7) THEN
XMEAN = XSUM / FLOAT(N)
YMEAN = YSUM / FLOAT(N)
XVAR = (FLOAT(N)*XSUM2 - XSUM*XSUM) / FLOAT(N)*FLOAT(N - 1)
XSD = SQRT(XVAR)
YVAR = (FLOAT(N)*YSUM2 - YSUM*YSUM) / FLOAT(N)*FLOAT(N - 1)
YSD = SQRT(YVAR)
WRITE(NHSTRY, 1120) XMEAN, YMEAN, XVAR, YVAR, XSD, YSD
ENDIF

BEGIN REGRESSION

ITER = ITER + 1
IF(ITER .GT. MAXIT) THEN
CALL MESS(2)
WRITE(NHSTRY, 900)
IERR = -11
WRITE(NHSTRY, 1045) MAXIT, ITER
GOTO 60
ENDIF

EVALUATE Z VECTOR (FUNCTION VALUE)

EQUATION OF FORM LN(PRESI - A + B/C + T)

DO 60 I=1, N
Z(I) = A(I) + B(C) + X(I) + B(T)
CONTINUE

CALC ANALYTICAL DERIVATIVES (PJ VECTOR)
CONTINUE

CALC DERIVATIVE

IF(NDATA(2) .GT. 0) THEN
IERR=-10
CALL MESS(1)
WRITE(NHSTRY,900)
WRITE(NHSTRY,1090)IERR
GOTO 9000
ENDIF

C
C IF(LDBUG.GE.7) THEN
WRITE(NHSTRY,1000)ITER,NDATA(1),{OUTPUT(1),J=1,5}
YMVC = 0.000
SS = 0.000
SSAS=0.000
DO 90 I=1,N
YMVC=YMVC+(Y(I)-Z(I))**2
SS=SS+(Z(I)-YMEAN)**2
SSAS=SSAS+(Y(I))**2-YMEAN**2)
CONTINUE
90
CALC R-SQUARE(SAS VERSION) AND ADJ R-SQUARE
1-VARIANCE OF FULL MODEL/VARIANCE OF MEAN MODEL

RSQU=SS/(SS+YMVC)
IF(SSAS.NE.0.00) THEN
RSUSAS=1.00-YMVC/(SSAS)
ELSE
RSUSAS=0.00
ENDIF
IF(DEGFR.EQ.0.00) THEN
ADJRSQU=0.00
ELSE
ADJRSQU=1.00-(1.00-RSQU)**2/FLOAT(N)-1.00)/DEGFR
ENDIF
IF(RSQU-RSQUAS).GE.1.00 THEN
WRITE(NHSTRY,1112)RSQU,ADJRSQU,RSUSAS,ADJRSUSAS
ELSE
WRITE(NHSTRY,1110)RSQU,ADJRSQU
ENDIF

DO 100 J=1,K
WRITE(NHSTRY,1030)J,H(J)
100
CONTINUE
C
C IF(LDBUG.EQ.0) THEN
WRITE(NHSTRY,1040)
DO 110 I=1,N
YMVC=YMVC+(Y(I)-Z(I))**2
SS=SS+(Z(I)-YMEAN)**2
PERERR=ABS(Z(I)-Y(I))/ABS(Y(I))
IF(NDATA(1).EQ.1.00) THEN
WRITE(NHSTRY,1095)I,Z(I),Y(I),Z(I)-Y(I),PERERR
ENDIF
110
CONTINUE
ENDIF

C
C CALL LSOLVE (E, H, NDATA, DATA, B, BW, BWAN, BHIN, Y, Z, WJ, 
1  OUTPUT, E, A, AC)
C
C NDATA(2) - NCTOR, 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
C IF(NDATA(2)).EQ.00,70
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 TH 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 NOT BUT STILL
C LARGE
C IF = -5, IC NOT A VALID NUMBER ON ENTRY
C IF = -6, H(I) IS NOT WITHIN BMIR(I) TO DMAX(I)
C IF = -7, ZERO DIAGONAL ELEMENT IN EQUATION SOLVE

140 IF(NDATA(3)) LE 0, 140, 120
140	FINAL STATISTICAL RESULTS
150 CONTINUE
190 IF(IARDS. GE. 6) THEN
200 WRITE(NHSTRY, 900)
210 WRITE(NHSTRY, 1000) (TER, NDATA(3), (OUTPUT(J), J = 1, 5))
220 YMVC = 0.0D0
230 SS = 0.0D0
240 SSSAS = 0.0D0
250 DO 150 I = 1, N
260 YMVC = YMVC + Y(I) - M(I))^2
270 SS = SS + (Z(I) - YMEAN)^2
280 SSSAS = SSSAS + (Y(I) - YMEAN)^2
290 CONTINUE

300 CALC R-SQUARE(SAS VERSION) AND ADJ R-SQUARE
310 RSQU = SS/(SS + YMVC)
320 RRSQUAS = 1.0D0 - YMVC/(SSSAS)
330 IF (BEGFR EQ 0.0D0) THEN
340 ADJRJSQU = 0.0D0
350 ADJRJSQAS = 0.0D0
360 ELSE
370 ADJRJSQU = 1.0D0 - (1.0D0 - RSQU)^((FLOAT(N)-1.0D0)/DEGFR)
380 ADJRJSQAS = 1.0D0 - (1.0D0 - RRSQUAS)^((FLOAT(N)-1.0D0)/DEGFR)
390 ENDIF
400 IF (IARDS. RRSQUA - RRSQUAS) GT 1.0D0 THEN
410 WRITE(NHSTRY, 1102) RSQU, ADJRJSQU, RRSQUAS, ADJRJSQAS
420 ELSE
430 WRITE(NHSTRY, 1110) RSQU, ADJRJSQU ENDIF

440 FINAL PARAMETERS
450 DO 160 J = 1, R
460 WRITE(NHSTRY, 1630) J, B(J)
470 CONTINUE

160 CONTINUE
170 FINAL SUMMARY
170 WRITE(NHSTRY, 1040)
180 DO 170 I = 1, N
190 PERERR = AHIS * (1 - Y(I))/AHIS(Y(I))/100.0D0
200 WRITE(NHSTRY, 1095) I, Y(I), Z(I), Z(I) - Y(I), PERERR
210 CONTINUE
220 ENDIF
C LOAD DATA INTO PLANT ARRAY
C IERR = NDATA(3)
DO 180 JJ = 1, 9
PLXANT(I,J) = 0.0D0

180 CONTINUE
C
C IF (IERR .EQ. 0) THEN
C CONVERGED
C
PLXANT(1,JC) = R(1)
PLXANT(2,JC) = R(2)
PLXANT(3,JC) = R(3)
PLXANT(4,JC) = ST
PLXANT(9,JC) = BT
C
IF (DBG .GT. 1) THEN
WRITE (NHOSTY, 900)
WRITE (NHOSTY, 1000) ITER, NDATA(3), (OUTPUT(J), J = 1, 5)
ELSE IF (IERE.R .GT. -1) THEN
PLXANT(1,JC) = B(1)
PLXANT(2,JC) = B(2)
PLXANT(3,JC) = B(3)
PLXANT(4,JC) = ST
PLXANT(9,JC) = BT
CALL MESS(1)
WRITE (NHOSTY, 900)
WRITE (NHOSTY, 1000) ITER, NDATA(3), (OUTPUT(J), J = 1, 5)
WRITE (NHOSTY, 1001)
ELSE IF (IERE.R .GT. -2) THEN
PLXANT(1,JC) = A(1)
PLXANT(2,JC) = A(2)
PLXANT(3,JC) = A(3)
PLXANT(4,JC) = ST
PLXANT(9,JC) = BT
CALL MESS(1)
WRITE (NHOSTY, 900)
WRITE (NHOSTY, 1000) ITER, NDATA(3), (OUTPUT(J), J = 1, 5)
WRITE (NHOSTY, 1002)
ELSE IF (IERE.R .LT. 0) THEN
CALL MESS(2)
WRITE (NHOSTY, 900)
WRITE (NHOSTY, 1000) ITER, NDATA(3), (OUTPUT(J), J = 1, 5)
WRITE (NHOSTY, 1003)
ELSE IF (IERE.R .LT. -1) THEN
PLXANT(1,JC) = A(1)
PLXANT(2,JC) = A(2)
PLXANT(3,JC) = A(3)
PLXANT(4,JC) = ST
PLXANT(9,JC) = BT
CALL MESS(2)
WRITE (NHOSTY, 900)
WRITE (NHOSTY, 1000) ITER, NDATA(3), (OUTPUT(J), J = 1, 5)
WRITE (NHOSTY, 1004)
ELSE IF (IERE.R .LT. -2) THEN
CALL MESS(3)
WRITE (NHOSTY, 900)
WRITE (NHOSTY, 1000) ITER, NDATA(3), (OUTPUT(J), J = 1, 5)
WRITE (NHOSTY, 1005)
ELSE IF (IERE.R .LT. -3) THEN
CALL MESS(3)
WRITE (NHOSTY, 900)
WRITE (NHOSTY, 1000) ITER, NDATA(3), (OUTPUT(J), J = 1, 5)
WRITE (NHOSTY, 1006)
ELSE IF (IERE.R .LT. -4) THEN
CALL MESS(3)
WRITE (NHOSTY, 900)
WRITE (NHOSTY, 1000) ITER, NDATA(3), (OUTPUT(J), J = 1, 5)
WRITE (NHOSTY, 1007)
ELSEIF
PLXREG(1,JC)=FLOAT(ITER)
PLXREG(2,JC)=FLOAT(NDATA(3))
PLXREG(3,JC)=OUTPUT(1)

C FORMATS

900 FORMAT(1X, 'IN MODULE MAXNUM')
1000 FORMAT(/,
1 1X, 'ITERATION: ', I9, '/,
2 1X, 'ERR' = ', F15.6, /
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 PH STILL LARGE'), /
1005 FORMAT(1X, 'JC NOT A VALID NUMBER ON ENTRY'), /
1006 FORMAT(1X, 'X(1) IS NOT WITHIN XMIN(1) TO XMAX(1)'), /
1007 FORMAT(1X, 'ZERO DIAGONAL ELEMENT IN EQUATION SOLVE'), /
1008 FORMAT(/, 1X, 'OBS. Y-CALC 1  % ERROR', /
1 1X, 'K (NUMBER OF PARAMETERS TO BE VARIED) = ', I4, ',/
2 5X, 'N (NUMBER OF DATA POINTS) = ', I4, '/',
3 5X, 'INITIAL B R-MIN R-MAX', /
4 'VARY FLAG', /
1009 FORMAT(2X, '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, 'G15.6')
1030 FORMAT(1X, 'R(''12,'') = ', G13.5)
1039 FORMAT(A10, 1X, 'Y-ACTUAL Y-ERROR', /
1 1X, 'DIFF', /
1055 FORMAT(1X, 4(1X, G13.5))
1100 FORMAT(/, 10X, 'INPUT DATA', /
1 1X, 'X-VALUE Y-VALUE ', /
2 5X, '------ ------ ', /
1110 FORMAT(1X, 'R-SQUARE' = ', F15.6, /
1 1X, 'ADJUSTED R-SQUARE' = ', F15.6, /
1112 FORMAT(1X, 'R-SQUARE' = ', F15.6, /
1 1X, 'ADJUSTED R-SQUARE' = ', F15.6, /
2 1X, 'R-SQUARE = ', F15.6, /
3 1X, 'R-SQUARE = ', F15.6, /
4 1X, 'R-SQUARE = ', F15.6, /
1120 FORMAT(/, 10X, 'STATISTICS', /
1 5X, 'X-VALUES ', 26X, 'Y-VALUES', /
2 5X, '------- ', 26X, '------- ', /
3 5X, 'MEAN = ', G15.5, 6X, 'MEAN = ', G15.5, /
4 5X, 'VARIANCE = ', G15.5, 6X, 'VARIANCE = ', G15.5, /
5 5X, 'STDEV. = ', G15.5, 6X, 'STDEV. = ', G15.5, /
1045 FORMAT(/, 'EXCEEDED MAXIT OF ', 15, ' ITER = ', 15, /
1096 FORMAT(1X, 'ERROR = ', 15, ' TRY TO CALC', /
1 1X, 'DERIVATIVE ANALYTICALLY, CALC. ABORTED')
9006 CONTINUE
RETURN
END

C SUBROUTINE MAXNUM(MABPF, UOPK, SG, TF, MAXIT, PA, IERR)
C
C
NAME OF MODULE - MAXBN2

MODULE TITLE - VAPOR PRESSURES USING MAXWELL-BONELL

PURPOSE - TO CALCULATE VAPOR PRESSURES USING MAXWELL-BONELL

METHOD OF TRIAL AND ERROR FOR THE ESTIMATION OF PRESSURES BASED

UPON BENZENE AS A STANDARD. REFERENCE: I*EC, VOL. 49, 1187, JULY 1957

FOR ONE TEMPERATURE

MODIFIED - 11-4-85

VARIABLES USED-

** VARIABLE I/O TYPE SPEC DIMENSION DESCRIPTION AND RANGE **

- MAFF I R - MEAN AVG BOILING POINT DEG F
- UOF R OR WATSON R
- SG I R - SPECIFIC GRAVITY [60/60]
- TF I R - TEMPERATURE OF VP (F)
- MAXIT I I - MAXIMUM ITERATIONS ON CALC
- PA O R - VAPOR PRESSURE (PA)
- IERR O I - ERROR CODE

0 = OK
-1 = NO IMPROVEMENT POSSIBLE IN THE VALUE OF VP EVEN THOUGH CONVERGENCE HAS NOT BEEN REACHED.
-2 = MORE UNKNOWNS THAN FUNCTIONS AND UNIQUE SOLUTION GENERALLY IS IMPOSSIBLE.
-3 = TOTAL NUMBER OF VARIABLES TO BE VARIED IS ZERO
-4 = CONVERGENCE CRITERION NOT BUT FLA STILL LARGE
-5 = IC NOT A VALID NUMBER ON ENTRY
-6 = X(I) IS NOT WITHIN XMIN(I) TO XMAX(I)
-7 = ZERO DIAGONAL ELEMENT IN EQUATION SOLVE
-16 = TRY TO CALC. DERIVATIVE ANALYTICALLY
-11 = RUN EXCEEDED MAXIT SPECIFIED

IMPLICIT REAL*8 (A-H,O-Z)
IMPLICIT INTEGER*4 (I-N)

REAL*8 MAFF

COMMON /TO / XMIN, XOUT, HISTHY, NREPT
COMMON /DEBUG / LDEBUG, LDEBUG

DIMENSION NDATA(261), DATA(16), OUTPUT(6)

DIMENSION X(?), XMIN(1), XMAX(1), Y(?), YMIN(1), YMAX(1)

11 Z(?), P(?), P(14), A(14), AC(3)

IF (LDEBUG .GT. 7) WRITE (HISTHY, 000)

SET DEFAULTS

NUMBER OF UNKNOWNS
K=1

NUMBER OF EQUATIONS
N=1

ITER = 0

INITIAL GUESS

X(1) = 10. D0**(1-2.31D-2*MAFF)
X(1) = 500. D0

NDATA(1)=1
DO 10 I=1,5
DATA(I)=0.0D0
10 CONTINUE
DO 20 I=1,K
XV(I)=1.0D0
Y(I)=1.0D0
XMAX(I)=500000.0D0
XMIN(I)=1.0D-20
20 CONTINUE
IF(X(1).LT.XMIN(I))X(1)=XMIN(I)
IF(X(1).GT.XMAX(I))X(1)=XMAX(I)
TR=459.67D0
CALC BEGINS
RTF=TF*TR
IF(UOPK.LE.0.0D0) UOPK=MAHFPP*(1.0D0/3.0D0)/SG
MAX. BON. CONV. LOOP BEGINS
ITER=ITER+1
IF(ITER.GT.MAXIT)THEN
ITER=11
CALL HESS(I)
WRITE(11,HISTORY,900)
WRITE(11,HISTORY,1000)MAXIT,ITER
GOTO 9000
ENDIF
CHECK IF MEAN AVE BP IS GE 400
IF(MAHFPP.GE.400.0D0)THEN
T=MAHFPP+TR+(2.5D0*(UOPK-12.0D0)*(1.0D0/X(1))/2.302559D0))
ENDIF
CHECK IF MEAN AVE BP IS LE 100
ELSE IF(MAHFPP.LE.100.0D0) THEN
T=MAHFPP
ELSE
MEAN AVE BP IN RANGE 200 TO 400.
EFK=0.065100*MAHFPP-1.0D0
FIRST TRIAL FROM BOILING POINT
T=MAHFPP+((2.5D0*(UOPK-12.0D0)*(1.0D0/X(1))/2.302559D0))
ENDIF
AX=T*(((1.0D0/RTF)-0.8802867D0)/(1.0D0-0.2145307D0))
IF(AX.GE.0.0621044D0) THEN
FOR VAPOR PRESSURE BELOW 2 MMHG (AX<0.002184)
PRE=2576.66161D0*AX-3.916261D0/((13.0D0*AX)-0.987672D0)
ELSE IF(AX.LT.0.0013676D0) THEN
FOR VAPOR PRESSURE AT 760 MMHG (AX>0.001367)
PRE=12666.376D0*AX-3.56155D0/((36.0D0*AX)-0.989679D0)
ELSE
FOR VAPOR PRESSURE IN RANGE 2-760 MMHG (AX=0.001367-0.002184)
PRE=(2387.262D0*AX-1.192572D0)/((95.76D0*AX)-0.972546D0)
ENDIF
PSAVE AND X(I) ARE IN ATM
PSAV = 10.00 \times 10^6

Z(1) = PSAV - X(1)

CALL YSOLVE (K, N, NDATA, DATA, X, XV, XMAX, XMIN, Y, Z, PJ, J, OUTPUT, P, A, AC)

IF (LDBG. GT. 5) THEN
  WRITE(NHSTRY, 900)
  WRITE(NHSTRY, 1000) ITER, NDATA(3), (OUTPUT(J), J = 1, 5)
ENDIF

CALL FUNCTION

IF (NDATA(2) .EQ. 0) THEN
  GOTO 50
ENDIF

CALL DERIVATIVE

ELSE IF (NDATA(2) .GT. 0) THEN
  IERR = -10
  CALL MESS(3)
  WRITE(NHSTRY, 900)
  WRITE(NHSTRY, 1000) IERR
  GOTO 9000
ENDIF

NDATA(2) < 0 CHECK NDATA(3)
NDATA(3) = NUMBER OF VARIABLES NOT SATISFYING CONV. CRITERION
IF (NDATA(3) .GT. 0) GOTO 50

IERR = NDATA(3)

CONVERGED OR PROBLEM

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 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, 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 (ITERM.EQ.-7) THEN
    CALL MESS(2)
    WRITE(NHSTRY,900)
    WRITE(NHSTRY,1000)ITER,NDATA(3),IOUTPUT(1,3),J=1,5
    WRITE(NHSTRY,1001)
END IF

IF (DEBUG.GT.5) THEN
    WRITE(NHSTRY,900)
    WRITE(NHSTRY,1000)ITER,NDATA(3),IOUTPUT(1,3),J=1,5
    WRITE(NHSTRY,1100)TF,X(1),Z(1),PA
END IF

FORMATS

900 FORMAT (X,'IN MODULE MAXMIN')
1000 FORMAT (/,
1 IX,'ITERATION: ',15,’/,
2 IX,'ITER' = ',+15,'/,
3 IX,'SUM OF SQUARES' = ',G15.0,'/,
4 IX,’ANGLE (DEGREES)' = ',G15.2,'/,
5 IX,’NUMBER OF TIMES YSOLVE CALLED' = ',F15.1,'/,
6 IX,’NUMBER OF FUNCTIONAL EVALUATIONS' = ',F15.1,'/,
7 IX,’NUMBER OF ANALYTICAL DERIVATIVE EVALUATIONS' = ',F15.1,'/)
1001 FORMAT (X,’NO IMPROVEMENT POSSIBLE IN THE VALUE OF',/
1 IX,’... EVEN THOUGH CONVERGENCE HAS NOT BEEN REACHED',/
1002 FORMAT (X,’MORE UNKNOWNS THAN FUNCTIONS AND UNIQUE',/
1003 FORMAT (X,’TOTAL NUMBER OF VARIABLES TO BE VARIED = ',/)
1004 FORMAT (X,’CONVERGENCE CRITERION NOT MET BUT F (X) STILL LARGE’,/)
1005 FORMAT (X,’IS NOT A VALID NUMBER ON ENTRY',/)
1006 FORMAT (X,’X(I) IS NOT WITHIN XMIN(I) TO XMAX(I)',/)
1007 FORMAT (X,’ZERO DIAGONAL ELEMENT IN EQUATION SOLVE',/)
1008 FORMAT (/,
1 IX,’****RUN EXCEEDED MAXIT OF ’,15,’ ITERATION’,/
2 ’**’*’*’*’*)
1050 FORMAT (X,’ERROR = ’,G15.1,’ ’, ’TRY TO CALC.’,/
1 ’ ’ DERIVATIVE ANALYTICALLY, CALC. ABORTED’)
1100 FORMAT (X,’TEMPERATURE (DEG F) = ’,G15.2,’/
1 FZA = ’,G15.2,’ DELTA = ’,G15.2,’ PRESS(PSI) = ’,G15.2)
9000 CONTINUE
   RETURN
END

SUBROUTINE MESS(IERROR)

NAME OF MODULE - MESS
MODULE TITLE - WRITE OUT CALC MESSAGES
PURPOSE - TO WRITE OUT MESSAGES
MODIFIED - 10-28-88

VARIABLES USED -

VARIABLE / TYPE-SPEC DIMENSION / DESCRIPTION AND RANGE / ERROR
I / I / - / ERROR FLAG

0 = NONE
1 = ‘WARNING’ (POSSIBLE PROBLEM)
2 = ‘ERROR’ (CONTINUE ON ERROR)
3 = ‘SEVERE ERROR’ (STOP ON ERROR)

IMPLICIT INTEGER(-N)

COMMON / IO / MN,ROUT,NHSTRY,NREPT
COMMON / IERR / IAMV,INERR,INERR
COMMON / IROR / GOTO 999
IF (IERR.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 FORMATS
C
1000 FORMAT (5X, 'WARNING')
2000 FORMAT (5X, 'ERROR')
3000 FORMAT (5X, 'SEVERE ERROR')
C
CONTINUE
RETURN
END

C SUBROUTINE NEED(IERR)
C
NAME OF MODULE - NEED
MODULE TITLE - CALC NEEDED PARAMETERS
PURPOSE - TO CALC NEEDED PARAMETERS FROM INPUT DATA
MODIFIED - 10-28-88

VARIABLES USED -

VARIABLE I/O TYPE SPEC DIMENSION DESCRIPTION AND RANGE
IERR G 0 1 - ERROR CODE
0 = OK
-1 = BOTH API AND UOP K VALUES SPEC.
-2 = BOTH API AND UOP K VALUES SPEC.
   LESS THAN ZERO
-3 = ALL CALC OUT OF SPEC RANGE

IMPLICIT REAL*8 (A-H,O-Z)
IMPLICIT INTEGER (1-1)

REAL*8 HAPI, HAPIK, HAPIPO
C
PARAMETER (MNC=25)
C
CHARACTER*32 CHAIN
C
COMMON /IG/ NH,MOUT,NHSTRY,NREPT
COMMON /DEBUG/ LDBUG,LDEBUG
C
COMMON /NROP1/ NCOMP,CHAIN(MNC),ICT
COMMON /NROP2/ VAPI(MNC),SAPI(MNC),CARAPI(MNC),HAPI(MNC),HAPIPO(MNC)
COMMON /NROP3/ UAPI(MNC),AAPI(MNC),SCAPI(MNC),MMAPI(MNC)
COMMON /NROP4/ DAPI(MNC),FAPI(MNC),FPAPI(MNC),IFP
COMMON /CALCV/ NCAL(VMNC)
C
COMMON /LDBGUL/ XFAP(MNC),XFAPI(MNC)
C
IF (LDBGUG.GT.7) WRITE (NHSTRY, 900)
C
IERR = 0
C
C OT = 1.00/1.00
C
DO 10 JC = 1, NCOMP
NCALC(JC)=1

CALL CAMP AND MABP FROM VABP AND SLOPE OF TBP CURVE OR ASTM CURVE

CALL TCON(VABP(JC),VABP(JC),J1,IERT)
IF (ICF.EQ.1) THEN
   CALL ASTMCF(VABP(JC),SLOP(JC),CABPO,MABPO,IERC)
ELSE
   CALL TBPCF(VABP(JC),SLOP(JC),CABPO,MABPO,IERC)
ENDIF
CALL TCON(CABPO,CABP(JC),14,IERT)
CALL TCON(MABPO,MABP(JC),14,IERT)

CALC MEAN AVER BP

MEABP(JC)=(CABP(JC)+MABP(JC))/2.D0

CHECK REST OF INPUT (SG,AP1,WK)

ALL SPECIFIED

IF (API(JC).GT.0.D0.AND. UOPK(JC).GT.0.D0.AND. SG(JC).GT.0.D0) THEN
   UOPK(JC)=0.D0
   SG(JC)=0.0D0
   CALL MESS(1)
   WRITE(NHSTRY,900)
   WRITE(NHSTRY,1000)
   IERR=-1
ENDIF

NOT ENOUGH DATA

IF (API(JC).LE.0.D0.AND. UOPK(JC).LE.0.D0.AND. SG(JC).LE.0.D0) THEN
   CALL MESS(2)
   WRITE(NHSTRY,900)
   WRITE(NHSTRY,2000)
   NCALC(JC)=0
   IERR=-2
ELSE IF (API(JC).GT.0.D0.AND. UOPK(JC).LE.0.D0.AND. SG(JC).LE.0.D0) THEN
   SG(JC)=141.5D0/1API(JC)+131.5D0
   CALL TCON(MEABP(JC),TEMPR,42,IERT)
   UOPK(JC)=TEMPR**OT/SG(JC)
ELSE IF UOPK GIVEN CALL API AND SG
ELSE IF API(GIVEN CALL WATSON K AND SG)
ELSE IF SG GIVEN CALL API AND UOPK
ELSE IF API(JC).LE.0.D0.AND. UOPK(JC).GT.0.D0.AND. SG(JC).LE.0.D0) THEN
   API(JC)=141.5D0/SG(JC)-131.5D0
   CALL TCON(MEABP(JC),TEMPR,42,IERT)
   UOPK(JC)=TEMPR**OT/SG(JC)
ELSE IF API AND SG GIVEN USE API TO CALC SG AND UOPK
ELSE IF(API(JC)).GT.0.00.AND.UOPK(JC).LE.0.00.AND.1
SG(JC) = 141.50/(API(JC)+131.50)

CALL TCON(MEABP(JC),TEMPR,42,IERT)
UOPK(JC) = TPRR*0.0/T/SG(JC)

IF UOPK AND SG GIVEN USE SG TO CALC API AND UOPK

ELSE IF(API(JC)).LE.0.00.AND.UOPK(JC)).GT.0.00.AND.
SG(JC)).GT.0.00.AND.
API(JC) = 11.50/SG(JC)-131.50
CALL TCON(MEABP(JC),TEMPR,42,IERT)
UOPK(JC) = TPRR*0.0/T/SG(JC)

IF UOPK AND API GIVEN USE API TO CALC SG AND UOPK

ELSE IF(API(JC)).GT.0.00.AND.UOPK(JC)).GT.0.00.AND.
SG(JC)).LE.0.00.AND.
SG(JC) = 141.50/(API(JC)+131.50)

CALL TCON(MEABP(JC),TEMPR,42,IERT)
UOPK(JC) = TPRR*0.0/T/SG(JC)
ELSE
ERROR
CALL MESS(2)
WRITE(NHSTRY,900)
WRITE(NHSTRY,2010)
IERR = 2
ENDIF

CALC HOLE UT IF NEEDED

IF(AMW(JC)).LE.0.00.AND.
CALL TCON(MEABP(JC),TEMPR,42,IERT)
CALL RDMP(TEMPR,API(JC),SG(JC),AMW(JC),IERT)
IF(IERR).LT.0.01 IERR = -3
ENDIF

CHECK PERCENT PARAFFINS ETC

PSUM = PA(JC)+PN(JC)+PI(JC)

IF(PSUM).LE.0.00.OR.IPF.EQ.0) THEN
ESTIMATE % PARA, NAP, AND AO
CALL MESS(1)
WRITE(NHSTRY,900)
WRITE(NHSTRY,3060)
CALL TCON(MEABP(JC),TF,41,IERT)
CALL ESTMP(TF,JC,IERT)
ELSE IF(PSUM).EQ.100.D0 THEN
CALL XA,XH,YF
XA0(JC) = PA(JC)/PSUM
YNAP(JC) = PA(JC)/PSUM
XPAR(JC) = PA(JC)/PSUM
ELSE
WRITE WARNING & NORMALIZE
XA0(JC) = PA(JC)/PSUM
PA(JC) = XA0(JC)*100.D0
YNAP(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),
  XPAR(JC),XNAP(JC),XARO(JC)
ENDIF

10 CONTINUE
C
CHECK FOR PROPERTIES NEEDED FOR SYSOP
C
CALL CHESOP(IERC)
C
FORMAT
C
500 FORMAT('IN MODULE NEED')
1000 FORMAT('BOTH API AND UOP & VALUES SPECIFIED',/,
  1     'API VALUE USED AND CALC. CONTINUES')
2000 FORMAT('BOTH API AND UOP & VALUES SPECIFIED ARE LESS THAN 0.0',/,
  1     'CALC. BYPASSED FOR THIS COMPOUND')
2010 FORMAT('INVALID SPECIFICATION',/,
  1     'CALC. BYPASSED FOR THIS COMPOUND')
3000 FORMAT('PERCENT PARAFFINS,NAPHTHENES, AND AROMATICS ARE ALL',/,
  1     '0.0 VALUES WILL BE ESTIMATED.')
4000 FORMAT('PERCENT PARAFFINS,NAPHTHENES, AND AROMATICS INCORRECTLY',/,
  1     'SPECIFIED. VALUES WILL BE NORMALIZED.')
5000 FORMAT('VALUES FOR PARAFFINS,NAPHTHENES, AND AROMATICS',/,
  1     'PERCENT:',3(I1,13.6),'/
  2     'FRACTIONS:',3(I1,13.6))
C
RETURN
END
C
SUBROUTINE NFMP(TBK,SG,XP,XN,XA,FPT,IERR)
C
NAME OF MODULE - NFMP
C
MODULE TITLE - TO CALC NORMAL FREEZING/HEATING POINT
C
PURPOSE - TO CALC NORMAL FREEZING/HEATING POINT OF A PETROL. FRACT.
C
MODIFIED - 12-19-88
C
VARIABLES USED-
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 NAPHTHENES
C   XA I R - MOLE FRACTION AROMATICS
C   FPT O H - NORMAL FREEZING/HEATING POINT DEG K
C   IERR O I - ERROR CODE
C
IMPLICIT REAL*4(A-H,O-Z)
IMPLICIT INTEGER*4(I-N)
C
COMMON /M0 / MH,HT,HOUT,NHSTRY,KEPT
COMMON /LDBG/LDBG,LDDBG
C
1000 IERH=0
IF(LDBUG.GE.7) WRITE(NHSTRY,900)
C
DATA REGRESSED FOR PARAFFINS
C
AP=EXP(-3.3158D0)
BP=1.4185D0
CP=-0.85142D-1
FMPP = AP * TBK + BP * SG + CP

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. 310.0D0) THEN
CALL MESS(1)
WRITE(NHSTRY, 900)
WRITE(NHSTRY, 1100)FMPP
FMPP = 310.0D0
ENDIF

DATA REGRESSED FOR NAPHTHENES

AN = EXP(10.396D0)
BN = -0.63128D0
CN = 5.6091D0

FMN = AN * TBK + BN * SG + CN

IF (FMN .LT. 130.7D0 .AND. XN .GT. 0.D0) THEN
CALL MESS(1)
WRITE(NHSTRY, 900)
WRITE(NHSTRY, 2000)FMN
FMN = 130.7D0
ENDIF

IF (FMN .GT. 265.0D0) THEN
CALL MESS(1)
WRITE(NHSTRY, 900)
WRITE(NHSTRY, 2100)FMN
FMN = 265.0D0
ENDIF

DATA REGRESSED FOR AROMATICS

AA = EXP(6.297D0)
RB = -0.67363D0 - 1
CA = 4.0603D0

FMF = AA * TBK + BA * SG + CA

IF (FMF .LT. 173.7D0 .AND. XA .GT. 0.D0) THEN
CALL MESS(1)
WRITE(NHSTRY, 900)
WRITE(NHSTRY, 3000)FMF
FMF = 173.7D0
ENDIF

IF (FMF .GT. 352.5D0) THEN
CALL MESS(1)
WRITE(NHSTRY, 900)
WRITE(NHSTRY, 3100)FMF
FMF = 352.5D0
ENDIF

EST. FOR FRACTION

FPT = XP * FMPP + XN * FMN + XA * FMF

FORMATS

900 FORMAT(IX, 'IN MODULE NFMP')
1000 FORMAT(IX, 'FPT VALUE FOR PARAFFINS IS LESS THAN 110.251 ',/,
1 IX, 'FPT VALUE OF ', G15.6, ' SET TO 110.251 CALC. CONTINUES')
1100 FORMAT(IX, 'FPT VALUE FOR PARAFFINS IS GREATER THAN 310.0 ',/,
1       'FPT-VALUE OF ',G15.6,' SET TO 310 CALC. CONTINUES')
2000  FORMAT(1X,'FPT VALUE FOR NAPHTHENES IS LESS THAN 130.71 ',/,
         1  'FPT-VALUE OF ',G15.6,' SET TO 265 CALC. CONTINUES')
2100  FORMAT(1X,'FPT VALUE FOR NAPHTHENES IS GREATER THAN 265.0 ',/,
         1  'FPT-VALUE OF ',G15.6,' SET TO 265 CALC. CONTINUES')
3000  FORMAT(1X,'FPT VALUE FOR AROMATICS IS LESS THAN 173.7 ',/,
         1  'FPT-VALUE OF ',G15.6,' SET TO 173.7 CALC. CONTINUES')
3100  FORMAT(1X,'FPT VALUE FOR ANOMATICS IS GREATER THAN 352.0 ',/,
         1  'FPT-VALUE OF ',G15.6,' SET TO 352 CALC. CONTINUES')
C
RETURN
END
C**********************************************************************
C
SUBROUTINE OPENFITYP, IERR
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 .INF
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  1        OPEN CALC FLAG
C       0 = ALL (.INF,.HIS,.REP)
C       1 = INPUT FILE (.INF)
C       2 = HISTORY FILE (.HIS)
C       3 = REPORT FILE (.REP)
C IERR  I/O  1    ERROR CODE
C       0 = OK
C       1 = FILE SPEC ERROR ON .INF FILE
C       2 = FILE SPEC ERROR ON .HIS FILE
C       3 = FILE SPEC ERROR ON .REP FILE
C
C PARAMETER (MAXFIE=100)
C
C IMPLICIT INTEGER(*)
C C CHARACTER*32 FILE, FILINF, FILHIS, FILREP
C COMMON /IO/ NINF, NOBT, NSTR, NREPT
C COMMON /FILES/ FILE
C COMMON /ERRMSG/ LRANG, LEBLANG, LTBANG
C
C .INF FILE
C IF( ITYP.EQ.1.OR.ITYP.EQ.0)THEN
C FILE = FILINF
C C INPUT FILE FILINF
C C IFINF=0
C 100 IF(INF.EQ.FILINF)THEN
C IF(INF.EQ.498)THEN
C IERR=2
C WRITE(' F',5000)
C WRITE(4,900)
C WRITE(4,10000)
C GOTO 9999
C ENDIF
C OPEN(UNIT=NINF, FILE=FILINF, STATUS='OLD', DEFAULTFILE='.'.
C
ENDIF

WRITE FINAL FLAG
CALL SECOND(TIME)
WRITE(HISTORY, 1000) NCOMP, TIME, IWARN, INERR, ISERR

FORMATS

100 FORMAT(2X, 'Enter input data file name ', $)
200 FORMAT(A32)

250 FORMAT(5X, 'SUCCESSFUL OPEN OF INPUT FILE '' ')
300 FORMAT(5X, 'SUCCESSFUL OPEN OF HISTORY FILE '' ')
500 FORMAT(5X, 'INPUT READ COMPLETE '' ')
510 FORMAT(5X, ' WARNING IN READ (SEE .HIS) '' ')
520 FORMAT(5X, ' ERR IN READ (SEE .HIS) '' ')
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) '' ')
800 FORMAT(5X, ' CALCULATE NEEDED VALUES COMPLETE '' ')
810 FORMAT(5X, ' ERROR/WARNING IN NEED ROUTINE (SEE .HIS) '' ')
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, ' ESTPHO ENDS EXECUTION '' ')
2 T5, ''
3 T5, ' NUMBER OF COMPOUNDS ...................... I10, ''
4 T5, ''
5 T5, ' CPU TIME .................................. JX, G12.6, ''
6 T5, ' NUMBER OF WARNINGS PRINTED ........... I10, ''
7 T5, ''
8 T5, ' NUMBER OF ERRORS PRINTED ............ I10, ''
9 T5, ''
10 T5, ''

STOP
END

SUBROUTINE ANDRA(JC, IERR)

NAME OF MODULE - ANDRA
MODULE TITLE - CALCULATE MODIFIED ANDRADE MODEL PARAMETERS
PURPOSE - TO CALC PARAMETERS FOR MODIFIED ANDRADE MODEL
FOR LIQ VISCOSITY FROM DATA OBTAINED FROM LETSOU-STIEL(1973)
MODEL
MODIFIED - 10-19-88
FOR 0.75<TR<0.98

VARIABLES USED:

VARIABLE I/O TYPE SPEC DIMENSION   DESCRIPTION AND RANGE

JC  I   1    -   COMPONENT ARRAY ID
IERR  0   1    -   ERROR CODE
0 = OK
-1 = NO IMPROVEMENT POSSIBLE IN
   THE VALUE OF PH EVEN THOUGH
   CONVERGENCE HAS NOT BEEN REACHED.
-2 = MORE UNKNOWNS THAN FUNCTIONS AND
UNIQUE SOLUTION GENERALLY IS IMPOSSIBLE.

-3 = TOTAL NUMBER OF VARIABLES TO BE
VARIED IS ZERO
-4 = CONVERGENCE CRITERION MET BUT FLA
STILL LARGE
-5 = IC NOT A VALID NUMBER ON ENTRY
-6 = X(J) IS NOT WITHIN XM(K(I)) TO
XMAX(I)
-7 = ZERO DIAGONAL ELEMENT IN EQUATION
SOLVE
-10 = TRY TO CALC. DERIVATIVE
ANALYTICALLY
-11 = RUN EXCEEDED MAXIT SPECIFIED

IMPLICIT REAL*8 (A-H,O-Z)
IMPLICIT INTEGER(I-M)

REAL*8 MULAND, MULREG

PARAMETER (MNC=25)

COMMON /IO/ NIN, NOUT, NINTRY, NNEPT
COMMON /NLPOP3/ UOPK(MNC), API(MNC), SG(MNC), AMW(MNC)
COMMON /CPPUL/ TC(MNC), PC(MNC)
COMMON /CPPUL0/ OMEGA(MNC)
COMMON /CPPUL09/ MULAND(5, MNC), MULREG(3, MNC)

DIMENSION NDATA(24), DATA(16), OUTPUT(6)

DIMENSION X(50), XV(50), XMAX(30), XM(K(I)), Y(50),
Z(100), PJ(50), P(206), AM15, AC15

DIMENSION H(61, BV), ZXMAX(3), DHM(3)

CONSTANTS
OS=1.D0/6.D0
OH=1.D0/2.D0
TT=2.D0/3.D0

X1=2.173564'TC(JC)'/OS / AM(WJC)' 'OH ' PC(JC)' TT

SET UP RANGE FOR LETSOU-STEIL

THL=0.76D0
TRH=0.98D0
TRD=1TRH-TRL)/50.5D0

TH=TRL-TRD

MARQUARDT SET DEFAULTS

NUMBER OF UNKNOWNS
k=3
NUMBER OF DATA POINTS
N=50

IF (LHUG.GE.5) THEN
DEGF=FLOAT(N-k)
ENDIF

ITER = 0
IF (MAXIT.LE.0) MAXIT=10000

SET EQUAL TO 1 FOR INITIAL CALL
NDATA(1)=1
SET INPUT PARAMETER DATA

DATA(1) - FNU, FACTOR USED TO CHANGE FLA. SET INTERNALLY TO 10.0 IF ZERO ON INITIAL CALL.

DATA(2) - FLA, FACTOR USED TO COMBINE GRADIENT AND NEWTON-RAPHSON METHODS. SET INTERNALLY TO .01 IF ZERO ON INITIAL CALL.

DATA(3) - TAU, USED IN CONVERGENCE TEST. SET INTERNALLY TO 0.001 IF ZERO ON INITIAL CALL.

DATA(4) - EPS, USED IN CONVERGENCE TEST. SET INTERNALLY TO 0.000002 IF ZERO ON INITIAL CALL.

DATA(5) - BEHMIN, WHEN PH .LT. BEHMIN, PARTIAL DERIVATIVES FROM THE PREVIOUS ITERATION ARE USED INSTEAD OF COMPUTING THEM AGAIN.

DATA(61 THRU DATA(161)) - VARIABLES USED INTERNALLY

DO 10 I=1,5
DATA(11)=0.000000
10 CONTINUE

BV = VARY VECTOR (0=HOLD PARAMETER CONST, 1=ALLOW TO VARY)

DO 20 I=1,5
BV(I)=1.000
20 CONTINUE

INITIAL VALUES OF PArms

B(1)=1.000
B(2)=1.000
B(3)=0.000

MIN AND MAX VALUES

BM(1)=2000.000
BMN(1)=-2000.000
BM(2)=200000.000
BMN(2)=-500000.000
BM(3)=2000.000
BMN(3)=-2000.000

IF(LDBUG.GE.7)THEN
WRITE(HISTRY,1000)I,J
GO TO 10
WRITE(HISTRY,1001),BMIN(I),BM(1),BY(I)
GO TO 10
WRITE(HISTRY,1010)
WRITE(HISTRY,1100)
1000 XSUH=0.000
XSOH=0.000
YSUH=0.000
YESH=0.000
END IF

BEGIN CALC (CALC 50 POINTS TO BE FIT)
LOG(ETA)=A0*TEMP(I) + C*log(TEMP(K))

UNIVERSAL FUNCTIONS FOR LETSOH-STIEL MODEL

UF0 = (H X )
UF1 = (H X 1 )

DO 90 I=1,50
TR=TR+TRD
UF0=0.01517100-0.0214500*TR+0.0075000*TR*TR
UF1=0.04255200-0.0767400*TR+0.0340000*TR*TR
Y(I)=LOG(UF0+UF1+OMEGA(JC))/X1
X1=TR+TC(JC)
90 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
CONTINUE
MEANS, VARIANCES AND STANDARD DEV.

IF(LDBG.GE.7) THEN
XMEAN=XSUM/REAL(N)
XVAR=(REAL(N)*XSUM2-XSUM*XSUM)/REAL(N/REAL(N-1))
XSD=SQRT(XVAR)
YMEAN=YSUM/REAL(N)
YVAR=(REAL(N)*YSUM2-YSUM*YSUM)/REAL(N/REAL(N-1))
YSD=SQRT(YVAR)
WRITE(NHSTRY,120)XMEAN,YMEAN,XVAR,YVAR,XSD,YSD
ENDIF

BEGIN REGRESSION
ITER=ITER+1
IF(ITER.GT.MAXIT) THEN
TERM=-11
WRITE(NHSTRY,1045)MAXIT,ITER
GOTO 9000
ENDIF

EVALUATE Z VECTOR (FUNCTION VALUE)

REGRESS TO MODIFIED LANDAE MODEL
V1=NLAND(1)+NLAND(2)/T+NLAND(3)*LN(T)

DO 60 I=1,N
V1(I)=V1(I)+B(I)*X(I)
CONTINUE

CALC ANALYTICAL DERIVATIVES (PJ VECTOR)
CONTINUE

CALC DERIVATIVE

IF(NDATA(I).GT.0) THEN
TERM=-10
WRITE(NHSTRY,1090)TERM
GOTO 9000
ENDIF

IF(LDBG.GE.7) THEN
WRITE(NHSTRY,1000)TERM,NDATA(I),OBSERVED(I),T,I,5

RMYC = 0.000
SS = 0.000
SSSAS=0.000
DO 90 I=1,N
YMYC=RMYC+Y(I)**2
SS=SS+2(I)-YMEAN**2
SSSAS=SSSAS+Y(I)**2-YMEAN**2
CONTINUE

CALC R-SQUARE (SAS VERSION) AND ADJ R-SQUARE

1-VARIANCE OF FULL MODEL/VARIANCE OF MEAN MODEL

RSQ=SS/(SS+RMYC)
IF(SSSAS.NE.0.0) THEN
RSQUSAS=1.0-RMYC/(SSSAS)

ELSE
    RSQUSAS=0.D0
ENDIF
IF (DEGRF.EQ.0.D0) THEN
    ADJRSQU=0.0D0
ELSE
    ADJRSQU=1.0D0-(1.0D0-RSQU)*(FLOAT(N)-1.0D0)/DEGRF
ENDIF
IF (ABS(RSQUSAS).GT.1.0D0) THEN
    WRITE(NHSTRY,1112)HSQU,ADJSQUS,RSQUSAS,ADJRSQUS
ELSE
    WRITE(NHSTRY,1110)HSQU,ADJRSQU
ENDIF
C
DO 100 J=1,K
    WRITE(NHSTRY,1030)J,NHSTRY
100 CONTINUE
C
IF (LDBG, 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(Y(I)-Z(I))/ABS(Y(I))*100.D0
        WRITE(NHSTRY, 1095)I, Y(I), Z(I), Y(I)-Z(I), PERERR
110 CONTINUE
ENDIF
C
120 CALL YSOLVE (K, N, NDATA, DATA, N, NV, BMX, BMIN, Y, Z, P3,
     1 OUTPUT, P, R, AC)
C
NDATA(2) - VECTOR, USED FOR CONTROL IN CALLING PROG.
    IF = 0, CALCULATE FUNCTION
    IF = 1, CALCULATE DERIVATIVE
    IF = -1, EXAMINE EACH FOR WHAT TO DO NEXT
C
IF (NDATA(2)) 130, 50, 70
C
NDATA(3) - LEVR, MAY TAKE ON VARIOUS VALUES
    IF POSITIVE, CONTAINS THE NUMBER OF VARIABLES NO
SATISFYING CONVERGENCE CRITERION
    IF = 0, CONVERGENCE SATISFIED AND SOLUTION RETU
    IF = -1, NO IMPROVEMENT POSSIBLE IN THE VALUE OF
        E EVEN THOUGH CONVERGENCE HAS NOT BEEN
        REACHED.
    IF = -2, MORE UNKNOWNS THAN FUNCTIONS AND UNIQUE
        SOLUTION GENERALLY IS IMPOSSIBLE.
    IF = -3, TOTAL NUMBER OF VARIABLES TO BE VARY
        ED 0
    IF = -4, CONVERGENCE CRITERION NOT MET BUT MLA STILL
        LARGE
    IF = -5, IF NOT A VALID NUMBER OR ENTRY
    IF = -6, B(I) IS NOT WITHIN BMX(I) AND BMX(I)
    IF = -7, ZERO DIAGONAL ELEMENT IN EQUATION SOLVE
C
130 IF (NDATA(3)) 140, 150, 120
C
FINAL STATISTICAL RESULTS
C
140 CONTINUE
IF (LDBG.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
150
C
145
SS = SS + (Z(I) - YMEAN)**2
SSAS = SSAS + (Y(I)**2 - YMEAN)**2

CONTINUE

CALC R-SQUARE (SAS VERSION) AND ADJ R-SQUARE

RSQUAS = 1 - VARIANCE (FULL MODEL) / VARIANCE (MEAN MODEL)

RSQU = SS / (SS + YMYC)

ADJRSQU = 1 - (1 - RSQU) * (FLOAT(N) - 1) / DEGFR

ADJRSQUAS = 1 - (1 - RSQUAS) * (FLOAT(N) - 1) / DEGFR

END IF

WRITE(NHSTRY, 112) RSQU, ADJRSQU, RSQUAS, ADJRSQUAS

ENDIF

FINAL PARAMETERS

DO 160 J = 1, K

WRITE(NHSTRY, 1041) J, B(J)

160 CONTINUE

END

FINAL SUMMARY

WRITE(NHSTRY, 1040)

DO 170 T = 1, N

PERERR = ABS(Z(I) - Y(I)) / ABS(Y(I)) * 100.0

WRITE(NHSTRY, 10551) T, Z(I), Y(I), Z(I) - Y(I), PERERR

170 CONTINUE

END IF

LOAD DATA INTO MULAND ARRAY

IF (IERR.EQ.0) THEN

MULAND(3, JC) = 0.0

ENDIF

IF (IERR.EQ.1) THEN

MULAND(3, JC) = B(3)

ENDIF

WRITE(NHSTRY, 1000) ITER, NDATA(3), OUTPUT(J), J = 1, 5

ENDIF

END

146
MULAND(1,JC) = TRL*TC(JC)
MULAND(5,JC) = TH*TC(JC)
WRITE(NHSTRY,1000)IB, NDATA(3), (OUTPUT(J), J=1,5)
WRITE(NHSTRY,1002)
ELSE IF (IERR.EQ.-3) THEN
WRITE(NHSTRY,1000)IB, 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) = TH*TC(JC)
WRITE(NHSTRY,1000)IB, NDATA(3), (OUTPUT(J), J=1,5)
WRITE(NHSTRY,1004)
ELSE IF (IERR.EQ.-5) THEN
WRITE(NHSTRY,1000)IB, NDATA(3), (OUTPUT(J), J=1,5)
WRITE(NHSTRY,1005)
ELSE IF (IERR.EQ.-6) THEN
WRITE(NHSTRY,1000)IB, NDATA(3), (OUTPUT(J), J=1,5)
WRITE(NHSTRY,1006)
ELSE IF (IERR.EQ.-7) THEN
WRITE(NHSTRY,1000)IB, NDATA(3), (OUTPUT(J), J=1,5)
WRITE(NHSTRY,1007)
ENDIF
MULREG(1,JC) = FLOAT(IB)
MULREG(2,JC) = FLOAT(NDATA(3))
MULREG(3,JC) = OUTPUT(1)

C
C FORMATS
C
1000 FORMAT(/,IX,' 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 'SOLVE' CALLED = ',F15.1,/, 6 ' 1X,'NUMBER OF FUNCTIONAL EVALUATIONS = ',F15.1,/, 7 ' 1X,'NUMBER OF ANALYTICAL DERIVATIVE EVALUATIONS = ',F15.1,/) 1001 FORMAT(IX,' NO INCREASE POSSIBLE IN THE VALUE OF ',/ 1 ' 1X,'IN EVEN THOUGH CONVERGENCE HAS NOT BEEN REACHED ',/) 1002 FORMAT(IX,' MORE UNKNOWNS THAN FUNCTIONS AND UNIQUE ',/) 1003 FORMAT(IX,' TOTAL NUMBER OF VARIABLES TO BE VARIED = 0 ',/) 1004 FORMAT(IX,' CONVERGENCE CRITERION NOT BUT FLA STILL LARGE ',/) 1005 FORMAT(IX,'IC NOT A VALID NUMBER ON ENTRY ',/) 1006 FORMAT(IX,'IC NOT A DECREASE IN FUNCTIONAL 'MAX(1) TO 'MAX(1) ',/) 1007 FORMAT(IX,'ZERO DIAGONAL ELEMNT IN EQUATION SOLVE ',/) 1008 FORMAT(/,5X,'**MARQUARDT METHOD REGRESSION ******** ',/ 1 5X,'K (NUMBER OF PARAMETERS TO BE VARIED) = ',F15.1,/, 2 5X,'N (NUMBER OF DATA POINTS) = ',I13,/, 3 5X,'INITIAL B ',B_MIN B_MAX ', 4 'VARY FLAG ',/) 1009 FORMAT(IX,4(G15.5,1X)) 1010 FORMAT(IX,' VARY FLAG : ',/ 1 ' 10X,' 0 = HOLD PARAMETER CONSTANT ',/ 2 ' 10X,' 1 = VARY PARAMETER USING NUMERICAL DERIVATIVE ',/ 3 ' 10X,' 1 = VARY PARAMETER USING ANALYTICAL DERIVATIVE ',/) 1020 FORMAT(IX,3G15.6) 1030 FORMAT(IX,'B(',12,'I = ',G13.5) 1040 FORMAT(IX,1X,'OBS. Y-CALC Y-ACTUAL DIFF. ',/ 1 ' 1X,' 0 = ERROR ',/) 1095 FORMAT(IX,1X,4(I12,G13.5)) 1100 FORMAT(/,10X,'INPUT DATA ',/ 1 5X,'X-VALUE Y-VALUE ',/ 2 ' 5X,'------- '------- ',/) 1110 FORMAT(1X,'R-SQUARE = ',F15.8,/, 2 ' 1X,'ADJ R-SQUARE = ',F15.8,/)
1112 FORMAT (1X, 'R-SQUARE = ', F15.8, /)
1120 FORMAT (//, 10X, 'STATISTICS', //)
1125 5X, 'X-VALUES', 2G8, 'Y-VALUES', //
1130 5X, '-----', 2G8, '-----', //
1135 5X, 'MEAN = ', G15.5, 'LEN = ', G15.5, //
1140 5X, 'VARIANCE = ', G15.5, 'STD. DEV. = ', G15.5, //
1015 FORMAT (//, 1X, 'DERIVATIVE ANALYTICALLY, CALC. ABORTED')
1090 FORMAT (1X, 'IN ANDRA', //)
1095 1X, '**** num exceeded max of ', 15, ' ITER = ', 15, '****', //
0000 CONTINUE
RETURN
END

C SUBROUTINE ASTMCF (VABP, SASTM, CABP, HABP, IERR)

C NAME OF MODULE - ASTMCF
C
C MODULE TITLE - PROCEUDRE 241.1 API DATA BOOK P2-11,12 (1980)
C
C PURPOSE - METHOD FOR CHARACTERIZE PETROLEUM FRACTION BOILING
C POINTS OF ASTM D86
C
C MODIFIED - 1-6-85
C
C LIMITATIONS:
C ASTHM SLOPE  0-9.0
C VABP  203-800
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 CABP  O  R  -  CUBIC AVERAGE BOILING POINT (DEG F)
C HABP  O  R  -  HORIZONTAL AVERAGE BOILING POINT (DEG F)
C IERR  O  I  -  ERROR CODE
C
C IERR=0
C -1 = ASTM NOT IN RANGE ABOVE
C -2 = CABP NOT IN RANGE ABOVE
C
C IMPLICIT REAL*8 (A-H.O-Z)
C IMPLICIT INTEGER(1-N)
C
REAL*8  HABP, HABPC
COMMON /IO / NINFO, NOUT, NISTRY, IFCPT
COMMON /DEBUG / LDEBUG, LDDEBUG

DIMENSION CC(8), CW(81), CH(4)

IERR=0

IF (LDEBUG, GT, 7) THEN (NISTRY, 900)

CHECK IF IN RANGE

IF (SASTM, LT, 0.00 OR SASTM, GT, 9.0) THEN
IERR=-1
CALL MESS(1)
WRITE(NISTRY, 900)
WRITE(NISTRY, 1000) SASTM

148
READONLY, ERR=100)

.HIS FILE

ELSE IF (ITYP.EQ.2 OR ITYP.EQ.0) THEN

HISTORY FILE FILE HIS

FILHIS = FILE
IOPHIS = 0
IOPHIS = IOPHIS + 1
IF (IOPHIS.GT.MAXOPE) THEN
WRITE(*,5000)
WRITE(*,9000)
IERR = 3
WRITE(*,2000) FILHIS
WRITE(*,2000) FILHIS
GOTO 9999
ENDIF

OPEN (UNIT=HISTORY, FILE=FILHIS, STATUS='NEW', DEFAULTFILE='.HIS',
1 ERR=2001)

.REP FILE

ELSE IF (ITYP.EQ.3 OR ITYP.EQ.0) THEN

REPORT FILE FILE.REP

FILEREP = FILE
IOPREP = 0
IOPREP = IOPREP + 1
IF (IOPREP.GT.MAXOPE) THEN
WRITE(*,5000)
WRITE(*,9000)
IERR = 4
WRITE(*,2000) FILREP
GOTO 9999
ENDIF

OPEN (UNIT=REPFILE, FILE=FILREP, STATUS='NEW', DEFAULTFILE='.REP',
1 CARRIAGECONTROL='LIST', ERR=300)

ELSE
WRITE(*,5000)
WRITE(*,9000)
WRITE(*,4000)
STOP
ENDIF

FORMATS

500 FORMAT (I5, 'IN MODULE OPEN')
1000 FORMAT (I5, 'PROBLEM ON OPEN OF INPUT FILE ', A32)
2000 FORMAT (I5, 'PROBLEM ON OPEN OF HISTORY FILE ', A32)
3000 FORMAT (I5, 'PROBLEM ON OPEN OF REPORT FILE ', A32)
4000 FORMAT (I5, 'PROBLEM ON OPEN FILE TYPE')
5006 FORMAT (I5, '***SEVERE ERROR***')

9995 CONTINUE
RETURN
END
NAME OF MODULE - OUTP
MODULE TITLE - OUTPUT OF RESULTS OF PROPS
PURPOSE - TO OUTPUT RESULTS TO FILE IN ASPEN INPUT FORMAT
OR DFNS INPUT FORMAT
MODIFIED - 12-19-88

VARIABLES USED:

<table>
<thead>
<tr>
<th>VARIABLE</th>
<th>TYPE</th>
<th>SPEC</th>
<th>DIMENSION</th>
<th>DESCRIPTION AND RANGE</th>
</tr>
</thead>
<tbody>
<tr>
<td>IC</td>
<td></td>
<td>1</td>
<td></td>
<td>COMPONENT ARRAY ID</td>
</tr>
<tr>
<td>IERR</td>
<td></td>
<td>0</td>
<td>1</td>
<td>ERROR CODE</td>
</tr>
</tbody>
</table>

IMPLICIT REAL*8 (A-H,O-Z)
IMPLICIT INTEGER(I-N)

REAL*8            HABP, HEABP, MULAND, MUP, MULREG
PARAMETER        (MNC=25)
CHARACTER*62      TITLE
CHARACTER*60      DESC(MNC), REC
CHARACTER*32      CRANE

COMMON /IO / NIN, NOUT, NSTR, NREPT
COMMON /DEBUG / LDBG, LDBUG
COMMON /INFO / TITLE, DESC, IDESC
COMMON /PRINT / ITYPE
COMMON /SYS1 / RHL2
COMMON /SYS2 / NSYSR, NPCVEC(12)

COMMON /NPROP/ NCOMP, CRANE(MNC), ICF
COMMON /NPROP2/ VARP(MNC), SLOP(MNC), CASP(MNC), NABP(MNC), HEABP(MNC)
COMMON /NPROP3/ UGPK(MNC), AP1(MNC), SG(MNC), AMG(MNC)
COMMON /NPROP4/ PA(MNC), PHMNC(MNC), PHN(MNC), IIF

COMMON /CPRP01/ TC(MNC)
COMMON /CPRP02/ EC(MNC)
COMMON /CPRP03/ VC(MNC)
COMMON /CPRP04/ ZC(MNC)
COMMON /CPRP05/ OMEGA(MNC)
COMMON /CPRP06/ TLXANT(5,MNC), TLXREG(3,MNC)
COMMON /CPRP07/ CPFG(11,MNC), CPREG(3,MNC)
COMMON /CPRP08/ DHYDNT(5,MNC)
COMMON /CPRP09/ NULAND(5,MNC), NULREG(3,MNC)
COMMON /CPRP10/ DLFORM(MNC)
COMMON /CPRP11/ LGFORM(MNC)
COMMON /CPRP12/ EKTRAH(MNC), EKTRREG(3,MNC)
COMMON /CPRP13/ BLCVTV(MNC)
COMMON /CPRP14/ TR(MNC)
COMMON /CPRP15/ VRH(MNC)
COMMON /CPRP16/ DFLX(MNC)
COMMON /CPRP17/ TPL(MNC)
COMMON /CPRP18/ DELTAM(MNC)
COMMON /CPRP19/ MUP(MNC)
COMMON /CPRP20/ RGZ(MNC)
COMMON /CPRP21/ PLCVTV(1,MNC), PLCVREG(3,MNC)
COMMON /CPRP22/ VLCSV(MNC)

IERR=0

MAIN LOOP

CALC ORDER

<table>
<thead>
<tr>
<th>TC</th>
<th>PC</th>
<th>VC</th>
<th>ZC</th>
<th>OMEGA</th>
</tr>
</thead>
</table>
PLXANT, CPEG, DHFORM, DGFORM, DHLCVT,
PLXANT, CPEG, DHFORM, DGFORM, DHLCVT,

TITLE AND DESCRIPTIONS

IF (IJC.EQ.1) THEN
  IF (IPTYP.EQ.1) THEN
    WRITE(NREPT,1000) TITLE
  ELSE
    WRITE(NREPT,1000) TITLE
  ENDIF

DO 10 JJ=1, NDESC
  CALL FEND(DESC(JJ), IEND, IERF)
  WRITE(NREPT,3100) DESC(JJ), IEND
CONTINUE

IF (IPTYP.EQ.1) THEN
  WRITE(NREPT,1100)
ENDIF

DO 20 JJ=1, NCOMP-1
  REC=CNAME(JJ)
  CALL FEND(REC, IEND, IERF)
  WRITE(NREPT,1300) CNAME(JJ), IEND, CNAME(JJ)

CONTINUE

WRITE(NREPT,1300) CNAME(NCOMP), CNAME(NCOMP)

ENDIF

FOR INPUT TO 'DFHS'

IF (IPTYP.EQ.1) THEN
  WRITE(NREPT,1400) CNAME(JC),
    AMM(JC), TEP(JC), TC(JC), PC(JC), YC(JC),
    ZC(JC), OMEGA(JC), RE724A(JC), VB(JC),
    (CPEG(IV,JC),IV=1,IV),
    DELTA(JC), MUP(JC),
    (PLXANT(IV,JC),IV=1,IV),
    (MULAND(IV,JC),IV=1,5),
    (DHFORM(JC),DGFORM(JC),DIUVB(JC),
    (DHLWRT(IV,JC),IV=1,5),
    (PLCAV(TIV,JC),IV=1,5),
    (DHLCVT(JC),VLCVT1(JC),RGYR(JC))
ENDIF

ELSE

FOR INPUT DIRECTLY INTO ASHEN .INP FILE

INPUT AND CALCULATED VALUES FOR COMPONENT

IF (LDRUG.GT.0) THEN
  WRITE(NREPT,1110) CNAME(JC), VARP(JC), AMM(JC)
ELSE
  WRITE(NREPT,1110) SLOP(JC)
ENDIF

WRITE(NREPT,1120) CARB(JC), MABP(JC), MMABP(JC)
WRITE(NREPT,1130) UOPK(JC), API(JC), SG(JC)
WRITE(NREPT,1140) PA(JC), PN(JC), PP(JC)

IF (NS5OP.GT.0) THEN
  WRITE(NREPT,1150) FLOAT(NS5OP)
ELSE

COMPONENT NAME

WRITE(NREPT,1200) CNAME(JC)
WRITE(NREPT,1300) ANM(JC), TC(JC), PC(JC), VC(JC), ZC(JC), OMEGA(JC)
WRITE(NREPT,2000) PLXREG(IV,JC), IV=1,3
WRITE(NREPT,3400) PLXANT(IV,JC), IV=1,9
WRITE(NREPT,2000) CPREG(IV,JC), IV=1,3
WRITE(NREPT,3500) CPZG(IV,JC), IV=1,11
WRITE(NREPT,3800) DHFORM(JC), DGFORM(JC)

IF(NPCVEC(10).EQ.1) THEN
WRITE(NREPT,3010) DHLCUT(JC)
ENDIF
WRITE(NREPT,3820) TB(JC), V0(JC)
WRITE(NREPT,3830) DHVLWT(IV,JC), IV=1,5
IF(ERTREG(1,JC).NE.0) THEN
WRITE(NREPT,2000) ERTREG(IV,JC), IV=1,1
ENDIF
WRITE(NREPT,3810) RTZRA(JC)
IF(NPCVEC(15).EQ.1) THEN
WRITE(NREPT,3850) DhVLR(JC)
ENDIF
IF(NPCVEC(6).EQ.1) THEN
WRITE(NREPT,3860) DFP(JC)
ENDIF
IF(NPCVEC(7).EQ.1) THEN
WRITE(NREPT,3870) DELTA(JC)
ENDIF
WRITE(NREPT,3880) MUF(JC)
WRITE(NREPT,2000) IMULREG(IV,JC), IV=1,3
WRITE(NREPT,3890) (MULAND(IV,JC), IV=1,5)
IF(NPCVEC(20).EQ.1) THEN
WRITE(NREPT,3900) RGYR(JC)
ENDIF
IF(NPCVEC(11).EQ.1) THEN
WRITE(NREPT,2000) ICREG(IV,JC), IV=1,3
IF(DRUGT.31) THEN
WRITE(NREPT,4040) OMEGA(JC), IV=0,1412315760
ENDIF
WRITE(NREPT,3901) DLCWAT(IV,JC), IV=1,11
ENDIF
IF(NPCVEC(121).EQ.1) THEN
WRITE(NREPT,1200) VLCVT(JC)
ENDIF

ENDIF

FORMATS

1000 FORMAT('TITLE ',1H',A62,1H')
1100 FORMAT('NO-ECHO',/,'FILE ASPENPCD ASPENPCD NEW'/,'FILE USHPFIA 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 '9X,  
5 'MULAND 5/DHVLB 1/VC'  
7 4X,'PROP-LIST MW 1/TFP 1/TB 1/TC 1/PC  
8 '1/VC 1/9X,  
9 '9X, 'DHVLW 5/MULAND 1/VC'  
1400 FORMAT(4X,'PVAL ',A32,/)

2 PLCAVT 1/0,'SUM OF SQUARES               = ',G15.8,/, 5X,G20.10,1X,'/.

3000 FORMAT('; TITLE ',A62)

3100 FORMAT(';A),

3110 FORMAT(';',  
1 'SUMMARY FOR COMPONENT ',A32,/)
2 '9X, 'VOLUME AVERAGE BOILING POINT (DEG K) = ',G12.6,/,  
3 '9X, 'AVERAGE MOLWT.'

3112 FORMAT(';5X,'SLOPE OF THE TBP CURVE = ',G12.6)

3114 FORMAT(';5X,'SLOPE OF THE ASTMD6 CURVE = ',G12.6)

3120 FORMAT(';5X,'HCIC AVERAGE BOILING POINT (DEG K) = ',G12.6,/,  
1 '9X, 'MOLAL AVERAGE BOILING POINT (DEG K) = ',G12.6,/,  
2 '9X, 'MEAN AVERAGE BOILING POINT (DEG K) = ',G12.6)

3130 FORMAT(';5X,'UPD (WATSON) K CHAP. FACTOR = ',G12.6,/,  
1 '9X, 'API GRAVITY = ',G12.6,/,  
2 '9X, 'SG GRAVITY (60/60 F) = ',G12.6)

3140 FORMAT(';5X,'PERCENT AROMATICS = ',G12.6,/,  
1 '9X, 'PERCENT NAPHTHENS = ',G12.6,/,  
2 '9X, 'PERCENT PARAFINS = ',G12.6)

3150 FORMAT(';5X,'SYSP SELECTED = ',5X,'A32)

3152 FORMAT(';5X,'SYSP SELECTED = ',5X,'A32)

3160 FORMAT(';PROP-DATA',/2X,'PROP-LIST ',A32)

3162 FORMAT(';PROP-DATA',/2X,'PROP-LIST ',A32)

3164 FORMAT(';PROP-DATA',/2X,'PROP-LIST ',A32)

3166 FORMAT(';PROP-DATA',/2X,'PROP-LIST ',A32)

2000 FORMAT(';',  
1 ' REGRESSION SUMMARY',/  
2 ' ITERATION = ',G12.8,/,  
3 ' NUMBER OF FARMS UNFIT = ',F15.0,/,  
4 ' SUM OF SQUARES = ',G12.8,/,  
5 '')
3400  FORMAT(1,5X,'CVAL Pixerat 1 ',G20.10,'/2',2X,G20.10,'/','/',1,
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 CPNIG 1 ',G20.10,'/2 ',2X,G20.10,'/','/',1,
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,'/','/',1)
3800  FORMAT(5X,'CVAL DHFORM 1 ',G20.10,'/','/',1,
1,5X,'CVAL DGFORM 1 ',G20.10,'/','/',1
3810  FORMAT(5X,'CVAL DHLCT 1 ',G20.10,'/','/',1
3820  FORMAT(5X,'CVAL TB 1 ',G20.10,'/','/',1
3830  FORMAT(1,5X,'CVAL DHVLWT 1 ',G20.10,'/2 ',2X,G20.10,'/','/',1,
2,5X,12X,'3 ',G20.10,'/4 ',2X,G20.10,'/','/',,
3,5X,12X,'5 ',G20.10,'/','/',
3840  FORMAT(5X,'CVAL RETZRA 1 ',G20.10,'/','/',1
3850  FORMAT(5X,'CVAL DHVV 1 ',G20.10,'/','/',1
3860  FORMAT(5X,'CVAL TFF 1 ',G20.10,'/','/',1
3870  FORMAT(5X,'CVAL DELTA 1 ',G20.10,'/','/',1
3880  FORMAT(5X,'CVAL HUP 1 ',G20.10,'/','/',1
3890  FORMAT(1,5X,'CVAL MULAND 1 ',G20.10,'/2 ',2X,G20.10,'/','/',1,
2,5X,12X,'3 ',G20.10,'/4 ',2X,G20.10,'/','/',,
3,5X,12X,'5 ',G20.10,'/','/',
3900  FORMAT(5X,'CVAL RGVR 1 ',G20.10,'/','/',1
4040  FORMAT(1,8S,'1ST CAVETT VAPOR PRES. CONST. OMEGA/0.24123337 = ',1,
1,12S,'/','/',2,8S,'2ND CAVETT VAPOR PRES. CONST. RANGE (-0.2 TO 0.2) = ',1,
2,12S,'/','/',2,5X,'CVAL VLCAVT 1 ',G20.10,'/2 ',2X,G20.10,'/','/',,
2,5X,12X,'3 ',G20.10,'/4 ',2X,G20.10,'/','/',
2,5X,'RETURN 1 ',G20.10,'/','/',1,13S,'SUBROUTINE FEND(REC, IEND, IERR)
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 VARIABLES USED=
C VALUEABLE I/O TYPE SPEC DIMENSION DESCRIPTION AND RANGE
C REC I/O C 80 RECORD TO BE WRITTEN
C IEND I 1 LAST NON BLANK CHARACTER
C IERR 0 1 ERROR FLAG
C 0 = OK
C 1 = NO CHARACTERS IN RECORD
C IMPLICIT INTEGER(I-N)
C CHARACTER*80 REC
C IERR=0
C DO 10 IEND=80,1,-1
10 IF(REC(IEND:IEND).NE. ' ')GOTO 20
10 CONTINUE
   IF(EEND=1) THEN
     IERR=1
   END IF
20 RETURN
9990 RETURN
END

SUBROUTINE PROPS(IERR)

NAME OF MODULE - PROPS
MODULE TITLE - CALC PROPERTIES OF PETROLEUM FRACTIONS
PURPOSE - TO CALC PROPERTIES OF PETROLEUM FRACTIONS
MODIFIED - 12-22-88

VARIABLES USED:

VARIABLE I/O TYPE SPEC DIMENSION DESCRIPTION AND RANGE
IERR 0 I 0 = ERROR CODE
G=6 NUMBER OF CALLS TO PROPERTIES

IMPLICIT REAL*8 (A-H,O-Z)
IMPLICIT INTEGER(N-N)

REAL*8 HABP, HABPF, HABPF, HULAND, HULREG, HUP

CHARACTER*32 CHNAME
CHARACTER*80 REC

PARAMETER (MNC=25)

COMMON /IDO/ MIN, NOUT, NISTRY, NREPT
COMMON /DEBUG/ LDEBUG, LDBG
COMMON /SYS2/ NSYSOP, MVEG (22)
COMMON /SYS3/ IERCAL (22)

COMMON /NPROP1/ NCMP, CHNAME (MNC), ICF
COMMON /NPROP2/ VARP (MNC), SLOP (MNC), CPA (MNC), HABP (MNC), HABPF (MNC)
COMMON /HPROP3/ VOPK (MNC), APV (MNC), SG (MNC), AMH (MNC)
COMMON /HPROP4/ PA (MNC), PN (MNC), FP (MNC), IPF
COMMON /CALC/ BCALC (MNC)

COMMON /XPROP1/ XPRM (MNC), XHPR (MNC), XARO (MNC)
COMMON /XPROP2/ HBAT (MNC), ST (MNC), BT (MNC)

COMMON /CPRP0/ T1 (MNC)
COMMON /CPRP0/ PC (MNC)
COMMON /CPRP0/ VC (MNC)
COMMON /CPRP0/ ZC (MNC)
COMMON /CPRP0/ OMEMA (MNC)
COMMON /CPRP0/ PLZANT (MNC), PLZREG (1, MNC)
COMMON /CPRP0/ CPNF (1, MNC), CPNF (3, MNC)
COMMON /CPRP0/ DHVLP (3, MNC)
COMMON /CPRP0/ HULAND (5, MNC), HULREG (3, MNC)
COMMON /CPRP0/ DHFORM (MNC)
COMMON /CPRP11/ DGFORM (MNC)
COMMON /CPRP12/ RKTZRA (MNC), RKTZREG (3, MNC)
COMMON /CPRP13/ DLVCT (MNC)
COMMON /CPRP14/ TI (MNC)
COMMON /CPRP15/ VB (MNC)
COMMON /CPRP16/ DHVLB (MNC)
COMMON /CPRP1/ TFP(MNC)
COMMON /CPRP18/ DELTA(MNC)
COMMON /CPRP19/ MUP(MNC)
COMMON /CPRP20/ RGYR(MNC)
COMMON /CPRP21/ PLCAVT(1,MNC), PLCREG(1,MNC)
COMMON /CPRP22/ VLCVT(1,MNC)

IF(LDBG GT 7)WRITE(HSTRY,900)
JERR=0

NPCVEC IS 1 CALC PROP IF NPCVEC IS 0 NO CALC

CALC ORDER

   1   2   3   4   5
TC  ,  PC  ,  VC  ,  RC  ,  OMEGA
   6   7   8   9   10
PLXANT, CPIC, DIFORM, DGFORM, DLCAVT,
   11  12  13  14  15
TH  ,  VB  ,  DHLMT, HRTZBA, DHVLB,
   16  17  18  19  20
TFP  ,  DELTA, MUP  ,  MULAND, RGYR,
   21  22
PLCAVT , VLCVT

DO 200 JCN=1,NCP

NOT ENOUGH DATA FOR CALCULATION

IF(NCALC(JCN).EQ.0)GOTO 100

CALC TC (CRITICAL TEMP)

CONVERT TO CALLED SUBROUTINE UNITS

IF(NPervas1).EQ.1 THEN
   CALL TCON(MEABP(JCN),TEMPR,12,IERHT1)
   CALL RTTC(MHW(JCN),THPR,AP(JCN),SG(JCN),TEMPRO,IERCAL1))
   CALL TCUM(TEMPRO,VC(JCN),23,IERHT2)
ENDIF

CALC PC (CRITICAL PREP)

IF(NPervas2).EQ.1 THEN
   CALL RPC(MHW(JCN),TEMPR,AP(JCN),SG(JCN),PRPSIA,IERCAL2))
   CALL PCOR(PRES,PC(JCN),15,IERHP1)
ENDIF

CALC VC (CRITICAL VOL)

IF(NPervas3).EQ.1 THEN
   CALL RPVC(MHW(JCN),TEMPR,SG(JCN),VOL,IERCAL3))
   VC(JCN)=VOL
ENDIF

CALC ZC (CRITICAL COMPRES. FACTOR)

IF(NPervas4).EQ.1 THEN
   CALL ZCCAL(TC(JCN),ZC(JCN),VC(JCN),ZC(JCN),IERCAL4))
ENDIF

CALC OMEGA (ACENTRIC FACTOR)

IF(NPervas5).EQ.1 THEN
   CALL TCON(MEABP(JCN),TEMPR,12,IERHT2)
   CALL TCON(TC(JCN),TCR,42,IERHT3)
   CALL PCOR(PC(JCN),PSI5,91,IERHP1)
CALL GYKL(TEMPR, TCH, PRPSIA, UOPK(JC), API(JC), OMEGA(JC), IERCAL(51))
ENDIF

CALL PLXANT (VAPOR PRESSURE) AND REGRESS INTO FORM LN(PA) = A + B/T + C

IF(NPCVEC(6).EQ.1) THEN
CALL TCON(MABP(JC), MABFF, 41, IERRT4)
ENDIF

CALL MAXBN1(MABP, UOPK(JC), SG(JC), MAXIT, MDAT, ST(JC), BT(JC), JC, IERCAL(61))
ENDIF

CALL CPIG (IDEAL GAS HEAT CAPACITY) AND REGRESS INTO FORM

IF(NPCVEC(7).EQ.1) THEN
CALL HDCPIG(VABP(JC), SG(JC), MAXIT, JC, IERCAL(71))
ENDIF

CALL DHFMR (STANDARD HEAT OF FORMATION)

IF(NPCVEC(8).EQ.1) THEN
CALL DHFMR(MABP(JC), XPAR(JC), XNAP(JC), XARO(JC), DHFMR(JC), IERCAL(81))
ENDIF

CALL DGFORM (STANDARD FREE ENERGY OF FORMATION)

IF(NPCVEC(9).EQ.1) THEN
CALL DGFORM(MABP(JC), XPAR(JC), XNAP(JC), XARO(JC), DGFORM(JC), IERCAL(91))
ENDIF

CALL DHLUT (CAVATT EQUATION FOR ENTHALPY)

IF(NPCVEC(10).EQ.1) THEN
CALL CAVENT(JC, IERCAL(10))
ENDIF

CALL TB (BOILING POINT)

IF(NPCVEC(11).EQ.1) THEN
CALL TBCALC(JC, IERCAL(111))
ENDIF

CALL VB (LIQUID MOLAR VOLUME AT THE BOILING POINT)

IF(NPCVEC(12).EQ.1) THEN
CALL LVVANP(JC, IERCAL(121))
ENDIF

CALL DHVLT (WATSON HEAT OF VAPORIZATION)

IF(NPCVEC(13).EQ.1) THEN
CALL WATHOV(JC, IERCAL(131))
ENDIF

CALL RZHA (RACKET EQUATION FOR LIQ. VOLUME)

IF(NPCVEC(14).EQ.1) THEN
IRRTZ=1
CALL REFV(JC, IRRTZ, IERCAL(141))
ENDIF

CALL DHVLE (HEAT OF VAPORIZATION AT BP)

IF(NPCVEC(15).EQ.1) THEN
CALL HVABP(JC, IERCAL(151))
ENDIF
CALC TFP (NORMAL FREEZING/MELTING POINT)

IF(NPCVEC(161).EQ.1) THEN
CALL MPH(MHAR(JC),SG(JC),XPAR(JC),XNAP(JC),XROR(JC),
       TFP(JC),IECALC(6))
ENDIF

CALC DELTA (SOLUBILITY PARAMETER)

IF(NPCVEC(17).EQ.1) THEN
CALL SOLPAR(JC,IECALC(17))
ENDIF

CALC MUP (DIPOLE MOMENT)

IF(NPVCVEC(18).EQ.1) THEN
CALL DIPOLE(JC,IECALC(18))
ENDIF

CALC HULAND (MODIFIED ANDRADE MODEL FOR LIQ VISCOSITY)

AND REGRESS TO FORM A+B/T+C'LOG(T)

IF(NPCVEC(19).EQ.1) THEN
CALL ANDRA(JC,IECALC(19))
ENDIF

CALC RGYR (RADIUS OF GYRATION)

IF(NPCVEC(20).EQ.1) THEN
CALL RGYR(JC,UGPK(JC),XPAR(JC),XNAP(JC),XROR(JC),
       RGYR(JC),IECALC(20))
ENDIF

CALC PLCVT (CAVETT EQUATION VAPOR PRESSURE CONST)

IF(NPCVEC(21).EQ.1) THEN
ICPLC=0
CALL CAVPT(JC,ICPLC,IECALC(21))
ENDIF

CALC VLVT (EXTENDED SCHATCHARD-HILDEBRAND CHARACTERISTIC VOLUME PARAMETER)

IF(NPVCVEC(22).EQ.1) THEN
CALL VPSH(TEMPH,SG(JC),JC,IECALC(22))
ENDIF

CALL OUTF(JC,IER)
CALL SECOND(TIME)

REC=NAME(JC)
CALL PRINTREC(I,IE,IER)
PRINT 1000, JC, CHAME(JC)(1:IE), TIME
WRITE(NTHSTRY,2000)JC,CHAME(JC)(1:IE),TIME
IER=6
DO 100 IEE=1,12
IF(IECALC(IEE).NE.6)IERR=1 IERR+1
100 CONTINUE
200 CONTINUE
CALL SECOND(TIME)

FORMAT

900 FORMAT(1X,'IN MODULE PROPS')
1000 FORMAT(1X,'FINISHED COMPONENT ','12,1X,',(','A,') C-TIME = ','G12.6)
2000 FORMAT(1X,'FINISHED COMPONENT ','12,1X,'(','A,')/')
SUBROUTINE RADGYR(AMW, UOPK, XP, XN, XA, RGY, IERR)

NAME OF MODULE - RADGYR

MODULE TITLE - CALC

PURPOSE - TO CALC RADIOUS OF GYRATION

MODIFIED - 12-13-88

METHOD - REGRESSION OF ASPEN DATA BANK FOR PARAIFINS, NAPHTHENES,
AND AROMATICS TO FORM: RADGYR=A'MNW+'B

VARIABLES USED-

C VARIABLE I/O TYPE SPEC DIMENSION DESCRIPTION AND RANGE
C AMW I R - AVERAGE MOLE WT.
C UOPK I R - UPF CHARACTERIZATION FACTOR
C XP I R - MOLE FRACTION PARAIFINS
C XN I R - MOLE FRACTION NAPHTHENES
C XA I R - MOLE FRACTION AROMATICS
C RGY O R - RADIUS OF GYRATION

IMPLICIT REAL*8 (A-H,O-Z)
IMPLICIT INTEGER(I-N)

COMMON /DEBUG/, /DEUG, LDBGUR
COMMON /IO/, / NIN, NOUT, NHSTRY, NRGP

IERR=0
IF (LDBGUR.GT.7) WRITE(NHSTRY, 906)

DATA REGRESSED FOR PARAIFINS
AP=EXP(-25.129D0)
BP=0.10375D0
CP=0.80725D0

RGF=AP*UOPK**BP*AMW**CP

IF (RGF.LT.0.3182D-9.AND.XP.GT.0.00) THEN
  CALL MESS(1)
  WRITE(NHSTRY, 901)
  WRITE(NHSTRY, 1000) RGF
  RGF=0.3182D-9
ENDIF
IF (RGF.GT.0.8318D-9.AND.XP.GT.0.00) THEN
  CALL MESS(1)
  WRITE(NHSTRY, 901)
  WRITE(NHSTRY, 1100) RGF
  RGF=0.8318D-9
ENDIF

DATA REGRESSED FOR NAPHTHENES
AN=EXP(-25.879D0)
BN=0.26866D0
CN=0.76607D0

RGN=AM*UOPK**BN*AMW**CN

IF (RGN.LT.0.285D-9.AND.XN.GT.0.00) THEN
  CALL MESS(1)
  WRITE(NHSTRY, 901)
WRITE (NHSTPY, 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 (NHSTPY, 2100) RGN
RGN = 0.4367D-9
ENDIF
IF (RGA.GT.0.4049D-9.AND.XA.GT.0.D0) THEN
  CALL MESS(1)
WRITE (NHSTRY, 900)
WRITE (NHSTPY, 3100) RGA
RGA = 0.4049D-9
ENDIF
C EST. FOR FRACTION
C
RGA = XP'RGN + XN'RGN + XA'RGA
C
FORMAT
C
900 FORMAT (4X, 'IN MODULE NAGGYR')
1000 FORMAT (4X, 'RGY VALUE FOR PARAFFINS IS LESS THAN 0.3182D-9', /)
  4X, 'RGY VALUE OF ', G15.6, ' SET TO 0.3182D-9 CALC. CONTINUES' )
1100 FORMAT (4X, 'RGY VALUE FOR PARAFFINS IS GREATER THAN 0.6184D-9', /)
  4X, 'RGY VALUE OF ', G15.6, ' SET TO 0.6184D-9 CALC. CONTINUES' )
2000 FORMAT (4X, 'RGY VALUE FOR NAPHTHENES IS LESS THAN 0.285D-9', /)
  4X, 'RGY VALUE OF ', G15.6, ' SET TO 0.285D-9 CALC. CONTINUES' )
2100 FORMAT (4X, 'RGY VALUE FOR NAPHTHENES IS GREATER THAN 0.4167D-9', /)
  4X, 'RGY VALUE OF ', G15.6, ' SET TO 0.4167D-9 CALC. CONTINUES' )
3000 FORMAT (4X, 'RGY VALUE FOR AROMATICS IS LESS THAN 0.10037D-9', /)
  4X, 'RGY VALUE OF ', G15.6, ' SET TO 0.10037D-9 CALC. CONTINUES' )
3100 FORMAT (4X, 'RGY VALUE FOR AROMATICS IS GREATER THAN 0.4849D-9', /)
  4X, 'RGY VALUE OF ', G15.6, ' SET TO 0.4849D-9 CALC. CONTINUES' )
C
RETURN
END
C SUBROUTINE RCHECK (AHW, THR, SG, ITYP)
C NAME OF MODULE - RCHECK
C MODULE TITLE - CHECK LIMITS ON RIAZI DAUBERT CORR.
C PURPOSE - TO CHECK LIMITS ON RIAZI DAUBERT CORR.
C MODIFIED - 10-1-88
C
LIMITATIONS:
C
MW 77.2-294.5
C TDEG R 569.67-1309.67
C SG 0.6247-1.0244
VARIABLES USED:

AMW  I  R  -  MOLAR WEIGHT
TBR  I  R  -  BOILING POINT TEMPERATURE (DEG F)
SG   I  R  -  SPECIFIC GRAVITY (60/60F)
ITYP I  I  -  TYPE OF CORRELATION

1 = MW
2 = TBR
3 = SG
4 = ITYP
5 = LAMBDA
6 = CP
7 = VB

IMPLICIT REAL*8 (A-H,O-Z)
IMPLICIT INTEGRAL(I-N)

COMMON /I0 / MIN,NOUT,INSTAT,INREP
COMMON /DEBUG / LDEBUG,LERROR

DATA NAMES /'AMW','TBR','SG','ITYP','LAMBDA','CP','VB'/

IF (AMW.LT.77.2D0.OR. AMW.GT.699.0D0) THEN
   CALL MESS(1)
   WRITE(INSTAT,960) MIN,NAMES(ITYP)
   WRITE(INSTAT,1000)AMW
ENDIF

IF (TBR.LT.569.6D0.OR. TBR.GT.1309.67) THEN
   CALL MESS(1)
   WRITE(INSTAT,960) MIN,NAMES(ITYP)
   WRITE(INSTAT,2000)TBR
ENDIF

IF (SG.LT.0.6247D0.OR. SG.GT.1.0244D0) THEN
   CALL MESS(1)
   WRITE(INSTAT,960) MIN,NAMES(ITYP)
   WRITE(INSTAT,3000)SG
ENDIF

FORMAT

SG0 FORMAT(5X,'USING PROCEDURE RD',A6)
1000 FORMAT(1X,'AMW VALUE IS NOT IN RANGE 77.2-699.0',/)
2000 FORMAT(1X,'TBR VALUE IS NOT IN RANGE 569.67-1309.67',/)
3000 FORMAT(1X,'SG VALUE IS NOT IN RANGE 0.6247-1.0244',/)

RETURN
END

SUBROUTINE RDCPIG(TBK,SG,MAXIT,JC,IERR)

NAME OF MODULE - RDCPIG
MODULE TITLE - TO ESTIMATE IDEAL GAS HEAT CAPACITY
PURPOSE - TO ESTIMATE IDEAL GAS HEAT CAPACITY USING RIAZI AND DAUBERT
METHOD
C VARIABLES USED:
C VARIABLE I/O TYPE SPEC DIMENSION DESCRIPTION AND RANGE
C THX 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 HARQUARDT
C 0 = CONVERGED CP
C -1 = NO IMPROVEMENT POSSIBLE IN THE VALUE OF PH EVEN THOUGH CONV. HAS NOT BEEN REACHED
C -2 = MORE UNKNOWNS THAN FUNCTIONS
C -3 = TOTAL NUMBER OF VARIABLES TO BE VARIED IS ZERO
C -4 = CONV. CRITERION MET BUT FLA STILL LARGE
C -5 = IC NOT A VALID NUMBER ON ENTRY
C -6 = XI(I) IS NOT WITHIN XMIN(I)-XMAX(I)
C -7 = ZERO DIAGONAL ELEMENT IN EQUATION
C 0 = SOLVE
C -10 = ASKED FOR ANALYTICAL DERIVATIVE
C -11 = ITERATIONS EXCEEDED MAXIT
C
C IMPPLICIT REAL*8(A-H,O-Z)
C IMPPLICIT INTEGER(1-N)
C
C PARAMETER
C (HNC=25)
C
C COMMON /IO / MIN, NOUT, NIND, NBKPT
C COMMON /DEBUG / LDEBUG, LDEBUG
C
C COMMON /CPREG 7, CPREG(11, HNC), CPREG(I, HNC)
C
C DIMENSION NDATA(24), DATA(16), OUTPUT(6)
C
C DIMENSION X(I), XMAX(I), XMIN(I), Y(I), Z(I), P(I), D(I), A(I), AC(I), XO(I)
C
C DIMENSION CP(I)
C
C IF (LDEBUG .GT. 7) WRITE (NIND, 900)
C
C CONVERT
C
C CALL TCON (THX, TB, 42, IERR)
C
C MAX ITERATIONS
C IF (MAXIT .EQ. 0) MAXIT = 1000
C
C CPTR(I, 2 AND 3)
C IDEAL GAS HEAT CAPACITY (IHTU/LB MOLE DEG F) AT 0 F
C CP00=4.9394D-7 ' TB**2(2.672D0), SG**4(-2.363D0)
C
C IDEAL GAS HEAT CAPACITY (IHTU/LB MOLE DEG F) AT 600 F
C CP600=4.935D-6 ' TB**2(2.4219D0), SG**4(-1.9436D0)
C
C IDEAL GAS HEAT CAPACITY (IHTU/LB MOLE DEG F) AT 1200 F
CP01200=8.352D-6 * TB**(2.3853D0) * SG**(-1.9320D0)  
C IDEAL GAS HEAT CAPACITY (J/KMOLE DEG K) AT 0 F  
CP00=CP00/9.486D-4/0.453593D0*1.8D0  
C IDEAL GAS HEAT CAPACITY (J/KMOLE DEG K) AT 600 F  
CP0600=CP0600/9.486D-4/0.453593D0*1.8D0  
C IDEAL GAS HEAT CAPACITY (J/KMOLE DEG K) AT 1200 F  
CP1200=CP1200/9.486D-4/0.453593D0*1.8D0  
C REGRESS CP VALUES USING MARQUARDT (ASPEN YSOLVE)  
C NUMBER OF unknowns  
n=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)=0.5D0  
10 continue  
DO 20 I=1,K  
xv(i)=1.D0  
v(i)=0.D0  
xmax(i)= 500000.D0  
xmin(i)=-500000.D0  
20 continue  
C  
ITER=ITER+1  
if(ITER.GT.MAXIT)then  
call mess(3)  
write(nhstry,900)  
iter=-1  
write(nhstry,1080)maxit,iter  
goto 9000  
endif  
C  
equation of form AX+BT+CT^T  
C  
TEMP1=(0.0D0+59.67D0)/1.8D0  
z(1)=x(1)+x(2)+TEMP1+x(3)+TEMP2*TEMP1 - CP00  
TEMP2=(600.0D0+59.67D0)/1.8D0  
z(2)=x(1)+x(2)+TEMP1+x(3)+TEMP2*TEMP2 - CP0600  
TEMP3=(1200.0D0+59.67D0)/1.8D0  
z(3)=x(1)+x(2)+TEMP1+x(3)+TEMP3*TEMP3 - CP1200  
C  
B6 call ysolve IK, N, NDATA, DATA, X, XV, XMAX, XMIN, Y, Z, PJ,  
output, F, A, AC)  
C  
calc function  
if(ndata(2).eq.0)then  
goto 50  
C  
calc derivative  
else if(ndata(2).gt.0)then  
izze=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
C       IF (NDATA(3) .GT. 0) GOTO 80
C
C       IERR = NDATA(3)
C
C       CONVERGED              C       IF (IERR .EQ. 0) THEN
C       CP(1) = X(1)            C       CP(1) = X(1)
C       CP(2) = X(2)            C       CP(2) = X(2)
C       CP(3) = X(3)            C       CP(3) = X(3)
C       CALL MESS(1)            C       CALL MESS(1)
C       WRITE (NHSTRY, 900)     C       WRITE (NHSTRY, 900)
C       WRITE (NHSTRY, 1000)     C       IF (NDATA(3), (OUTPUT(J), J = 1, 5)
C       WRITE (NHSTRY, 1001)     C       WRITE (NHSTRY, 1002)
C       ELSE IF (IERR .EQ. -1) THEN              C       ELSE IF (IERR .EQ. -3) THEN
C       CP(1) = X(1)            C       CALL MESS(2)
C       CP(2) = X(2)            C       WRITE (NHSTRY, 900)
C       CP(3) = X(3)            C       WRITE (NHSTRY, 1000)     C       IF (NDATA(3), (OUTPUT(J), J = 1, 5)
C       CALL MESS(1)            C       WRITE (NHSTRY, 1001)     C       WRITE (NHSTRY, 1002)
C       WRITE (NHSTRY, 900)     C       ELSE IF (IERR .EQ. -3) THEN              C       ELSE IF (IERR .EQ. -9) THEN
C       WRITE (NHSTRY, 1000)     C       CALL MESS(2)
C       IF (NDATA(3), (OUTPUT(J), J = 1, 5)         C       WRITE (NHSTRY, 900)
C       WRITE (NHSTRY, 1001)     C       WRITE (NHSTRY, 1000)     C       ELSE IF (IERR .EQ. -9) THEN              C       ELSE IF (IERR .EQ. -6) THEN
C       IF (NDATA(3), (OUTPUT(J), J = 1, 5)         C       CALL MESS(2)
C       WRITE (NHSTRY, 1000)     C       WRITE (NHSTRY, 1006)
C       ELSE IF (IERR .EQ. -7) THEN     C       WRITE (NHSTRY, 900)
C       CALL MESS(2)
C       WRITE (NHSTRY, 1000)     C       WRITE (NHSTRY, 1007)
ENDIF

C                                C       ASPEN
C
C       C1IG(1, JC) = CP(1)
C       CPXG(2, JC) = CH(2)
C       CPXG(3, JC) = CP(3)
C       CPXG(4, JC) = 0.00
C       CPXG(5, JC) = 0.00
C       CPXG(6, JC) = 0.00
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)=(CPIG1+CPIG2)/(TEMP2-TEMP1)
CPIG(5,JC)=1.00*CPIG(10,JC)*TEMP1+CPIG1
CPIG(11,JC)=1.00

C
CPREG1(JC)=FLOAT(ITER)
CPREG2(JC)=FLOAT(INDATA(3))
CPREG3(JC)=OUTPUT11)

C
FORMATS

960 FORMAT(IX,'IN MODULE RDCPIG')
1000 FORMAT(/,1X,'ITERATION: ',I9,/) ;
1001 FORMAT(IX,'NO IMPROVEMENT POSSIBLE IN THE VALUE OF',/)
1002 FORMAT(IX,'I5 EVEN THOUGH CONVERGENCE HAS NOT BEEN REACHED',/) ;
1003 FORMAT(IX,'TOTAL NUMBER OF VARIABLES TO BE VARIED = 0',/)
1004 FORMAT(IX,'CONVERGENCE CRITERION NOT MET BUT FLA STILL LARGE',/)
1005 FORMAT(IX,'I5 NOT A VALID NUMBER ON ENTRY',/)
1006 FORMAT(IX,'X(I) IS NOT WITHIN XMIN(I) TO XMAX(I)',/)
1007 FORMAT(IX,'ZERO DIAGONAL ELEMENT IN EQUATION SOLVE',/)
1008 FORMAT(/,IX,'RUN EXCEEDED MAXIT OF ',I5,' ITER = ',I5,)
1009 FORMAT(IX,'I5 TRY TO CALC.',/)
1010 FORMAT(IX,'I5 DERIVATIVE ANALYTICALLY, CALC. ABORTED')
9000 CONTINUE
RETURN
END

C SUBROUTINE RHDW(MEABP,API,SG,AWW,ITRR)
C
C NAME OF MODULE - RHDW
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(DG F) 97-1036
C API 14.4-93.1
C AWW 78-724
C
C VARIABLES USED--

C VARIABLE I/O TYPE SPEC DIMENSION DESCRIPTION AND RANGE
C MEABP I R - MEAN BOILING POINT (DG F)
C API I R - API GRAVITY
C SG I R - SPEC. GRAVITY
C AWW O R - PSEUDOCRITICAL AVE MOL WT OF PET. FRAC.
C IERR O I - ERROR CODE
C
C -1 = MEABP NOT IN RANGE ABOVE
C -2 = API NOT IN RANGE ABOVE
-3 = AMW NOT IN RANGE ABOVE

```
IMPLICIT REAL*8 (A-H,O-Z)
IMPLICIT INTEGER(I-N)

REAL*8 MEANP

PARAMETER (MN=25)

COMMON /ID/ NIN,HOUT,NSTRY,NNP
COMMON /DEBUG/ LDBUG,LDEBUG

IF (LDBUG.GT.7) WRITE(NSTRY,900)

IERR=0

CHECK IF IN RANGE

IF (MEANP.LE.555.57D0.OR.MEANP.GT.1495.67D0) THEN
   IERR=-1
   WRITE(NSTRY,900)
   CALL HESS111
   WRITE(NSTRY,1000) MEANP
END IF

IF (API.LE.14.406.OR.API.GT.93.1D0) THEN
   IERR=-2
   WRITE(NSTRY,900)
   CALL HESS111
   WRITE(NSTRY,2000) API
END IF

CALC AVE MW

AMW=2.0436D2 * EXP(-0.9021D0*MEANP) * EXP(-3.07D0*SG)
   * (MEANP^2.0118D0) * (SG^2.168D0)

IF (AMW.LE.70.00.OR.AMW.GT.724.00) THEN
   IERR=-3
   WRITE(NSTRY,900)
   CALL HESS111
   WRITE(NSTRY,3000) AMW
END IF

FORMATS

900 FORMAT (IX, ' IN MODUKE EDNW'

1000 FORMAT
   1 IX, 'MEAN Values IN RANGE 555.67-1495.67',/
   2 IX, 'API VALUE = ',API, ' CALC. CONTINUES'

2000 FORMAT
   1 IX, 'API VALUE IS NOT IN RANGE 14.4-93.1',/
   2 IX, 'API VALUE = ',API, ' CALC. CONTINUES'

3000 FORMAT
   1 IX, 'MEAN VALUE IS NOT IN RANGE 70-724',/
   2 IX, 'MEAN VALUE = ',AMW, ' CALC. CONTINUES'

RETURN

SUBROUTINE RUPC (AMW,TBR,API,SG,PC,IERR)

END```

NAME OF MODULE - API4D4P1
MODULE TITLE - PROCEDURE 4D4.1 API DATA BOOK P4-57 (1980)
PURPOSE - METHOD FOR THE PSEUDOCRITICAL PRESSURE OF PETROLEUM FRACTIONS
MODIFIED - 10-3-88

LIMITATIONS:
  MW          82-694
  TB(CTRL F)  100-850
  API         6.6-95.0

VARIABLES USED:

<table>
<thead>
<tr>
<th>VARIABLE</th>
<th>TYPE</th>
<th>SPEC</th>
<th>DIMENSION</th>
<th>DESCRIPTION AND RANGE</th>
</tr>
</thead>
<tbody>
<tr>
<td>AMW</td>
<td>I</td>
<td>R</td>
<td></td>
<td>Mole Weight</td>
</tr>
<tr>
<td>TBR</td>
<td>I</td>
<td>R</td>
<td></td>
<td>Mean Average Boiling Point</td>
</tr>
<tr>
<td>SG</td>
<td>I</td>
<td>R</td>
<td></td>
<td>Specific Gravity (60/60F)</td>
</tr>
<tr>
<td>FC</td>
<td>O</td>
<td>R</td>
<td></td>
<td>PSEUDOCRITICAL PRES. OF PET. FRACTION</td>
</tr>
<tr>
<td>IERR</td>
<td>O</td>
<td>T</td>
<td></td>
<td>ERROR CODE</td>
</tr>
</tbody>
</table>

3 = API NOT IN RANGE ABOVE
-2 = TB NOT IN RANGE ABOVE
-1 = MW NOT IN RANGE ABOVE
0 = OK

IMPLICIT REAL*8 (A-H,O-Z)
IMPLICIT INTEGER (I-N)
PARAMETER (MNC=25)
COMMON /IO / NIN, NOUT, NINTRY, NKEFT
COMMON /DEBUG / LDEBUG, LDDEBUG
IERR=0
CHECK IF IN RANGE

IF (AMW .LT. 82.0D0 .OR. AMW .GT. 694.0D0) THEN
  WRITE (NINTRY, 900)
  CALL MESS(1)
  IERR=-1
  WRITE (NINTRY, 1000) AMW
ENDIF

CALL TCON(TBR, TB, 21, IERR)

IF (TB(CTRL F) .LT. 100.0D0 .OR. TB(CTRL F) .GT. 850.0D0) THEN
  WRITE (NINTRY, 900)
  CALL MESS(1)
  IERR=-2
  WRITE (NINTRY, 2000) TB(CTRL F)
ENDIF

IF (AMW .LT. 6.6D0 .OR. AMW .GT. 95.0D0) THEN
  WRITE (NINTRY, 900)
  CALL MESS(1)
  IERR=-3
  WRITE (NINTRY, 3000) AMW
ENDIF

PSEUDOCRITICAL PRES. OF FRACTION, PA

PC=3.12281D9 * TBR**(3.3125D0) * SG**(2.3201D0)

FORMATS
C SUBROUTINE ROLC(AMW,THR,API,SG,TC,IERR)
C
C NAME OF MODULE - ROLC
C MODULE TITLE - PROCEDURE 103.1 API DATA BOOK PI-51 (1980)
C PURPOSE - METHOD FOR THE PSEUDOCRITICAL TEMP. OF PETROLEUM
C         FRACTIONS
C MODIFIED - 10-3-88
C
C LIMITATIONS:
C      MM  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 THR  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 (DEG R)
C IERR  O  I   -  ERROR CODE
C
C -1 = MM NOT IN RANGE ABOVE
C -2 = TB NOT IN RANGE ABOVE
C -3 = API NOT IN RANGE ABOVE
C
C IMPLICIT REAL*8 (A-H,O-Z)
C IMPLICIT INTEGER(1-N)
C
C PARAMETER (NHC=25)
C COMMON /O / MIN,NOPT,MHC, NPT
C COMMON /DEBUG / LDBUG, LDBG
C IF (LDBG.GT.7) WRITE (NHYRSTY, 9000)
C IERR=0
C
C CHECK IF IN RANGE
C IF (AMW.LT.100.D0.OR.AMW.GT.850.D0) THEN
C WRITE (NHYRSTY, 900)
C CALL MEAS(1)
C IERR=-1
C WRITE (NHYRSTY, 1000) AMW
C ENDF
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

IF(API.LT.6.6D0.OR.API.GT.95.D0)THEN
  IERR=-3
  WRITE(NHSTRY,900)
  CALL MESS(1)
  WRITE(NHSTRY,3000)API
ENDIF

PSEUDOCRITICAL TEMP. OF FRACTION, IN DEGREES R

TC=24.2787D0  *  TBR**(0.58848D0)  *  SG**(0.3596D0)

FORMATS

900  FORMAT(1X,'IN MODULE RDTC')
1000  FORMAT(1X,'MW VALUE IS NOT IN RANGE 82-694',/,
  1  1X,'MW VALUE = ',6D12.6,' CALC. CONTINUES')
2000  FORMAT(1X,'TH(DEG F) VALUE IS NOT IN RANGE 100-850',/,
  1  1X,'TH-VALUE = ',6D12.6,' CALC. CONTINUES')
3000  FORMAT(1X,'API VALUE IS NOT IN RANGE 6.6-95',/,
  1  1X,'API VALUE = ',6D12.6,' CALC. CONTINUES')

RETURN
END

SUBROUTINE RDTC(MW,TBR,SG,VC,IERR)

NAME OF MODULE = RDTC

MODULE TITLE -- TO ESTIMATE PHYSICAL PROPS BY RIAZI DAUBERT MTH

PURPOSE -- TO ESTIMATE PHYSICAL PROPERTIES USING RIAZI AND DAUBERT

METHOD

REF: HYDROCARBON PROCESSING MARCH 1980 P115-116

RIAZI AND DAUBERT

MODIFIED -- 10-3-88

LIMITATIONS:

MW  77.2-291.5
TBR(DEG F)  100-850
SG  0.6247-1.0244

VARIABLES USED--

VARABLE  I/O  TYPE  SPEC  DIMENSION  DESCRIPTION AND RANGE

MW   I   R   -   MOLE WEIGHT
TBR   I   R   -   MEAN AVERAGE BOILING POINT (DEG F)
SG   I   R   -   SPECIFIC GRAVITY (60/60F)
VC   I   R   -   MOLAR CRITICAL VOLUME (M^3/KG-MOLE)
IERR  O   I   -   ERROR CODE

-1 = TH NOT IN RANGE ABOVE

IMPLICIT REAL*8 (A-H,O-Z)
IMPLICIT INTEGER(I-N)

PARAMETER (MNC=25)
COMMON /IO / MIN,MOUT,RETRY,NETRT
COMMON /DEBUG / LDBUG,LDBUGR

IF(LDBUG.GT.7)WRITE(NHSTRY,900)
IERR=0
ITYP=4

CALL RDCHECK(AMW,TBR,SG,ITYP)

MOLAR CRITICAL VOLUME (FT^3/LB-MOLE)

VCM=7.0434D-7 + TBR*(2.3829D6 + SG*(-1.683D0))

CONVERT CRITICAL VOLUME TO CORRECT UNITS (M^3/KG-MOLE)

VC=VCM/15.3155D0/0.453592D0

FORMATS

900 FORMAT(1X,'IN MODULE Rdvc')
RETURN
END

SUBROUTINE RDVC(JC,ICT,IERR)

NAME OF MODULE - RDVC
MODULE TITLE - RACKETT EQUATION FOR LIQUID VOLUME
PURPOSE - TO ESTIMATE THE RACKETT EQUATION LIQUID VOLUME
PARAMETER RTENA
MODIFIED - 10-5-88
METHOD - GENERATE VALUES FOR MODIFIED RACKETT EQUATION
BY DEFAULT ZC OR FITTING GUNN YAMADA METHOD.

VARIABLES USED-

VARIABLE I/O TYPE SPEC DIMENSION DESCRIPTION AND RANGE
JC I 1 1 COMPONENT ARRAY ID
ICT I 1 I 1 CALC TYPE
0 = VSL ZC
1 = FLY DATA
IERR 0 1 I ERROR CODE
0 = OK
-1 = NO IMPROVEMENT POSSIBLE IN THE VALUE OF YH EVEN THOUGH CONVERGENCE HAS NOT BEEN REACHED.
-2 = MORE UNKNOWNS THAN FUNCTIONS AND UNIQUE SOLUTION GENERALLY IS IMPOSSIBLE.
-3 = TOTAL NUMBER OF VARIABLES TO BE VARIED IS ZERO
-4 = CONVERGENCE CRITERION NOT BUT ITL STILL LARGE
-5 = L/1 NOT A VALID NUMBER ON ENTRY
-6 = X1(I) IS NOT WITHIN XMIN(I) TO XMAX(I)
-7 = ZERO DIAGONAL ELEMENT IN EQUATION SOLVE
-10 = TRY TO CALC. DERIVATIVE ANALITICALLY
-11 = RUN EXCEEDED MAXIT SPECIFIED

IMPLICIT REAL*8 (A-H,O-Z)
IMPLICIT INTEGER(I-M)

PARAMETER (MNC=25)
COMMON /IO / MIN,NOUT,NHSTRY,NHEPT
COMMON /DEBUG / LDSUG,LDBUGR
COMMON /HEFS / TREF,PREF,RGAS

COMMON /CPRP01/ TC(MNC)
COMMON /CPRP02/ PC(MNC)
COMMON /CPRP03/ SC(MNC)
COMMON /CPRP05/ RMEGA(MNC)
COMMON /CPRP12/ RKTZRA(MNC),RKTREG(3,MNC)
COMMON /CPRP14/ TB(MNC)

COMMON /CPRP15/ VD(MNC)

DIMENSION X(50),Y(50), Z(100),PJ(50),P(102),A(15),AC(5)
DIMENSION B(2),BV(1),BMAX(1),BMIN(1)

IF(LDBUG.GT.7)WRITE(NHSTRY,900)

IF(ICT.EQ.0)THEN
RKTZRA(JC)=ZC(JC)
ELSE
     FIT GUMA YHADA IN RANGE 0.2*TH<0.9
     SET DEFAULTS
     MAXIT=1000
     NUMBER OF UNKNOWNS
     K=1
     NUMBER OF DATA POINTS
     N=50
     ITER = 0
     INITIAL GUESS
     B(1) = ZC(JC)
     NDATA(1)=1

DO 10 I=1,5
     DATA(I)=0.000
10  CONTINUE
DO 20 T=1,6
     BV(I)=1,00
     BMAX(I)= 0.9900
     BMIN(I)= 0.0100
20  CONTINUE
     IF(B(I).LT.BMIN(I))B(I)=BMIN(I)
     IF(B(I).GT.BMAX(I))B(I)=BMAX(I)

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)
XSUM=0.0D0
XSUM2=0.0D0
YSUM=0.0D0
YSUM2=0.0D0
ENDIF

BEGIN CALC (CALC 50 POINTS TO BE FIT)
I-CALC=0

DEL=(0.99D0-0.20D0)/FLOAT(N)
TRD=0.20D0-DEL
OMEGA=OMEGA(JC)
VR=V(jc)
TR=TB(JC)/TC(JC)

DO 40 I=1,N
TRD=TRD+DEL

CALL GUNYAH(VR,TR,OMEGA,TRD,I-CALC,VD,IERR)
X(I)=TRD*TC(JC)
Y(I)=VD

IF(LDBUG.GE.7)THEN
WRITE(NHSTRY,1120)X(I),Y(I)
XSUM=XSUM+X(I)
XSUM2=XSUM2+X(I)**2
YSUM=YSUM+Y(I)
YSUM2=YSUM2+Y(I)**2
ENDIF

MEANS, VARIANCES AND STANDARD DEV.

IF(LDBUG.GE.7)THEN
XMEAN=XSUM/FLOAT(N)
XVAR=(FLOAT(N)*XSUM2-XSUM*XSUM)/FLOAT(N)/FLOAT(N-1)
XSD=SQRAT(XVAR)
YMEAN=YSUM/FLOAT(N)
YVAR=(FLOAT(N)*YSUM2-YSUM*YSUM)/FLOAT(N)/FLOAT(N-1)
YSD=SQRAT(YVAR)
WRITE(NHSTRY,1120)XMEAN,YMEAN,XVAR,YVAR,XSD,YSD
ENDIF

40 CONTINUE

MARQUARDT LOOP BEGINS TO FIT REZRA

ITER=ITER+1
IF(ITER.GT.MAXIT)THEN
IERR=-11
CALL MESS(2)
WRITE(NHSTRY,900)
WRITE(NHSTRY,1043)MAXIT,ITER
GOTO 9000
ENDIF

EVALUATE \& VECTORS [FUNCTION VALUE]

VNL=RTC*FC*REZRA**((1+1-TR)**2+7)

TS=2.50/1.00
DO 60 I=1,N
TR=X(I)/TC(JC)
VNL=EGAS*TC(JC)/TC(JC)*TR**11***(1.00+(1.00-TR)**2*TS)
60 CONTINUE

CALC ANALYTICAL DERIVATIVES (PJ VECTOR)

CONTINUE

CALC DERIVATIVE
IF (NDATA(2).GT.0) THEN
  IERR=-10
  CALL MESS(3)
  WRITE(NHSTRY,900)
WRITE(NHSTRY,10900)
WRITE(NHSTRY,1022)
  RKTZRA(JC)=ZC(JC)
ENDIF

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.D0
ELSE
  ADJRSQU=1.D0-(1.D0-RSQU)*(FLOAT(N1-1.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

DO 100 J=1,K
  WRITE(NHSTRY,10100) J, B(J)
100 CONTINUE

IF (LDBUG.EQ.8) THEN
  WRITE(NHSTRY,1015)
DO 110 J=1,N
  YMYC=YMYC+(Y(J)-Z(J))**2
  SS=SS+(Z(J)**2-YMEAN)**2
  PERERR=ABS(Y(J)-Z(J))/ABS(Y(J))*100.D0
  WRITE(NHSTRY,10950) Z(J), Y(J), Z(J)-Y(J), PERERR
110 CONTINUE
ENDIF

ENDIF

CALL YSGLED (K, N, NDATA, ITRP, MV, LV, UM, VM, Y, 2, J, I,
1  OUTPUT, NV, 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).EQ.130, 50, 70
C
C  NDATA(3) - IERR, MAY TAKE ON VARIOUS VALUES
IF POSITIVE, CONTAINS THE NUMBER OF VARIABLES NO SATISFYING CONVERGENCE CRITERION
IF = 0, CONVERGENCE SATISFIED AND SOLUTION RETU
IF = -1, NO IMPROVEMENT POSSIBLE IN THE VALUE OF
PH EVEN THOUGH CONVERGENCE HAS NOT BEEN
REACHED.
IF = -2, MORE UNKNOWNS THAN FUNCTIONS AND UNIQUE
SOLUTION GENERALLY IS IMPOSSIBLE.
IF = -3, TOTAL NUMBER OF VARIABLES TO BE VARIED
IS ZERO
IF = -4, CONVERGENCE CRITERION MET BUT FLM STILL
LARGE.
IF = -5, IS NOT A VALID NUMBER ON ENTRY
IF = -6, X(I) IS NOT WITHIN BMNI(I) TO BMX(I)
IF = -7, ZERO DIAGONAL ELEMENT IN EQUATION SOLVE

130 IF(NDATA(3)) .EQ. 140, 140, 120

FINAL STATISTICAL RESULTS

CONTINUE
IF(FDSVGE.5) THEN
WRITE(NHYST, 900)
WRITE(NHYST, 1000) DATA(I), OUTPUT(I), I=1, 5
YMYC = 0.000
SS = 0.000
SSAS = 0.000
DO 150 I=1, N
YMYC = YMYC + (Y(I) - Z(I))**2
SD = SS * (N(N-1)/NMEAN)**(1/2)
SSAS = SSAS + (Y(I) - Z(I))**2

150 CONTINUE

CALC R-SQUARE(SAS VERSION) AND ADJ R-SQUARE

RSQAS = 1.0 - YMYC/(SSAS)
IF(DEGFR.EQ.0.000) THEN
ADJRSQAS = 0.000
ELSE
ADJRSQV = 1.0 - (1.0 - RSQV)/(FLOAT(N) - 1.0)/DEGFR
ADJRSQAS = 1.0 - (1.0 - RSQAS)/(FLOAT(N) - 1.0)/DEGFR
ENDIF
IF(DRSQV<RSQV) THEN
WRITE(NHYST, 1112) RSQV, ADJRSQV, RSQAS, ADJRSQAS
ELSE
WRITE(NHYST, 1110) RSQV, ADJRSQV
ENDIF

FINAL PARAMETERS

DO 166 I=1, K
WRITE(NHYST, 1030) I, X(I)

166 CONTINUE

FINAL SUMMARY

WRITE(NHYST, 1030)
DO 170 I=1, N
PERERR = ABS(Z(I) - Y(I))/ABS(Y(I)) * 100.00
WRITE(NHYST, 1035) I, Z(I), Y(I), Z(I) - Y(I), PERERR
170 CONTINUE

ENDIF

LOAD DATA INTO RKTZRA ARRAY
IERR=NDATA(3)  
IF (IERR.EQ.0) THEN  
  CONVERGED  
  RKTZRA(JC)=ZC(JC)  
ENDIF  
ELSE IF (IERR.EQ.-1) THEN  
  RKTZRA(JC)=ZC(JC)  
  CALL MS(1)  
  WRITE (NHSTRY, 900)  
  WRITE (NHSVRY, 1000) IITER, NDATA(3), (OUTPUT(J), J=1, 5)  
ENDIF  
ELSE IF (IERR.EQ.-2) THEN  
  RKTZRA(JC)=ZC(JC)  
  CALL MS(1)  
  WRITE (NHSVRY, 900)  
  WRITE (NHSVRY, 1000) IITER, NDATA(3), (OUTPUT(J), J=1, 5)  
  WRITE (NHSVRY, 1002)  
  WRITE (NHSVRY, 1022)  
  RKTZRA(JC)=ZC(JC)  
ELSE IF (IERR.EQ.-3) THEN  
  CALL MS(2)  
  WRITE (NHSVRY, 900)  
  WRITE (NHSVRY, 1000) IITER, NDATA(3), (OUTPUT(J), J=1, 5)  
  WRITE (NHSVRY, 1004)  
  WRITE (NHSVRY, 1022)  
  RKTZRA(JC)=ZC(JC)  
ELSE IF (IERR.EQ.-4) THEN  
  CALL MS(2)  
  WRITE (NHSVRY, 900)  
  WRITE (NHSVRY, 1000) IITER, NDATA(3), (OUTPUT(J), J=1, 5)  
  WRITE (NHSVRY, 1005)  
  WRITE (NHSVRY, 1022)  
  RKTZRA(JC)=ZC(JC)  
ELSE IF (IERR.EQ.-5) THEN  
  CALL MS(2)  
  WRITE (NHSVRY, 900)  
  WRITE (NHSVRY, 1000) IITER, NDATA(3), (OUTPUT(J), J=1, 5)  
  WRITE (NHSVRY, 1006)  
  WRITE (NHSVRY, 1022)  
  RKTZRA(JC)=ZC(JC)  
ELSE IF (IERR.EQ.-6) THEN  
  CALL MS(2)  
  WRITE (NHSVRY, 900)  
  WRITE (NHSVRY, 1000) IITER, NDATA(3), (OUTPUT(J), J=1, 5)  
  WRITE (NHSVRY, 1007)  
  WRITE (NHSVRY, 1022)  
  RKTZRA(JC)=ZC(JC)  
ENDIF  
RKTREG(1, JC)=FLOAT(ITER)  
RKTREG(2, JC)=FLOAT(NDATA(3))  
RKTREG(3, JC)=OUTPUT(1)  
ENDIF
C

FORMATS

900 FORMAT('IN MODULE REFLV')
1000 FORMAT(/,1X,'ITERATION: ',I9,/,1X,'ERR: ',F15.8,/,1X,'SUM OF SQUARES: ',G15.8,/,1X,'ANGLE (DEGREES): ',F15.3,/,1X,'NUMBER OF TIMES YSOLVE CALLED: ',F15.1,/,1X,'NUMBER OF FUNCTIONAL EVALUATIONS: ',F15.1,/,1X,'NUMBER OF ANALYTICAL DERIVATIVE EVALUATIONS: ',F15.1,/) 1001 FORMAT('NO IMPROVEMENT POSSIBLE IN THE VALUE OF: ',/),1X,'IT EVEN THOUGH CONVERGENCE HAS NOT BEEN REACHED. ')
1002 FORMAT('MORE UNKNOWNS THAN FUNCTIONS AND UNIQUE: '/)
1003 FORMAT('TOTAL NUMBER OF VARIABLES TO BE VARIED: ',I9,/,/)
1004 FORMAT('CONVERGENCE CRITERION NOT BUT PLA STILL LARGE: '/)
1005 FORMAT('J IS NOT A VALID NUMBER ON ENTRY: '/)
1006 FORMAT('X(I) IS NOT WITHIN XMIN TO XMAX(I): '/)
1007 FORMAT('ZERO DIAGONAL ELEMENT IN EQUATION SOLVE: '/)
1008 FORMAT('/,5X,'* NESTED METHOD REGRESSION ***, '/),1X,'K (NUMBER OF PARAMETERS TO BE VARIED) = ',I9,/,1X,'H (NUMBER OF DATA POINTS) = ',I9,/,1X,'N-H = N-HAX',/)
1009 FORMAT('VARY FLAG: '/)
1010 FORMAT(5X,'VARY FLAG: '/),1X,'1 = HOLD PARAMETER CONSTANT: ',/)
1011 FORMAT(5X,'1 = VARY PARAMETER USING NUMERICAL DERIVATIVE: ',/),1X,'-1 = VARY PARAMETER USING ANALYTICAL DERIVATIVE: ')
1012 FORMAT('X, ',15X,15F15.4)
1013 FORMAT('VALUE IS DEFAULTED TO ZC: *****)
1014 FORMAT('H, ',15X,1F15.5)
1015 FORMAT(1X,'% ERROR: '/)
1016 FORMAT(1X,15I1,1X,15F15.5)
1017 FORMAT(1X,'INPUT DATA: '/),1X,'',/)
1018 FORMAT(/,5X,'X-VALUE: ',F15.4,1X,'Y-VALUE: ',F15.4,/,1X,'-------',/)
1110 FORMAT(1X,'R-SQUARE: ',F15.8,/,1X,'ADJ R-SQUARE: ',F15.8,/) 1111 FORMAT(1X,'R-SQUARE: ',F15.8,/,1X,'ADJ R-SQUARE: ',F15.8,/) 1112 FORMAT(/,5X,'R-SQUARE: ',F15.8,/,1X,'ADJ R-SQUARE: ',F15.8,/,1X,'R-SQUARE: ',F15.8,/,1X,'ADJ R-SQUARE: ',F15.8,/) 1120 FORMAT(/,1X,'R-SQUARE: ',F15.8,/,1X,'ADJ R-SQUARE: ',F15.8,/,1X,'R-SQUARE: ',F15.8,/,1X,'ADJ R-SQUARE: ',F15.8,/) 1045 FORMAT(1X,'RUN EXCEEDED MAXIT OF ',15X,'ITER = ',15X,'**',/) 1050 FORMAT('X, ',15F15.5,15F15.5)
5000 CONTINUE
RETURN
END

SUBROUTINE SOLPAR(JC, JERR)

NAME OF MODULE - SOLPAR
MODULE TITLE - CALCULATION OF SOLUBILITY PARAMETER AT 25 DEG C
PURPOSE - TO CALC SOLUBILITY PARAMETER AT 25 DEG C
MODIFIED - 11-12-88

METHOD - ESTIMATE SOLUBILITY PARAMETER PER API REPORT API-1-77,
USING HEAT OF VAPORIZATION AT 25 C BY WATSON METHOD AND
VOLUME AT 20 C AND 1 ATM BY RAIZI DAUBERT METHOD
AND CORRECT TO 25 C BY GUNN & YAMADA METHOD.

VARIABLES USED:

VARIABLE I/O TYPE SPEC DIMENSION DESCRIPTION AND RANGE
JC I I - COMPONENT ARRAY ID
IERR 0 I - ERROR CODE

0 = OK
-1 = GUNYAM REDUCED TEMP > 0.99
-2 = GUNYAM REDUCED TEMP < 0.2
-3 = TB OUT OF RANGE
-4 = SG OUT OF RANGE
-5 = WATSON CALC OUT OF RANGE

IMPLICIT REAL*8 (A-H,O-Z)
IMPLICIT INTEGER(I-N)

PARAMETER
(MNC=25)

COMMON /TO / MIN, NOUT, NISTRY, NREPT
COMMON /DEBUG / LDEBUG, LDEBUGR
COMMON /RECS / TREF, PREF, ROAS

COMMON /HPROP/) /UGPR(MNC), API(MNC), SG(MNC), AMW(MNC)

COMMON /CRP1/) /TC(MNC)
COMMON /CRP15/) /OMEGA(MNC)
COMMON /CRP16/) /DHVLWT5(MNC)
COMMON /CRP14/) /TH(MNC)
COMMON /CRP13/) /DELTA(MNC)

IERR=0
IF(LDEBUG.GT.7) WRITE(NISTORY,300)

CALC HEAT OF VAPORIZATION (BTU/IB-MOLE) AT 25 C USING ASEFEN'S
WATSON EQUATION

T25=THREF

IF(T25.GT.1.50) THEN
  CALL MESS111
  WRITE(NISTORY,300) T25
ENDIF

HVA25=DHVLWT1(JC)+HVA25

CONVERT TO CAL/GH

HVA25=HVA25*0.239018/1000.DO/AMW(JC)

CALC ENERGY OF VAPORIZATION AT 25 C

CALL TCON(T25C,JT,25C,42,IERR1)
EVA25=HVA25 * 1.98719DO * T25C/AMW(JC)

LIQUID MOLAR VOLUME AT 20 DEG C AND 1 ATM (CM^3/G-MOLE)
AT 1 BTU/LB-MOLE AT TB AND SG

CALL TCON(TB>JC,THB,42,IERR2)
CALL TCON(TBR, TBF, 21, IERR1)

IF (TBF.LT.100.D0 OR TBF.GT.850.D0) THEN
  IERR=-3
  CALL MESS(1)
  WRITE(MHSTRY, 900)
  WRITE(MHSTRY, 2000) TBF
ENDIF

SM=SG(JC)
IF (SM.LT.0.6247D0 OR SM.GT.1.0244D0) THEN
  IERR=-3
  CALL MESS(1)
  WRITE(MHSTRY, 900)
  WRITE(MHSTRY, 1000) SM
ENDIF

V=7.6211D-5 * TBR**2 (2.1262D0) * SM**(-1.8688D0)

CORRECT TO 25 C BY GUMYAH

VR=V
TH=293.15D0/TC(JC)
OMEGA1=OMEGA(JC)
TRD=TREF/TC(JC)
ICALC=0
CALL GUMYAH(VR, TH, OMEGA1, TRD, ICALC, VD, IERR)

DENSITY AT 25 C (G/M**3)
RHO=1.00/VD*AMW(JC)

CALC SOLUBILITY PARAMETER (CAL/M**3)
SOLP=EVA25*RHO

SOLUBILITY PARAMETER (CAL/M**3)**1/2
SOLP=SQR(SOLP)

SOLUBILITY PARAMETER (M/M**3)**1/2
CFAC=SQRT(1.0D6/33961D0)
DELTAC(JC)=SOLP*CFAC

FORMAT

900 FORMAT(IX, 'IN MODULE SOLPARI')
1000 FORMAT(IX, 'SG VALUE IS NOT IN RANGE 0.6247-1.0244', /,
          IX, 'SG VALUE = ', A12.6, ' CALC. CONTINUES')
2000 FORMAT(IX, 'TH(BOG FL) VALUE IS NOT IN RANGE 100-850', /,
          IX, 'BOG FL VALUE = ', A12.6, ' CALC. CONTINUES')
3000 FORMAT(IX, 'WATSON VALUE IS NOT IN RANGE 0-TC', /,
          IX, 'WATSON VALUE = ', A12.6, ' CALC. CONTINUES')
RETURN
END

SUBROUTINE TBCALC(JC, IERR)

NAME OF MODULE - TBCALC
MODULE TITLE - LOAD NORMAL BOILING POINT ARRAY
PURPOSE - TO LOAD NORMAL BOILING POINT ARRAY
MODIFIED - 10-28-88
METHOD - SET EQUAL TO INPUT VOLUME AVERAGE BOILING POINT
VARIABLES USED:

VARIABLE I/O TYPE SPEC DIMENSION DESCRIPTION AND RANGE
JC  I  I  - COMPONENT ARRAY ID
IERR  0  I  - ERROR CODE
D  =  OK

IMPLICIT REAL*8 (A-H,O-Z)
IMPLICIT INTEGER (I-N)

REAL*8  MABP,MEABP

PARAMETER (MNC=25)

COMMON /IO / NIN,NOUT,NHSTRY,NREPT
COMMON /DEBUG / LDEBUG,LDEBUGR

COMMON /NPROP2/ VABP(MNC),SLOP(MNC),CABP(MNC),HABP(MNC),HABP(MNC),HABP(MNC)

COMMON /CRPF4/ TB(MNC)

IF (LDEBUG.GT.7) WRITE(NHSTRY,990)
IERR=0

TB(JC)=VABP(JC)

FORMATS

990 FORMAT(1X,'IN MODULE TFCF')
RETURN
END

SUBROUTINE TFCF(VABP,STPF,CABP,MABP,IERR)

NAME OF MODULE - TFCF

MODULE TITLE - CHARACTERIZE PETROLEUM FRACTION BOILING PTS

PURPOSE - METHOD FOR CHARACTERIZE PETROLEUM FRACTION BOILING

POINTS

MODIFIED - 1-6-83

LIMITATIONS:

SLOPE  5  TO  10
CABP  200  TO  600

VARIABLES USED:

VARIABLE I/O TYPE SPEC DIMENSION DESCRIPTION AND RANGE
VABP1  I  H  - VOLUME AVERAGE BOILING POINT (deg F)
STPF  I  H  - SLOPE OF THE CURVE
(C70-T10)/0 1.6/deg F
CABP  O  H  - CURRIC AVERAGE BOILING POINT (deg F)
MABP  O  H  - HOURLY AVERAGE BOILING POINT (deg F)
IERR  0  I  - ERROR CODE
D  =  OK
-1 = SLOPE NOT IN RANGE ABOVE
-2 = CABP NOT IN RANGE ABOVE

IMPLICIT REAL*8 (A-H,O-Z)
IMPLICIT INTEGER (I-N)

REAL*8  MABP,MEABP,EMEX

COMMON /IO / NIN,NOUT,NHSTRY,NREPT
COMMON /DEBUG / LDEBUG,LDEBUGR
IERR = 0

IF (LDBUG.GT.7) WRITE (NHSTRY, 900)
CABPC = 0.0 DO
MABPC = 0.0 DO
VABP = VABPI

CHECK IF SLOPE IN RANGE (-10)

IF (STBP .LT. 0.0) THEN
IERR = -1
CALL MESS(1)
WRITE (NHSTRY, 900)
WRITE (NHSTRY, 1000) STBP
STBP = 0.0 DO
ENDIF

IF (STBP .GT. 10.0) THEN
IERR = -1
CALL MESS(1)
WRITE (NHSTRY, 900)
WRITE (NHSTRY, 2000) STBP
STBP = 10.0 DO
ENDIF

CHECK APPLICATION RANGE FOR MABP

IF (VABP .LT. 200.0 DO ) THEN
IERR = -2
CALL MESS(1)
WRITE (NHSTRY, 900)
WRITE (NHSTRY, 3000) VABP
HABPC = INDEX (200.0 DO, VC(STBP, 1), 300.0 DO, VC(STBP, 2), VABP)
ELSE IF (VABP .LE. 200.0 DO .AND. VABP .LT. 100.0 DO ) THEN
HABPC = INDEX (200.0 DO, VC(STBP, 1), 100.0 DO, VC(STBP, 2), VABP)
ELSE IF (VABP .LE. 100.0 DO .AND. VABP .LT. 500.0 DO ) THEN
HABPC = INDEX (100.0 DO, VC(STBP, 2), 500.0 DO, VC(STBP, 3), VABP)
ELSE IF (VABP .LE. 500.0 DO .AND. VABP .LT. 1000.0 DO ) THEN
HABPC = INDEX (500.0 DO, VC(STBP, 3), 1000.0 DO, VC(STBP, 4), VABP)
ELSE IF (VABP .GT. 600.0 DO ) THEN
IERR = -2
CALL MESS(1)
WRITE (NHSTRY, 900)
WRITE (NHSTRY, 3000) VABP
HABPC = VC(STBP, 1)
ENDIF

CHECK MABP

IF (HABPC .LE. 0.0 DO ) THEN
MABP = VABP + HABPC
ELSE
MABP = VABP
ENDIF

CHECK APPLICATION RANGE FOR CABP

IF (VABP .LT. 200.0 DO ) THEN
IERR = -2
CALL MESS(1)
WRITE (NHSTRY, 900)
WRITE (NHSTRY, 3000) VABP
CABPC = INDEX (200.0 DO, VC(STBP, 1), 300.0 DO, VC(STBP, 2), VABP)
ELSE IF (VABP .LE. 200.0 DO .AND. VABP .LT. 100.0 DO ) THEN
CABPC = INDEX (200.0 DO, VC(STBP, 2), 100.0 DO, VC(STBP, 3), VABP)
ELSE IF (VABP .LE. 100.0 DO .AND. VABP .LT. 500.0 DO ) THEN
CABPC = INDEX (100.0 DO, VC(STBP, 3), 500.0 DO, VC(STBP, 4), VABP)
ELSE IF (VABP .LE. 500.0 DO .AND. VABP .LT. 1000.0 DO ) THEN
CABPC = INDEX (500.0 DO, VC(STBP, 4), 1000.0 DO, VC(STBP, 5), VABP)
ELSE IF (VABP .GT. 1000.0 DO ) THEN
IERR = -2
CALL MESS(1)
WRITE (NHSTRY, 900)
WRITE (NHSTRY, 3000) VABP
CABPC = VC(STBP, 5)
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.LT.500.D0) THEN
   ERR=-2
   CALL MESS(1)
   WRITE(NHSTRY,900)
   WRITE(NHSTRY,4000)VABP
   CABPC=VC(STBP,4)
ENDIF

CORRECT CABP

IF (CABPC.LE.0.D0) THEN
   CABP=VABP+CABPC
ELSE
   CABP=VABP
ENDIF

FORMATS

900  FORMAT(1X,'IN MODULE TBPCF')
1000  FORMAT(1X,'SLOPE VALUE IS NOT IN RANGE 0-10.0',/,
         1     IX,' SLOPE= ',F12.6,/,
         2     IX,' SLOPE SET TO 0.0 AND CALC. CONTINUES')
2000  FORMAT(1X,'SLOPE VALUE IS NOT IN RANGE 0-10.0',/,
         1     IX,' SLOPE= ',F12.6,/,
         2     IX,' SLOPE SET TO 10.0 AND CALC. CONTINUES')
3000  FORMAT(1X,'VABP VALUE IS NOT IN RANGE 200-600',/,
         1     IX,' VABP= ',F12.6,/,
         2     IX,' CALC IS EXTRAPOLATION. HABP CALC CONTINUES')
4000  FORMAT(1X,'VABP VALUE IS NOT IN RANGE 200-600',/,
         1     IX,' VABP= ',F12.6,/,
         2     IX,' CALC IS EXTRAPOLATION. CBAP CALC CONTINUES')

RETURN

END

FUNCTION INEX(XL,YL,XH,YH,XW)

NAME OF MODULE - INEX

MODULE TITLE - INTERPOLATION/EXTRAPOLATION

PURPOSE - TO CALC LINEAR INTERPOLATION/EXTRAPOLATION

MODIFIED - 1-6-85

LIMITATIONS:

VARIABLES USED-

VARIABLE I TO TYPE SPEC DIMENSION   DESCRIPTION AND RANGE
C   XL  I   H   LOW VALUE DEPENDENT VARIABLE
C   YL  I   H   LOW VALUE INDEPENDENT VARIABLE
C   XH  I   H   HIGH VALUE DEPENDENT VARIABLE
C   YH  I   H   HIGH VALUE INDEPENDENT VARIABLE
C   XW  I   H   DESIRED VALUE INDEPENDENT VARIABLE

IMPLICIT REAL*8 (A-H,O-Z)
IMPLICIT INTEGER (I-N)
REAL*8   INEX

IF((XH-XL).NE.0.D0) THEN
   INEX=YL+((XW-XL)/(XH-XL))*(YH-YL)
ELSE
   INEX=(YL-YH)/2.D0
ENDIF
FUNCTION VM(STBP, TEMP)

NAME OF MODULE - VMC
MODULE TITLE - CORRECTION TO VABP VALUE FOR CABP
PURPOSE - CORRECTION OF VABP TO GIVE CABP FROM SLOPE OF TBP CURVE
MODIFIED - 1-6-83

LIMTATIONS:

VARIABLES USED:

VARIABLE I/O TYPE SPEC DIMENSION DESCRIPTION AND RANGE
STBP I A - SLOPE OF TBP CURVE
ITEMP I I - CALC TYPE
1 = 200
2 = 400
3 = 500
4 = 600+

IMPLICIT REAL A-N, I-E
IMPLICIT INTEGER E-M
REAL A

DIMENSION EQUA(5,1)
DIMENSION EQUA(5,1)

5 EACH 100 400 300 600
DATA EQUA / 1.97111112D0, 3.53376666D0, 2.40272166D0,
1 0.34331112D0, 0.36535353D0, 0.12343434D0,
3 0.76543210D0, 0.90112312D0, 0.23456789D0,
3 0.76543210D0, 0.90112312D0, 0.23456789D0,
3 0.76543210D0, 0.90112312D0, 0.23456789D0,
3 0.76543210D0, 0.90112312D0, 0.23456789D0,

C DATA EQUA / 1.97111112D0, 3.53376666D0, 2.40272166D0,
1 0.34331112D0, 0.36535353D0, 0.12343434D0,
3 0.76543210D0, 0.90112312D0, 0.23456789D0,
3 0.76543210D0, 0.90112312D0, 0.23456789D0,
3 0.76543210D0, 0.90112312D0, 0.23456789D0,
3 0.76543210D0, 0.90112312D0, 0.23456789D0,

IF (STBP .LT. LLM/ITEMP) THEN
VM = EQUA(5,ITEMP)/STBP+EQUA(5,ITEMP)*STBP+STBP
ELSE
VM = 0
ENDIF

RETURN
END

FUNCTION VM(STBP,ITEMP)
MODIFIED - 1-6-89

LIMITATIONS:

VARIABLES USED:

VARIABLE I/O TYPE SPEC DIMENSION DESCRIPTION AND RANGE
STBP I M - SLOPE OF TBP CURVE (T70-T10)/60 (DEG F/DEG F)
ITEMP I I - CALC TYPE
  1 = 200
  2 = 300
  3 = 400
  4 = 500+

IMPLICIT REAL*8 (A-H.O-Z)
IMPLICIT INTEGER(I-N)
REAL*8

DIMENSION EQVAL(2,4)
DIMENSION LLIM(4)

DATA EQVAL/6.0268357600,-7.3722554000,
  1 5.0019394900,-1.1081232000,
  2 2.5105675300,-1.6103920700,
  3 0.51730600100,-0.11555627900/

DATA LLIM/(1.067821D0,1.298701D0,1.500722D0,1.998557D0)/

IF(STBP.GT.LLIM(ITEMP))THEN VC=EQVAL(1,ITEMP)+EQVAL(2,ITEMP)*STBP
ELSE
  VC=0.D0
ENDIF

IF(VC.GT.0.0D0)VC=0.0D0
RETURN
END

SUBROUTINE PCON(PRESI,PRESO,ICALC,IERR)

NAME OF MODULE - PCON

MODULE TITLE - CONVERSION OF PRESSURES
PURPOSE - TO CONVERT PRESSURES
MODIFIED 5-13-88 (COMPLETED)

VARIABLES USED:

VARIABLE I/O TYPE SPEC DIMENSION DESCRIPTION AND RANGE
PRESI I R - INPUT PRESSURE
PRESO O W - OUTPUT PRESSURE
TCALC I I - INPUT CODE(1=PSIA,2=PSIG,3=ATH,
  4=MHG,5=FAM)
  12 FOR PSIA TO PSIG
  13 FOR PSIA TO ATH
  ETC.
  21 FOR PSIG TO PSIA
  ETC.
IERR O I - ERROR CODE
  0 = OK
  -1 = NOT VALID TCALC NUMBER

IMPLICIT REAL*8 (A-H.O-Z)
IMPLICIT INTEGER(I-N)
C
COMMON /IO / NIN,NOUT,NHSTRY,NREPT
COMMON /DEBUG / LDBUG,LDBGUR
IERR=0

C
PRES=PRES

C
IF (ICALC.EQ.12) THEN
   PSI A TO PSIG
   PRES=PRES-14.696D0
   ELSE IF (ICALC.EQ.13) THEN
   PSI A TO ATM
   PRES=PRES/14.696D0
   ELSE IF (ICALC.EQ.14) THEN
   PSI A TO MMHG
   PRES=PRES/14.696D0*760.D0
   ELSE IF (ICALC.EQ.15) THEN
   PSI A TO PA
   PRES=PRES/14.696D0*1.01325D5
   ELSE IF (ICALC.EQ.21) THEN
   PSIG TO PSI A
   PRES=PRES+14.696
   ELSE IF (ICALC.EQ.23) THEN
   PSIG TO ATM
   PRES=(PRES+14.696D0)/14.696D0
   ELSE IF (ICALC.EQ.24) THEN
   PSIG TO MMHG
   PRES=(PRES+14.696D0)/14.696D0*760.D0
   ELSE IF (ICALC.EQ.25) THEN
   PSIG TO PA
   PRES=(PRES+14.696D0)/14.696D0*1.01325D5
   ELSE IF (ICALC.EQ.31) THEN
   ATM TO PSI A
   PRES=PRES-14.696D0
   ELSE IF (ICALC.EQ.32) THEN
   ATM TO PSIG
   PRES=PRES-14.696D0-14.696D0
   ELSE IF (ICALC.EQ.34) THEN
   ATM TO MMHG
   PRES=PRES+760.D0
   ELSE IF (ICALC.EQ.35) THEN
   ATM TO PA
   PRES=PRES+1.01325D5
   ELSE IF (ICALC.EQ.41) THEN
   MMHG TO PSI A
   PRES=PRES+760.D0*14.696D0
   ELSE IF (ICALC.EQ.42) THEN
   MMHG TO PSIG
   PRES=PRES+760.D0*14.696D0-14.696D0
   ELSE IF (ICALC.EQ.43) THEN
   MMHG TO ATM
   PRES=PRES+760.D0
   ELSE IF (ICALC.EQ.45) THEN
   MMHG TO PA
   PRES=PRES+760.D0+1.01325D5
   ELSE IF (ICALC.EQ.51) THEN
   PA TO PSI A
   PRES=PRES+1.01325D5*14.696D0
   ELSE IF (ICALC.EQ.52) THEN
   PA TO PSIG
   PRES=PRES+1.01325D5*14.696D0-14.696D0
   ELSE IF (ICALC.EQ.53) THEN
   PA TO ATM
   PRES=PRES+1.01325D5
   ELSE IF (ICALC.EQ.53) THEN
   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
FORMATS
C
900 FORMAT(1X,'IN MODULE PCON')
1000 FORMAT(1X,'INVALID VALUE OF ICALC OF ',I10,/,1
   IX,'NO PRES CONVERSION (& CALC. CONTINUES')
RETURN
END
C
***************************************************************
C
SUBROUTINE TCON(TEMPI,TEMPO,ICALC,IERR)
C
***************************************************************
C
NAME OF MODULE - TCON
C
MODULE TITLE - CONVERSION OF TEMPERATURE
C
PURPOSE - TO CONVERT TEMPERATURES
C
MODIFIED - 9-14-88 (COMPLETED)
C
VARIABLES USED-
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
C
IMPLICIT REAL*8 (A-H,O-Z)
C
IMPLICIT INTEGER (I-N)
C
COMMON /IO / NIN,NOUT,NHSTRY,NREPT
C
COMMON /DEBUG / LDBUG,LDBUGE
C
IERR=0
C
TEMPI=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-32.00D0)/1.8D0
ELSE IF(ICALC.EQ.14)THEN
C
   F TO K
   TEMP=(TEMP-32.00D0)/1.8D0+273.15D0
ELSE IF(ICALC.EQ.21)THEN
C

C R TO F
  TEMP = TEMP - 459.6700
  ELSE IF (ICALC.EQ.23) THEN
    R TO C
    TEMP = TEMP / 1.8000 - 273.1500
    ELSE IF (ICALC.EQ.31) THEN
      C TO F
      TEMP = 1.8000 * TEMP + 32.00
      ELSE IF (ICALC.EQ.32) THEN
        C TO R
        TEMP = 1.8000 * TEMP + 32.00 + 459.6700
        ELSE IF (ICALC.EQ.34) THEN
          C TO K
          TEMP = TEMP + 273.1500
          ELSE IF (ICALC.EQ.41) THEN
            K TO F
            TEMP = 1.8000 * TEMP - 459.6700
            ELSE IF (ICALC.EQ.42) THEN
              K TO R
              TEMP = 1.8000 * TEMP
              ELSE IF (ICALC.EQ.43) THEN
                K TO C
                TEMP = TEMP - 273.1500
                ELSE
                  ERROR MESSAGE
                  CALL MSGS(21)
                  WRITE(NHSTRY,900)
                  WRITE(NHSTRY,1000)
                  IERR = -1
                ENDIF
  ENDIF
C TEMPO = TEMP
C C FORMATS
C 500 FORMAT(1X,'IN MODULE TCON')
C 1000 FORMAT(1X,'INVALID VALUE OF ICALC OF ',110,
            11X,'NO TEMP CONVERSION & CALC. CONTINUES')
C RETURN
C END
C SUBROUTINE VF5H(THR,SG,JC,IERR)
C C C NAME OF MODULE - VF5H
C C MODIFIED - 12-26-88
C C VARIABLES USED -
C C VARIABLE I/O TYPE SPEC DIMENSION DESCRIPTION AND RANGE
C C THR  I  R  -  BOILING POINT (DEG K)
C C SG  I  R  -  SPECIFIC GRAVITY (60/60)
C C JC  I  I  -  COMPONENT NUMBER ARRAY
C C IERR  O  I  -  ERROR CODE ID
C C 0 = OK
C C -1 = REDUCED TEMP > 0.99
C C -2 = REDUCED TEMP < 0.2
C C 1 = THR OUT OF RANGE
C C 2 = SG OUT OF RANGE
IMPLICIT REAL*8 (A-H,O-Z)
IMPLICIT INTEGER(I-N)

PARAMETER (MNC=25)

COMMON /IO / MIN,NOUT,NHSTRY,NREPT
COMMON /REF5 / TREF,PREF,RGAS

COMMON /CPP01/ TC(MNC)
COMMON /CPP05/ OMEGA(MNC)
COMMON /CPP22/ VLCVTJ(MNC)

IERR=0

CHECK LIMITS OF TBR AND SG

IF(TBR.LT.569.67D0.OR.TBR.GT.1309.67) THEN
  CALL MESS(1)
  WRITE(NHSTRY,900)
  WRITE(NHSTRY,1000) TBR
  IERR=1
ENDIF

IF(SG.LT.0.6247D0.OR.SG.GT.1.0244D0) THEN
  CALL MESS(1)
  WRITE(NHSTRY,900)
  WRITE(NHSTRY,2000) SG
  IERR=2
ENDIF

LIQUID MOLAR VOLUME AT 70 DEG C AND 1 ATM (CM^3/G-MOLE)

V=7.6211D-5 * TBR^-4 * (2.1262D0 + SG^-3 * (1.8688D0)

LIQUID MOLAR VOLUME AT 20 DEG C AND 1 ATM (M^3/KG-MOLE)

VR=V/1.061100

TR=293.15D0/TC(JC)
OMEGA=OMEGA(JC)
TDF=TDF/TC(JC)
ICALC=0

CORRECT TO 25 C BY RACKETT FOR GUNYAM

CALL GUNYAM(VR,TR,OMEGA,TDF,ICALC,VR,IERR)

IF(IERR.LT.0) THEN
  CALL MESS(1)
  WRITE(NHSTRY,900)
  WRITE(NHSTRY,3000) TBR
ENDIF

VLCVTJ(JC)=VR/(5.7881D0*TREF/TC(JC))

FORMATS

900 FORMAT(*X,'IN MODULE VCFH')
1000 FORMAT(*X,'TBR (DEG K) VALUE IS NOT IN RANGE 569.67-1309.67',/)
1     FORMAT(*X,'TBR VALUE = ',G12.6,' CALC. CONTINUES')
2000 FORMAT(*X,'SG VALUE IS NOT IN RANGE 0.6247-1.0244',/)
1     FORMAT(*X,'SG VALUE = ',G12.6,' CALC. CONTINUES')
3000 FORMAT(*X,'IN CALL TO GUNYAM IERR RETURNED = ',I5,' CALC CONT.')

RETURN
END
SUBROUTINE WATHOV(JC, IERR)

NAME OF MODULE - WATHOV
MODULE TITLE - WATSON HEAT OF VAPORIZATION
PURPOSE - EST OF WATSON HEAT OF VAPORIZATION PARAMETERS
MODIFIED - 12-20-88
METHOD - WATSON HEAT OF VAPORIZATION EQUATION
REF: REID, R.C. ET AL., "THE PROPERTIES OF GASES AND LIQUIDS"
    McGRAW-HILL, NY, 1977

VARIABLES USED-
VARIABLE I/O TYPE-SPEC DIMENSION        DESCRIPTION AND RANGE
   JC    I    I        COMPONENT ARRAY ID
   IERR  D    I        ERROR CODE
                   0 = OK
                   1 = TB(R) NOT IN OPT. RANGE
                   2 = SG NOT IN OPT. RANGE

IMPLICIT REAL*8 (A-H,O-Z)
IMPLICIT INTEGER (I-N)

PARAMETER (MNC=25)
COMMON /IO/, MIN, NOUT, NHSTRY, NHRT
COMMON /DEBUG/, LDEBUG, LDEBUG
COMMON /NSP03/, UDEF(MNC), API(MNC), SG(MNC), AMW(MNC)
COMMON /SP03/, DHVLWT(5, MNC)
COMMON /SP04/, TH(MNC)
IERR=0
IF (LDEBUG.GT.7) WRITE(NHSTRY, 900)
HEAT OF VAP (BTU/LB-MOLE) AT TB AND SG FOR COMPOUND
CALL TCON(TB(JC), T1, 42, IERR)
SJ=SG(JC)
IF (T1.LT.569.67D0 .OR. T1.GT.1309.67) THEN
    CALL MESS(1)
    WRITE(NHSTRY, 900)
    WRITE(NHSTRY, 2006) T1
    IERR=1
ENDIF
IF (SJ.LT.0.6247D0 .OR. SJ.GT.1.024D0) THEN
    CALL MESS(1)
    WRITE(NHSTRY, 900)
    WRITE(NHSTRY, 2000) SJ
    IERR=2
ENDIF
HVAP1=3.40585D0 + T1 * (1.3471D0 + SJ**4.0214D0)
HEAT OF VAP (J/KMOL)
HVAP1=HVAP1/9.486D-4/0.453592D0
DHVLWT(1, JC)=HVAP1
DHVLWT(2, JC)=TB(JC)
DHVLWT(3, JC)=0.38D0
FORMATS

900 FORMAT(1X,'IN MODULE WATHOV')
1000 FORMAT(1X,'TB DEG R1 VALUE IS NOT IN RANGE 569.67-1309.67',/)
      1X,'TB-VALUE = ', G12.6,  'CALC. CONTINUES')

RETURN
END

SUBROUTINE ZCAL(TC, PC, VC, ZC, IERR)

NAME OF MODULE - ZCAL
MODULE TITLE - CALC CRITICAL COMPRESS. FACTOR
PURPOSE - TO CALC CRITICAL COMPRES. FACTOR
MODIFIED - 10-3-88

LIMITATIONS:
ZC
0.26-0.28

VARIABLES USED-

INPLICIT REAL*8 (A-H,O-Z)
INPLICIT INTEGER(I-N)

PARAMETER (NMC=25)

COMMON /ID / NIH,NOUT,NSHTY,NREF
COMMON /IDRUG / LDRUG,LDRUGR
COMMON /REFS / TREF,PREF,RGAS

IERR=0
IF(LDRUG.GT.0)WRITE(NSHTY,900)

CRITICAL COMPRES. FACTOR

ZC=(PC*VC)/(TC*RGAS)

IF(ZC.LT.0.26D0 .OR. ZC.GT.0.28D0)THEN
   CALL MESS(1)
   WRITE(NSHTY,900)
   WRITE(NSHTY,1000)ZC
ENDIF

FORMATS

900 FORMAT(1X,'IN MODULE ZCAL')
1000 FORMAT(1X,'ZC VALUE IS NOT IN OPTIMAL RANGE 0.26-0.28',/)
      1X,'ZC-VALUE = ', G12.6,  'CALC. CONTINUES')
C     RETURN
C END
C*******************************************************************************
C SUBROUTINE SECOND(USED)
C*******************************************************************************
C NAME OF MODULE - SECOND
C MODULAR TITLE - CALC ELAPSED CPU TIME
C PURPOSE - CALC 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   M - CPU TIME USED
C
C INTEGER TIMESTATS,ELAPSED
C LOGICAL STATUS,LIB$INIT_TIMER,LIB$STAT_TIMER
C COMMON /TIMEDATA/ TIMESTATS
C
C DATA ISWT/1/
C
C SAVE TIMEDATA
C IF(I$W.T.EQ.1)CALL TIME_INIT
C ISWT=2
C STATUS=LIB$STAT_TIMER(2,ELAPSED,TIMESTATS)
C USED=FLOAT(ELAPSED)/100.0
C
C RETURN
C END
C*******************************************************************************
C SUBROUTINE TIME_INIT
C*******************************************************************************
C
C NAME OF MODULE - TIME_INIT
C MODULAR TITLE - INITIALIZE TIME ROUTINE
C PURPOSE - TO INITIALIZE COUNTERS FOR FUTURE REFERENCE
C (VAX DEPENDENT)
C MODIFIED - 3-23-89
C
C INTEGER TIMESTATS
C LOGICAL STATUS,LIB$INIT_TIMER,LIB$STAT_TIMER
C COMMON /TIMEDATA/ TIMESTATS
C
C SAVE TIMEDATA
C TIMESTATS=0
C STATUS=LIB$INIT_TIMER(TIMESTATS)
C
C RETURN
C END
C*******************************************************************************
C BEGIN ASPEN USER SUBROUTINE YSO LE
**NOTICE**

THIS CODE IS PART OF THE VAX SYSTEM DEVELOPED AT
MORGANTOWN ENERGY TECHNOLOGY CENTER, MORGANTOWN, WEST VIRGINIA

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CAMBRIDGE, MA

SUBROUTINE VSOLVE (K, N, NDATA, DATA, X, XMAX, XMIN, Y, Z, PJ,
OUTPUT, P, A, AC)

**TITLE**
- NONLINEAR ESTIMATION AND EQUATION SOLVING

**THE PURPOSE OF THIS SUBPROGRAM IS TO SOLVE SYSTEMS OF NONLINEAR
EQUATIONS.**

A - SCRATCH MATRIX OF LENGTH K*(K + 2)
AC - SCRATCH MATRIX OF LENGTH K*(K + 2)
DATA - ARRAY USED TO STORE VARIABLES USED IN SUBROUTINE
DATA(1) - FMU, FACTOR USED TO CHANGE FLA. SET INTERNALLY TO 10.0 IF ZERO ON INITIAL CALL.
DATA(2) - FLA, FACTOR USED TO COMBINE GRADIENT AND
NEWTON-RAPHSON METHODS. SET INTERNALLY TO
.51 IF ZERO ON INITIAL CALL.
DATA(3) - TAU, USED IN CONVERGENCE TEST. SET INTERNALLY TO
0.001 IF ZERO ON INITIAL CALL.
DATA(4) - EPS, USED IN CONVERGENCE TEST. SET INTERNALLY TO
0.0003 IF ZERO ON INITIAL CALL.
DATA(5) - PHMIN, WHEN PH .LT. PHMIN, PARTIAL DERIVATIVES FROM THE PREVIOUS ITERATION ARE USED
INSTEAD OF COMPUTING THEM AGAIN.
DATA(6) THRU DATA(16) - VARIABLES USED INTERNALLY
K - NUMBER OF INDEPENDENT VARIABLES, Unknowns
N - NUMBER OF EQUATIONS TO BE SOLVED
NDATA - ARRAY USED TO STORE INTEGER VARIABLES USED IN SUBROUTI
NDATA(1) = IC, MUST BE SET EQUAL TO ONE ON INITIAL
ENTRY TO VSOLVE. USED TO CONTROL SEQUEN
OF OPERATION.
NDATA(2) = MFACTOR, USED FOR CONTROL IN CALLING PROG
IF = 0, CALCULATE FUNCTION
IF = 1, CALCULATE DERIVATIVE
IF = -1, EXAMINE TERR FOR WHAT TO DO NEXT
NDATA(3) = TERR, MAY TAKE ON VARIOUS VALUES
IF POSITIVE, CONTAINS THE NUMBER OF VARIABLES NO
SATISFYING CONVERGENCE CRITERION
IF = 0, CONVERGENCE SATISFIED AND SOLUTION REACHED
IF = -1, NO IMPROVEMENT POSSIBLE IN THE VALUE OF
PH EVEN THOUGH CONVERGENCE HAS NOT BEEN
REACHED.
IF = -2, MORE UNKNOWNS THAN FUNCTIONS AND UNIQUE
SOLUTION GENERALLY IS IMPOSSIBLE.
IF = -3, TOTAL NUMBER OF VARIABLES TO BE VARIED
IS ZERO
IF = -4, CONVERGENCE CRITERION MET BUT FLA STILL
LARGE
IF = -5, IC NOT A VALID NUMBER ON ENTRY
IF = -6, XI(I) IS NOT WITHIN XMIN(I) TO XMAX(I)
NDATA(4) = J, INDEX TO INDICATE WHICH PARTIAL DERIV
ATIVE IS TO BE EVALUATED.
NDATA(5) THRU NDATA(6) = NOT USED
NDATA(7) THRU NDATA(26) - INTEGER VARIABLES USED INTERNALLY

OUTPUT - VECTOR OF OUTPUT VALUES
  OUTPUT(1) - PH, VALUE OF THE SUM OF THE SQUARES OF Y(I) - Z(I) AS I=1,N.
  OUTPUT(2) - GAMM, ANGLE IN DEGREES BETWEEN THE STEP ACTUALLY TAKEN AND THE STEEpest DESCENT DIRECTION.
  OUTPUT(3) - XITER, ITERATION COUNTER FOR YSOLVE.
  OUTPUT(4) - XFCNT, ITERATION COUNTER TO COUNT NUMBER OF TIMES THE FUNCTION WAS EVALUATED.
  OUTPUT(5) - XDER, ITERATION COUNTER TO COUNT NUMBER OF TIMES THE DERIVATIVE WAS EVALUATED.

OUTPUT(6) - VALUE OF PLA FOR CURRENT BASE POINT
P - VECTOR OF LENGTH K*(N+2)+K USED TO STORE PARTIAL DERIVATIVES AND AS A SCRATCH AREA.
PJ - VECTOR OF PARTIAL DERIVATIVES OF LENGTH N. THIS IS ONE ROW OF THE P VECTOR CORRESPONDING WITH X(J).
X - VECTOR OF LENGTH 2*K CONTAINING THE K BASE POINTS AND THE K UNKNOWNS
XMAX - VECTOR OF LENGTH K CONTAINING UPPER BOUNDS OF X
XMIN - VECTOR OF LENGTH K CONTAINING LOWER BOUNDS OF X
XV - VECTOR OF LENGTH K INDICATING WHICH OF THE X VARIABLES ARE TO BE VARIED
  IF XV(I) = 0., HOLD X(I) CONSTANT
  IF XV(I) = 1., ALLOW X(I) TO VARY AND USE NUMERICAL DERIVATIVES.
  IF XV(I) =-1., ALLOW X(I) TO VARY AND USE ANALYTIC DERIVATIVES CALCULATED BY USER
Y - VECTOR OF LENGTH K CONTAINING DESIRED FUNCTION VALUES
Z - VECTOR OF LENGTH 2*N CONTAINING COMPUTED FUNCTION VALUE AND BASE POINT FUNCTION VALUES

IMPLICIT REAL*8 (A - H, O - Z)
DIMENSION NDATA(26), DATA(16), X(1), XV(1), XMAX(1), XMIN(1),
  Y(1), Z(1), PJ(1), OUTPUT(6), P(1), PJ(1), XV(1), Z(1)

SET INTEGER VARIABLES USED IN SUBROUTINE EQUAL TO NDATA ARRAY

IC = NDATA(1)
NFCNTOR = NDATA(2)
IERR = NDATA(3)
J = NDATA(4)
KP1 = NDATA(7)
KP2 = NDATA(8)
KBI = NDATA(9)
KBI2 = NDATA(10)
KZ1 = NDATA(11)
J1 = NDATA(12)
J2 = NDATA(13)
J3 = NDATA(14)
J4 = NDATA(15)
J6 = 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)

SET VARIABLES USED IN SUBROUTINE EQUAL TO DATA ARRAY
FNU  = DATA(6)
TAU  = DATA(7)
EPS  = DATA(8)
PHMIN = DATA(9)
GN   = DATA(10)
FL   = DATA(11)
DM   = DATA(12)
DG   = DATA(13)
COSG = DATA(14)
PHI  = DATA(15)
DEN  = DATA(16)

C SET OUTPUT VARIABLES EQUAL TO OUTPUT ARRAY

PH   = OUTPUT(1)
GAHM = 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  = 1.0D+02
C6  = 1.0D-10
C7  = 9.0D+01
C8  = 9.5D+01
C9  = 1.0D+08
PI   = 3.14159265D0

C IF (IC .GT. 6 .AND. IC .LT. 6) GO TO 800
IF (IC .GT. 6 .AND. IC .LT. 6) GO TO 800
IERR = -5

GO TO 805
B60 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 NFDTH = -7
B805 GO TO 995

2 GO TO (10, 20, 30, 40, 13), IC
10 KPI = K + 1
KBI1 = K*N
KBI2 = KBI1 + K
KZI = KBI2 + K

C STORE INITIAL BASE POINT VALUES

DO 82 KK = 1, K
KKS = KK + K
82 X(KKS) = 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 ZERO ON ENTRY, SUBPROGRAM DEFINES THEN

IF (FNU .LE. 0.00) FNU = 1.0D0
IF (FLA .LE. 0.00) FLA = 0.1D0
IF (TAU .LE. 0.00) TAU = 0.01D0
IF (EPS .LE. 0D0) EPS = .00002D0
IF (PHMIN .LE. 0D0) PHMIN = 0D0
PH = 0D0
GAMM = 0D0
XITR = 0D0
XFCT = 1D0
XDER = 0D0

C
TEST TO SEE IF TOTAL NUMBER OF VARIABLES
TO BE VARIED IS ZERO
C
KE = 0
DO 11 KE = 1, K
IF (XV(KE) .NE. 0D0) KE = KE + 1
11 CONTINUE
IF (KE .GT. 0D0) GO TO 12
IEHR = -3
IC = -1
NFCTR = -1
GO TO 999
C
TEST TO SEE IF THERE ARE MORE UNKNOWNS
PRESENT THAN FUNCTIONS, THUS MAKING A
UNIQUE SOLUTION GENERALLY IMPOSSIBLE
C
12 IF (H .GE. KE) GO TO 13
IEHR = -2
IC = -1
NFCTR = -1
GO TO 999
13 J1 = 1
61 IF (XITR .GT. 0D0) GO TO 17
DO 14 J1 = 1, K
J2 = KB1 + J1
P(J2) = X(J1)
J3 = KB2 + J1
14 P(J3) = DABS(X(J3)) + C
GO TO 40
15 IF (PHMIN .GT. PH AND. IC .GT. 1) GO TO 34
J1 = 0
16 J1 = J1 + 1
NJ = (J1 - 1) + 1
IF (XV(J1)) 17, 35, 22
C
CALCULATE ANALYTICAL DERIVATIVES IN CALLING
PROGRAM
17 NFCTR = 1
J = J1
IC = 2
GO TO 999
C
RETURN FROM CALCULATING DERIVATIVE
C
20 DO 21 KK = 1, H
KEK = N + KK
21 P(KKE) = P(JKE)
XDER = XDER + 1D0
GO TO 35
C
CALCULATE NUMERICAL DERIVATIVES
22 DO 23 J2 = 1, K
J3 = KB1 + J2
LL = K + J2
23 P(J3) = X(LLL)
J3 = KB1 + J1
J4 = KB2 + J1
DEN = C2*DABS(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
56 NFCTR = 0
C
CALCULATE VALUE OF FUNCTION
DO 24 LL = 1, K
     LLL = KB11 + LL
24    X(LLL) = 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(MMM)
     XFCT = XFCT + ID0

DO 32 J2 = 1, N
     JB = J2 + M1
     JS = J2 + N
32    P(JB) = P(JB) - Z(JS)/DEN
35 IF (.EQ. K) GO TO 34
     GD TO 16

C SET UP CORRECTION EQUATIONS

34 DO 38 J1 = 1, K
     N1 = (J1 - 1)*N
     A(J1, KP1) = 0.
38 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) = 0.0
     N2 = (J2 - 1)*N
     N3 = N1 + J3
     N4 = N2 + J3
36    A(J1, J2) = A(J1, J2) + P(N3)*P(N4)

37 DO 37 J2 = 1, KP1
     A(J1, J2) = 0.0
     A(J1, J3) = 1.0
37 CONTINUE

C SCALE CORRECTION EQUATIONS

DO 39 J1 = 1, K
39    A(J1, KP2) = NSORT*(A(J1, J1));

DO 27 J1 = 1, K
     A(J1, KP1) = A(J1, KP1)/A(J1, KP2)
27    A(J1, J2) = A(J1, J2)/(A(J1, KP2)*A(J2, KP2))

FL = FLA/FLH

GO TO 3

62 DO 5 FL = FLH*FL
3    DO 4 J2 = 1, KP1
4    AC(J1, J2) = A(J1, J2)
5    AC(J1, J1) = AC(J1, J1) + FL.

C SOLVE CORRECTION EQUATIONS

DO 9 L1 = 1, K
8 IF (.EQ. 0.0) GO TO 80
     L2 = L1 + 1
9 DO 6 L3 = 1, L1
8    AC(L1, L3) = AC(L1, L3)/AC(L1, L1)
6    L3 = L2, KP1
6 DO 7 L4 = L2, KP1
7    L1 = L3, L4
7 DO 8 AC(L1, L4) = AC(L3, L4) - AC(L1, L4)*AC(L3, L1)
8 CONTINUE
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(J11), DMIN1(XMAX(J11), X(LL) + AC(J1, 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 SES MODIFICATION 2/85 TO AVOID DIV BY ZERO

VALUE=SQRT(DN*GN)
IF (VALUE.LE.0.D0) VALUE=VMIN
COSG=DG/VALUE

IF (COSG) 18, 19, 19
18 JGAM = 0
COSG = -COSG
19 JGAM = 1
COSG = DMIN1(COSG, C1)

C SES MODIFICATION 2/86 DANCOS TO DACOS

GAMM = DANCOS(COSG)*C5/PI
GAMM = DACOS(COSG)*C5/PI
IF (JGAM .GT. 0) GAMM = C5 - GAMM

DO 48 NFCTDR = 0
40 DO 42 HM = 1, N
HM = KBI1 + HM
42 XMHM = X(HM)
XFCT = XFCT + ID0
PHI = 0.
43 DO 44 J1 = 1, N
J2 = KBI1 + J1
J3 = PHI + IF(J2) - Y(J11)**2
44 IF (PHI .LT. C6) GO TO 50
45 IF (XMHM .GT. 0D0) GO TO 44
IERR = K
IC = 5
NFCTDR = -1
GO TO 56
46 IF (PHI .GE. PH) GO TO 47

C EPSILON TEST

IERR = 0
45 DO 49 J1 = 1, K
J2 = K + J1
49 IF (DABS(AC(J1, KP2))/TAN + DABS(X(J2))) .GT. EPS1 IERR=IERR + 1
45 CONTINUE

IF (IERR .EQ. 0) GO TO 46

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
IC = -1
NFCTDR = -1
GO TO 92

C
GAMMA EPSILON TEST

IF (FL .GT. C4 .AND. GAMM .LE. C81) IERR = -4
   IC = -1
   NFCTDR = -1
   GO TO 92

IF (11 - 2) .EQ. 49, 49, 50
   11 = 11 + 1
   GO TO (61, 15, 62), 11

IF (1FL .LT. C91) GO TO 62
   IERR = -1
   IC = -1
   NFCTDR = -1
   GO TO 92

IF (1ERR = 0
   IC = -1
   NFCTDR = -1
   GO TO 92

FLA = FL

DO 93 J2 = 1, K
   J3 = KB11 + J2
   LL = K + J2
   X(LL) = P(J3)
93   X(J2) = P(J3)

DO 94 J2 = 1, N
   J3 = KZ1 + J2
   LL = N + J2
   Z(LL) = P(J3)
94   Z(J2) = P(J3)

FU = PI

XITR = XITR + 100

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(5) = KPI
NDATA(6) = KP2
NDATA(7) = KB11
NDATA(8) = KB12
NDATA(9) = KZ1
NDATA(10) = J1
NDATA(11) = J2
NDATA(12) = J3
NDATA(13) = J4
NDATA(14) = J5
NDATA(15) = J6
NDATA(16) = J7
NDATA(17) = J8
NDATA(18) = J9
NDATA(19) = J10
NDATA(20) = J11
NDATA(21) = J12
NDATA(22) = J13
NDATA(23) = J14
NDATA(24) = J15
NDATA(25) = J16
NDATA(26) = JGAM

C
SET DATA ARRAY EQUAL TO VARIABLES FOR
C
RETURN TO CALLING PROGRAM

DATA(6) = FMU
DATA(7) = TAU
DATA(8) = EPS
DATA(9) = PMIN
DATA(IO) = GN
DATA(11) = FL
DATA(12) = DM
DATA(13) = DG
DATA(14) = COSG
DATA(15) = PHI
DATA(16) = DEN

C
C
SET OUTPUT ARRAY EQUAL TO OUTPUT VARIABLES
FOR RETURN TO CALLING PROGRAM

OUTPUT(1) = PH
OUTPUT(2) = GAMM
OUTPUT(3) = XITR
OUTPUT(4) = XFCT
OUTPUT(5) = XDEN
OUTPUT(6) = FLA

RETURN
END
APPENDIX C

ESTPRO/PROCESS™ Peng Robinson simulation summary
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. Doehne
DESC FOR SY50F4 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= 6
  REP-DBUG=8
  ASPENTOUT=INPUT
  REP-FILE= MASTEST
  PROP-OPT= SYSOP4
;
END-INPUT
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. ROCHÉ
10 DESC FOR SYSOF3 FENG ROBINSON
11 DESC
12;
13 T-UNITS= F
14 P-UNITS= PSI A
15;
16 PROP-DATA
17 COMPF-LIST HP225
18 CVAL VABF= 225.7
19 CVAL STBF= 0.0
20 COMPF-LIST HP275
21 CVAL VABF= 275.4
22 CVAL STBF= 0.0
23 CVAL API= 55.32
24 COMPF-LIST HP324
25 CVAL VABF= 324.9
26 CVAL STBF= 0.0
27 CVAL API= 50.12
28 COMPF-LIST HP375
29 CVAL VABF= 374.9
30 CVAL STBF= 0.0
31 CVAL API= 46.07
32 COMPF-LIST HP424
33 CVAL VABF= 424.9
34 CVAL STBF= 0.0
35 CVAL API= 42.40
36 COMPF-LIST HP475
37 CVAL VABF= 475.0
38 CVAL STBF= 0.0
39 CVAL API= 39.44
40 COMPF-LIST HP525
41 CVAL VABF= 525.1
42 CVAL STBF= 0.0
43 CVAL API= 36.66
44 COMPF-LIST HP575
45 CVAL VABF= 575.1
46 CVAL STBF= 0.0
47 CVAL API= 34.13
48;
49 PRINT-OPT
50 PRINT-OPT
51 PRINT-OPT
52 CAL-DBUG= 0
53 REP-DBUG= 8
COMPONENT ESTIMATION SUMMARY

*WARNING*
IN MODULE NEED
PERCENT PARAFFINS, NAPHTHENES, AND AROMATICS ARE ALL 0.0 VALUES WILL BE ESTIMATED.

*WARNING*
IN MODULE NEED
PERCENT PARAFFINS, NAPHTHENES, AND AROMATICS ARE ALL 0.0 VALUES WILL BE ESTIMATED.

*WARNING*
IN MODULE NEED
PERCENT PARAFFINS, NAPHTHENES, AND AROMATICS ARE ALL 0.0 VALUES WILL BE ESTIMATED.

*WARNING*
IN MODULE NEED
PERCENT PARAFFINS, NAPHTHENES, AND AROMATICS ARE ALL 0.0 VALUES WILL BE ESTIMATED.

*WARNING*
IN MODULE NEED
PERCENT PARAFFINS, NAPHTHENES, AND AROMATICS ARE ALL 0.0 VALUES WILL BE ESTIMATED.

*WARNING*
IN MODULE NEED
PERCENT PARAFFINS, NAPHTHENES, AND AROMATICS ARE ALL 0.0 VALUES WILL BE ESTIMATED.

*WARNING*
IN MODULE ESTFA
TH(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 = 13.2560

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 ZCCAL
ZC VALUE IS NOT IN OPTIMAL RANGE 0.26-0.28
ZC-VALUE = 0.226389      CALC. CONTINUES

WARNING
IN MODULE DIFIRM
TB(K) VALUE OF  515.261
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 = 0.220389      CALC. CONTINUES

WARNING
IN MODULE DIFIRM
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 = 0.221564      CALC. CONTINUES

WARNING
IN MODULE DIFIRM
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

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Figure C.1
ESTPRO report output file

; TITLE TEST RUN OF PROGRAM COMPEST
; MASTERS OF SCIENCE
; N. J. 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 SYOSIPI PENG ROBINSON
;
;
; SUMMARY FOR COMPONENT BP225
; VOLUME AVERAGE BOILING POINT (DEG K) = 380.761
; AVERAGE MOL. WEIGHT = 115.358
; SLOPE OF THE TBP CURVE = 0.0000000E+00
; CYCIC AVERAGE BOILING POINT (DEG K) = 380.761
; MOAL AVERAGE BOILING POINT (DEG K) = 380.761
; MEAN AVERAGE BOILING POINT (DEG K) = 380.761
; UOF (WATSON) K CHAM. FACTOR = 11.9652
; API GRAVITY = 60.5300
; SG GRAVITY (60/60 F) = 0.716864
; PERCENT AROMATICS = 8.84911
; PERCENT NAPHTHENES = 35.1108
; PERCENT PARAFLNS = 56.0400
; SYOSIP SELECTED = 4.00000
;
; PROP-DATA
; COMM-LIST BP225
; CVAL MW 1 1 115.3961836
; CVAL TC 1 1 563.8331613
; CVAL FC 1 1 293297.331
; CVAL VC 1 1 0.426801854
; CVAL ZC 1 1 0.2632750562
; CVAL CHEGA 1 1 0.00041405428
;
; REGRESSION SUMMARY
; ITERATION = 1230.0000
; NUMBER OF PARMS UNFIT = 0.
; SUM OF SQUARES = 0.390461807E-03
;
; CVAL FLMHRT 1 1 -0.035381523 /2 -3010.526307 /3
; 3 -53.96148665 /4 0.06000000000E+00 /5
; 5 0.0000000000E+00 /6 0.06000000000E+00 /7
; 7 0.0000000000E+00 /8 185.2860000 /9
; 9 265.7800000
;
; REGRESSION SUMMARY
; ITERATION = 21.000000
; NUMBER OF PARMS UNFIT = 0.
; SUM OF SQUARES = 6.22482929E-15
;
; CVAL CPG 1 1 -14960.63646 /2 6436.4331858 /3
; 3 -0.2415604396 /4 0.00000000000E+00 /5
; 5 0.00000000000E+00 /6 0.00000000000E+00 /7
; 7 255.3722222 /8 922.0388889 /9
; 9 21346.32947 /10 432.5373873 /11
; 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 0.1616069320
CVAL DHVLMT 1 1 32361763.75 /2 380.7611111 /4 0.0000000000E+00 /
CVAL 3 1 0.3800000000E+00
CVAL 5 1 0.0000000000E+00

REGRESSION SUMMARY
ITERATION = 5.0000000
NUMBER OF PRRMS UNFIT: = 0.
SUM OF SQUARES = 0.12979604E-04
CVAL RKZRA 1 1 0.2645291347
CVAL MUP 1 1 0.0000000000E+00

REGRESSION SUMMARY
ITERATION = 17.0000000
NUMBER OF PRRMS UNFIT: = 0.
SUM OF SQUARES = 0.12078411E-02
CVAL MULAND 1 1 102.4839674 /2 -7038.655840 /
3 -18.98690027 /4 428.5142028 /
5 552.5564981

SUMMARY FOR COMPONENT RP275
VOLUME AVERAGE BOILING POINT (DEG K) = 408.372
AVERAGE MOLE WEIGHT = 126.704
SLOPE OF THE TBP CURVE = 0.00000000E+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
UGP (WATSON) K CHAR. FACTOR = 14.9154
API GRAVITY = 55.3200
SG GRAVITY 160/60 F1 = 0.757414
PERCENT AROMATICS = 15.3000
PERCENT NAPHTHENES = 31.5340
PERCENT PARAFFINS = 50.0959
SYRUP SELECTED = 1.00000

PROP-DATA
COMP-LIST RP275
CVAL RN 1 1 128 2016122
CVAL RC 1 1 593.3872478
CVAL PC 1 1 2655001.461
CVAL VC 1 1 0.4747005866
CVAL ZC 1 1 0.2558277720
CVAL OMEGA 1 1 0.3392175151

REGRESSION SUMMARY
ITERATION = 119.30000
NUMBER OF PRRMS UNFIT: = 0.
SUM OF SQUARES = 0.00000000E+00
CVAL PLXANT 1 1 26.85607706 /2 -3259.021719 /
3 -50.09760168 /4 0.0000000008E+00 /
5 0.0000000000E+00/6 0.0000000000E+00 /
7 0.0000000000E+00/8 235.1060000 /
9 315.4000000

REGRESSION SUMMARY
ITERATION = 42.000000
NUMBER OF PRRMS UNFIT: = 0.
SUM OF SQUARES = 0.20290766E-15
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| CVAL DFORM | 1 1 | -172921695.8 |
| CVAL DGFORM | 1 1 | 47066750.39 |
| CVAL TB | 1 1 | 108.3722222 |
| CVAL VB | 1 1 | 0.18137656161 |
| CVAL DHVINT | 1 1 | 250.79719.90 /2 | 408.3722222 / |
|       |      | 3   | 0.3800000000 /4 | 0.0000000000E+00 / |
|       |      | 5   | 0.0000000000E+00 |

**REGRESSION SUMMARY**

| ITERATION | 7.0000000 |
| NUMBER OF PARNHS UNFIT | 0. |
| SUM OF SQUARES | 0.31044333E-04 |
| CVAL RKTZA | L 1 | 0.259318198 |
| CVAL MUP | L 1 | 0.0000000000E+00 |

**REGRESSION SUMMARY**

| ITERATION | 17.000000 |
| NUMBER OF PARNHS UNFIT | 0. |
| SUM OF SQUARES | 0.14154293E-02 |
| CVAL MULAND | L 1 | 110.5423513 /2 | -781.3264935 / |
|       |      | 3   | -19.91686762 /4 | 456.9743084 / |
|       |      | 5   | 581.5195029 |

**SUMMARY FOR COMPONENT BP324**

| VOLUME AVERAGE BOILING POINT (DEG K) | 435.872 |
| AVERAGE MOLE WEIGHT | 141.983 |
| SLOPE OF THE TBP CURVE | 0.00000000E+00 |
| CUBIC AVERAGE BOILING POINT (DEG K) | 435.872 |
| MOHAL AVERAGE BOILING POINT (DEG K) | 435.872 |
| HEAN AVERAGE BOILING POINT (DEG K) | 435.872 |
| UOF (WATSON) K CHAR. FACTOR | 11.0302 |
| API GRAVITY | 50.1200 |
| SG GRAVITY (60/60 F) | 0.779095 |
| PERCENT AROMATICS | 19.2952 |
| PERCENT HAPTHEMS | 33.2572 |
| PERCENT PARAFINS | 47.4476 |
| STSOF SELECTED | 4.00000 |

**PROP-DATA**

| COM-P-Lists BP324 |
| CVAL MW | l 1 | 141.9841370 |
| CVAL TC | l 1 | 622.0773567 |
| CVAL FC | l 1 | 1411898.559 |
| CVAL VC | l 1 | 0.5287254199 |
| CVAL ZC | l 1 | 0.241910966 |
| CVAL OMEGA | l 1 | 0.3804518343 |

**REGRESSION SUMMARY**

| ITERATION | 1548.0000 |
| NUMBER OF PARNHS UNFIT | 0. |
| SUM OF SQUARES | 0.37979416E-03 |

| CVAL PLXANT | L 1 | 20.97926728 /2 | -3513.104077 / |
|       |      | 3   | -6.275131879 /4 | 0.0000000000E+00 / |
|       |      | 5   | 0.0000000000E+00 /6 | 0.0000000000E+00 / |
|       |      | 7   | 0.0000000000E+00 /8 | 283.9000000 / |
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REGRESSION SUMMARY
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NUMBER OF PARMS UNFIT = 0.
SUM OF SQUARES = 0.7232330E-04

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REGRESSION SUMMARY
ITERATION = 37.000000
NUMBER OF PARMS UNFIT = 0.
SUM OF SQUARES = 0.16447130E-02

| CVAL | HULAND | 1 | 1 | 118.1029182 | /2 | -8618.951396 |
|------|--------|---|---|---------------|----|-------------|---|
|      |        | 3 |   | -20.82260320 | /4 | 473.3663526 | / |
|      |        | 5 |   | 610.3198115 | /10 | 513.2783800 | / |

REGRESSION SUMMARY
ITERATION = 1718.000000

SUMMARY FOR COMPONENT RP374
VOLUME AVERAGE BOILING POINT (DEG K) = 463.650
AVERAGE MOLD 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 = 11.0159
API GRAVITY = 46.0700
SG GRAVITY (60/60 F) = 0.7968669
PERCENT AROMATIC = 19.8892
PERCENT PARAFFINES = 33.3386
PERCENT NAPHTHA = 46.7722
SYNOPSIS SELECTED = 4.000000

PROP-DATA

| CVAL | MW | 1 | 1 | 157.5668619 |
|------|----|---|---|-------------|---|
| CVAL | TC | 1 | 1 | 651.1993778 |
| CVAL | PC | 1 | 1 | 2230426.910 |
| CVAL | VC | 1 | 1 | 0.5807697862 |
| CVAL | ZC | 1 | 1 | 0.2429568871 |
| CVAL | OMEGA | 1 | 1 | 0.4725734931 |

REGRESSION SUMMARY
ITERATION = 1718.000000
NUMBER OF PARMS UNFIT: = 0.
SUM OF SQUARES = 0.37564425E-03

CVALL PLXANT 1 1 21.10823177 /2 -3771.961827 /
3 -69.75129394 /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 = 0.42315661E-15

CVALL CPNG 1 1 -15456.45179 /2 872.17652083 /
3 -0.3319530380 /4 0.0000000000E+00 /
5 0.0000000000E+00/6 0.0000000000E+00 /
7 255.37222222 /8 922.0388289 /
9 3490.328338 /10 589.4516824 /
11 1.000000000

CVALL DFORMATION 1 1 -202697802.5
CVALL DERFORMATION 1 1 69516418.21
CVALL TB 1 1 463.6500000
CVALL VB 1 1 0.2303106469
CVALL DHALVMT 1 1 0.053199124 /2 463.6500000 /
3 0.3800000000E+00 /4 0.0000000000E+00 /
5 0.0000000000E+00

REGRESSION SUMMARY
ITERATION = 7.000000
NUMBER OF PARMS UNFIT: = 0.
SUM OF SQUARES = 0.13140176E-03

CVALL RENTZA 1 1 0.2499284050
CVALL NHF 1 1 0.0000000000E+00

REGRESSION SUMMARY
ITERATION = 37.000000
NUMBER OF PARMS UNFIT: = 0.
SUM OF SQUARES = 0.19329111E-02

CVALL MULAND 1 1 126.3882029 /2 -9497.811860 /
3 -21.82710698 /4 491.9116031 /
5 638.1754883

SUMMARY FOR COMPONENT BP424
VOLUME AVERAGE BOILING POINT (DEG K) = 491.428
AVERAGE MOL. WEIGHT = 174.749
SLOPE OF THE TBP CURVE = 0.0000000000E+00
CRITICAL 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 = 11.7074
API GRAVITY = 12.0000
SG GRAVITY (60/60 F) = 0.813686
PERCENT AROMATICS = 18.4543
PERCENT NAPHTHENS = 34.8047
PERCENT PARAFFINS = 46.7410
SYTOP SELECTED = 4.000000

PROP-DATA
COMP-LIST BP424
CVALL NW 1 1 174.7488357
CVALL TC 1 1 678.9631101
CVAL PC 1 1 2036124.655
CVAL VC 1 1 0.6510320188
CVAL ZC 1 1 0.23711125566
CVAL OMEGA 1 1 0.4741677501

REGRESSION SUMMARY
ITERATION = 1883.0000
NUMBER OF P ARMS UNFIT: = 0.
SUM OF SQUARES = 0.37239392E-03

CVAL PLXANT 1 1 21.23202054 2 -0.4010.305846
3 -75.62535664 4 0.00000000E+00
5 0.00000000E+00/6 0.00000000E+00
7 0.00000000E+00/8 364.9080000
9 -64.9080000

REGRESSION SUMMARY
ITERATION = 105.0000
NUMBER OF P ARMS UNFIT: = 0.
SUM OF SQUARES = 0.53198802E-15

CVAL CPTG 1 1 -11877.00033 2 960.0819410
3 -0.36697610 4 0.00000000E+00
5 0.00000000E+00/6 0.00000000E+00
7 0.00000000E+00/8 922.0388869
9 4665.17478 /10 648.0765964
11 1.00000000

CVAL HFORM 1 1 -215891179.6
CVAL DHFORM 1 1 63612010.62
CVAL TH 1 1 491.4277778
CVAL VH 1 1 0.2570688772
CVAL DHVLT 1 1 43319325.43 2 391.4277778
3 0.38000000E+00/4 0.00000000E+00
5 0.00000000E+00/60

REGRESSION SUMMARY
ITERATION = 7.000000
NUMBER OF P ARMS UNFIT: = 0.
SUM OF SQUARES = 0.21097444E-03

CVAL HTERA 1 1 0.235619566
CVAL HV 1 1 0.00000000E+00

REGRESSION SUMMARY
ITERATION = 37.000000
NUMBER OF P ARMS UNFIT: = 0.
SUM OF SQUARES = 0.22710492E-02

CVAL HULAND 1 1 134.91552861 2 -10430.36200
3 -22.6651436 /4 516.6115617
5 665.1818179

SUMMARY FOR COMPONENT #475
VOLUME AVERAGE BoILING POINT (DEG K) = 519.261
AVERAGE MOLWEIGHT = 194.945
SLOPE OF THE TBP CURVE = 0.000000E+00
CURVATURE 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 = 1.000000

PROP-DATA
COMP-LIST BP475
CVAL MW 1 1 194.0446714
CVAL TC 1 1 705.6792434
CVAL PC 1 1 18718.43631
CVAL VC 1 1 0.725985772
CVAL ZC 1 1 0.2315416125
CVAL OMEGA 1 1 0.5263636183

REGRESSION SUMMARY
ITERATION = 2053.0000
NUMBER OF PAMS UNFIT = 3.
SUM OF SQUARES = 0.370255441E+93

CVAL PLXANT 1 1 21.37752015 /2 -4305.991140 /4
3 -82.17116104 /4 0.0000000000E+00 /8
5 0.0000000000E+00 /8 0.0000000000E+00 /10
7 0.0000000000E+00 /8 0.0000000000E+00 /10
9 515.0000000

REGRESSION SUMMARY
ITERATION = 126.0000
NUMBER OF PAMS UNFIT = 0.
SUM OF SQUARES = 0.620612741E-15

CVAL CPTG 1 1 -13511.21343 /2 1055.066721 /4
3 -82.17116104 /4 0.0000000000E+00 /8
5 0.0000000000E+00 /8 0.0000000000E+00 /10
7 255.32722722 /8 922.0388889 /10
9 4764.1714949 /10 711.744498 /10
11 1.00000000

CVAL DHEFOM 1 1 -21521396.19
CVAL DCEFORM 1 1 1014.166308
CVAL TH 1 1 519.261111
CVAL V 1 1 0.2870122619
CVAL DHEVLWT 1 1 46131274.18 /2 519.261111 /4
3 0.0000000000E+00 /4 0.0000000000E+00 /8
5 0.0000000000E+00

REGRESSION SUMMARY
ITERATION = 7.000000
NUMBER OF PAMS UNFIT = 0.
SUM OF SQUARES = 0.308493037E-03

CVAL RKTZRA 1 1 0.2405432282
CVAL HUP 1 1 0.0000000000E+00

REGRESSION SUMMARY
ITERATION = 17.000000
NUMBER OF PAMS UNFIT = 0.
SUM OF SQUARES = 0.268684152E-02

CVAL MULAND 1 1 111.1112313 /2 -11137.15550 /4
3 -23.90895036 /4 536.3162250 /8
5 691.5656568

SUMMARY FOR COMPONENT BP525
VOLUME AVERAGE BOILING POINT (DEG K) = 547.094
AVERAGE MOLE WEIGHT = 215.384
SLOPE OF THE TBP CURVE = 0.00000000E+00
CUBIC AVERAGE BOILING POINT (DEG K) = 547.094
MALAL AVERAGE BOILING POINT (DEG K) = 547.094
MEAN AVERAGE BOILING POINT (DEG K) = 517.800
UGF (WATSON) K CHAR. FACTOR = 11.8235
API GRAVITY = 36.6600
SG GRAVITY (60/60 F) = 0.841461
PERCENT AROMATICS = 25.4703
PERCENT NAPHTHENES = 31.3743
PERCENT PARAFLNS = 43.1553
SYSOP SELECTED = 4.00000

PROF-DATA

COMP-LIST HRP525
CVAL RH  1 1  215.35369375
CVAL TC  1 1  732.0027722
CVAL PC  1 1  1726030.936
CVAL VC  1 1  0.7062679251
CVAL NC  1 1  0.22638092295
CVAL OMEGA 1 1  0.5602694600

REGRESSION SUMMARY
ITERATION = 2233 0000
NUMBER OF PARAMS UNFIT = 0.
SUM OF SQUARES = 0.368445078-03

CVAL PHTXANT 1 3 21.51843597 /2 -1517.992317
3 -85.043316046 /4 0.0000000000E+00
5 0.0000000000E+00 /6 0.0000000000E+00
7 0.0000000000E+00 /8 0.0000000000E+00
9 563.1000000

REGRESSION SUMMARY
ITERATION = 147.00000
NUMBER OF PARAMS UNFIT = 0.
SUM OF SQUARES = 0.71281249E-15

CVAL FTG 1 1 -11.60351835 /2 1153.508125
3 -0.116521270 /4 0.0000000000E+00
5 0.0000000000E+00 /6 0.0000000000E+00
7 255.3122222 /8 522.0388889
9 777.6476633 /10 554.11371
11 1.000000000

REGRESSION SUMMARY
ITERATION = 2 000000
NUMBER OF PARAMS UNFIT = 0.
SUM OF SQUARES = 0.418108589-03

CVAL HENTX 1 1 0.23775773
CVAL HOP 1 1 0.00000000E+00

REGRESSION SUMMARY
ITERATION = 37.00000
NUMBER OF PARAMS UNFIT = 0.
SUM OF SQUARES = 0.317412589-02

CVAL NULAND 1 1 153.6305521 /2 -12501.64628
3 -25.14670836 /4 556.3221070
5 717.3627168
**SUMMARY FOR COMPONENT BP575**

- **Volume Average Boiling Point (deg K)**: 574.872
- **Average Mole Weight**: 238.929
- **Slope of the TDL 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**: 33.1300
- **SG Gravity (60/60 F)**: 0.854114
- **Percent Aromatics**: 33.1600
- **Percent Paraffins**: 25.8704
- **Percent Naphthenes**: 40.6696
- **Sysop Selected**: 4.00000

**PROP-DATA**

**COMP-LIST BP575**

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**REGRESSION SUMMARY**

- **Iteration**: 2348.0000
- **Number of Parms Unfit**: 0
- **Sum of Squares**: 0.36696847E-03

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**REGRESSION SUMMARY**

- **Iteration**: 168.0000
- **Number of Parms Unfit**: 0
- **Sum of Squares**: 0.86049719E-15

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| CVAL | DHFORM | 1  | -154323072.6 |
|      | DGFOM | 1  | 124469506.9 |
|      | TH    | 1  | 574.6722222 |
|      | V7    | 1  | 0.3528850529 |

**REGRESSION SUMMARY**

- **Iteration**: 7.000000
- **Number of Parms Unfit**: 0
- **Sum of Squares**: 0.531000048E-03

| CVAL | RKTSA | 1  | 0.2342367825 |
|      | RUP   | 1  | 0.000000000E+00 |

**REGRESSION SUMMARY**
; ITERATION = 37.000000
; NUMBER OF PARMS UNFIT = 0.
; SUM OF SQUARES = 0.37192264E-02

; CUAL NULAND 1 1 165.1955236 /2 -13638.07707 /
  3  26.35087233 /4  575.9057879 /
  5 742.6153581
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) = A1
: OLDID = MSIC
: NEVID = MSIC
: DELETE FILES (EXCEPT .LOG, .HIS, .REP, .INF - G BUILDS PLD; Y/N/G) = Y
: VERSION (REFERS TO TEST/I OR PRODUCTION/P) = T
: BUILD A NEW INPUT TRANSLATOR (Y/N) = N
: PDF LENGTH (300 MAX) = 790
: TABLE (PATHNAME OF USER SDF) = NULL
: QUEUE (A, AASPLN ) = 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 = USRFPLA ARG = FOR021
: KEY = USRFPLB ARG = FOR022
: KEY = USRFPLL ARG = FOR023
: KEY = USRFPLC ARG = FOR024
: KEY = USRFPLC ARG = FOR025
: KEY = USRCOST ARG = FOR026
:
: END VAX/VMS PROCS
;
:
: TITLE 'ASPLN RUN OF ASP1C.IMP'
:
: DESCRIPTION &
: 'ALLIED CORPORATION
ASPLN SIMULATION OF ASPIC.IMP
PENG-ROBINSON:SYSOP4 (50/50)
S. E. SUND RUN=1C DATE 3/89'
:
: IN-UNITS ENG
: OUT-UNITS ENG
:
: MXID : Maximum number of INTEGER OVERFLOWS
: MXDO : Maximum number of FLOATING POINT OVERFLOWS
: MXDI : Maximum number of FLOATING POINT UNDERFLOWS
: MXID : Maximum number of INTEGER DIVIDES BY ZERO
: MXDD : Maximum number of FLOATING POINT DIVIDES BY ZERO
: MXON : Maximum number of FLOATING POINT OVERFLOWS IN MATH LIBRARY
: MXUN : Maximum number of FLOATING POINT UNDERFLOWS IN MATH LIBRARY
: MXEL : Maximum number of SIGNIFICANCE LOST IN MATH LIBRARY ERRORS
: MXLZ : Maximum number of LOGZERNEG ERRORS IN MATH LIBRARY
: MXEN : Maximum number of SQR doomed ERRORS IN MATH LIBRARY
: MXUE : Maximum number of UNDEFINED EXPONENTIATION ERRORS
:
: RUN-CONTROL MAX-TIME=54000. MAX-ERRORS=5000 &
HISTORY MSG-LEVEL PROPERTIES=2 SIMULATION=4
: PROPERTY-REPORT ALL
STREAM-REPORT
STANDARD OPTIONS=ALL
SUPPLEMENTAL 1 OPTIONS=MASS-FLOW
:
SIM-OPTIO NS MHB-RESULTS=2 SIZE-RESULTS=0
:
:------------------------------------------
:
PHYSICAL PROPERTY DATA
:
:------------------------------------------
:
COMPONENTS
BP225
BP275
BP324
BP374
BP424
BP475
BP525
BP575

TITLE
TEST RUN OF PROGRAM COMPEST
MUNI. J. I. T. CHEMICAL ENGINEERING DEPARTMENT
STEVEN E. SUND
FOR PARTIAL FULFILLMENT OF A
MUNI. OF SCIENCE IN CHE ENG.
FAUN 1988 SPRING 1989
ADVISOR DR. E. C. ROCHER
FOR SYSGI PENG ROBINSON
:
SUMMARY FOR COMPONENT BP225
VOLUME AVERAGE BOILING POINT (DEG K) = 380.761
AVERAGE MOL WT = 115.398
SLOPE OF THE TAU CURVE = 0.0060069E+00
CUBIC AVERAGE BOILING POINT (DEG K) = 380.761
HEAT 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 = 5.84911
PERCENT NAPHTHENES = 35.1108
PERCENT PARAFLNS = 56.0406
SYSGI SELECTED = 4.00890
:
PROPI-DATA
COMPLIT BP225
CVAL MW 1 1 115.3981836
CVAL TC 1 1 563.8331613
CVAL FC 1 1 2932997.331
CVAL VC 1 1 0.4208001854
CVAL ZC 1 1 0.2932750582
CVAL OMEGA 1 1 0.2971405438
:
REGRESSION SUMMARY
: ITERATION = 1230.0000
: NUMBER OF PARMS UNFIT: = 0
: SUM OF SQUARES = 0.39046387E-03


CVAL PLANT 1 1 20.73581523 /2 3010.526307 /3
3 -51.9048885 /4 0.0000000000E+00 /5
5 0.0000000000E+00 /6 185.7000000 /7
6 0.0000000000E+00 /8
REGRESSION SUMMARY
ITERATION = 21.000000
NUMBER OF PAPMS UNFIT = 0.
SUM OF SQUARES = 0.22382929E-15
CVAL CPU 1 1 -14960.62616 /2 6364331858 /3
3 -0.2415601390 /4 0.0000000000E+00 /5
5 0.0000000000E+00 /6 922.0388389 /7
7 21346.32947 /8 132.5373873 /9
9 1.000000000
REGRESSION SUMMARY
ITERATION = 5.000000
NUMBER OF PAPMS UNFIT = 0.
SUM OF SQUARES = 0.12979606E-04
CVAL ERTZA 1 1 0.2455251387
CVAL MVP 1 1 0.0000000000E+00
REGRESSION SUMMARY
ITERATION = 37.000000
NUMBER OF PAPMS UNFIT = 0.
SUM OF SQUARES = 0.12078111E-02
CVAL MULAND 1 1 102.8439674 /2 7038.655849 /3
3 -18.96690027 /4 428.5131262 /5
5 552.5554988
SUMMARY FOR COMPONENT HP27
VOLUME AVERAGE BOILING POINT (DEG K) = 408.372
AVERAGE MOLE WEIGHT = 120.204
SLOPE OF THE TBP CURVE = 0.00000000E+00
CURIC AVERAGE BOILING POINT (DEG K) = 408.372
MOLAL AVERAGE BOILING POINT (DEG K) = 408.372
MEAN AVERAGE BOILING POINT (DEG K) = 408.372
DGP (MATSON) K CHAR. FACTOR = 11.9151
API GRAVITY = 55.3200
SG GRAVITY (60/60 F) = 0.737414
PERCENT AROMATICS = 15.3600
PERCENT NAPTHENES = 31.5310
PERCENT PARAFLNS = 50.0859
SYSOP SELECTED = 4.00000
PROP-DATA
COMP-LIST BP27
CVAL WM 1 1 128.2036122
CVAL WC 1 1 593.3872478
CVAL PC 1 1 2659001.461
CVAL VC 1 1 0.4747008666
CVAL EC  1  1  0.2558727720
CVAL OMEGA  1  1  0.3392753513

REGRESSION SUMMARY
ITERATION  = 1392.0000
NUMBER OF PARMS UNFIT  = 0.
SUM OF SQUARES  = 0.3543110E-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  235.40000000 /
9   315.40000000

REGRESSION SUMMARY
ITERATION  = 42.000000
NUMBER OF PARMS UNFIT  = 0.
SUM OF SQUARES  = 0.202096E-15

CVAL CPIC  1  1  -15259.99359  /2  712.2214812 /
3   -0.2711031070  /3  0.0000000000E+00 /
5   0.0000000000E+00  /6  0.0000000000E+00 /
7   255.3722222  /8  922.0388888 /
9   255.1715000  /10  493.1080850 /
11  1.00000000

CVAL DHCPN  1  1  -13291169.8
CVAL DHCPH  1  1  470.62720.33
CVAL T4  1  1  408.3722222
CVAL VN  1  1  0.103376.9161
CVAL DHUWT  1  1  350.7011.90  /2  108.3722222 /
3   0.3860000000  /4  0.0000000000E+00 /
5   0.0000000000E+00

REGRESSION SUMMARY
ITERATION  = 7.000000
NUMBER OF PARMS UNFIT  = 0.
SUM OF SQUARES  = 0.3104355E-04

CVAL HARRHA  1  1  0.2553318988
CVAL HOP  1  1  0.000000000E+00

REGRESSION SUMMARY
ITERATION  = 17.000000
NUMBER OF PARMS UNFIT  = 0.
SUM OF SQUARES  = 0.141524E-02

CVAL HULAND  1  1  110.5123513  /2  -7813.261935 /
3   -19.91886742  /4  456.9743084 /
5   584.5196029

SUMMARY FOR COMPONENT 8324
VOLUME AVERAGE BOILING POINT (DEG F) = 435.872
AVERAGE MOL weight  = 131.584
SLOPE OF THE T/P CURVE  = 0.000000000
COMPO 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  = 11.6382
AIT GRAVITY  = 50.1200
SG GRAVITY [160/60 F]  = 0.779099
PERCENT AROMATICS  = 19.2952
PERCENT NAPHTHES  = 31.2572
PERCENT PARAFFINS  = 47.4176
SYSOP SELECTED  = 4.00000
PROP-DATA

COMP-LIST BP324

CVAL MW 1 1 111.9041320
CVAL TC 1 1 622.8773587
CVAL PC 1 1 24418.08559
CVAL VC 1 1 0.5287254199
CVAL ZC 1 1 0.2492940938
CVAL OMEGA 1 1 0.3904918363

REGRESSION SUMMARY
ITERATION = 1510.0000
NUMBER OF PARMS UNFIT = 0
SUM OF SQUARES = 0.37979416E-03

CVAL PLXANT 1 1 20.97026728 /2 3513.104077 /2
3 -6.27551879 /4 0.0000000000E+00
5 0.0000000000E+00 /6 0.0000000000E+00 /6
7 0.0000000000E+00 /8 284.9000000
9 364.9000000

REGRESSION SUMMARY
ITERATION = 63.000000
NUMBER OF PARMS UNFIT = 0
SUM OF SQUARES = 0.31543831E-15

CVAL CPTG 1 1 -15735.34137 /2 787.9762754 /2
3 -0.3017495065 /4 0.0000000000E+00 /4
5 0.0000000000E+00 /6 0.0000000000E+00 /6
7 255.1722222 /8 922.0388889
9 296.2903519 /10 533.2783800
11 1.000000000

CVAL DFORM 1 1 -1861.725071
CVAL DFFORM 1 1 50331118.91
CVAL TH 1 1 436.8722222
CVAL VB 1 1 0.2652125324
CVAL DHGLNT 1 1 3797128.46 /6 435.8722222 /6
3 0.3800000000 /6 0.0000000000E+00 /6
5 0.0600000000E+00

REGRESSION SUMMARY
ITERATION = 7.000000
NUMBER OF PARMS UNFIT = 0
SUM OF SQUARES = 0.72323879E-04

CVAL HETETA 1 1 0.2515433310
CVAL HUF 1 1 0.0000000000E+00

REGRESSION SUMMARY
ITERATION = 37.000000
NUMBER OF PARMS UNFIT = 0
SUM OF SQUARES = 0.16447130E-02

CVAL HULAND 1 1 110.1029102 /2 -610.9533396
3 -20.82264320 /4 473.3867926
5 610.4198115

SUMMARY FOR COMPONENT BP324
VOLUME AVERAGE BOILING POINT (DEG K) = 463.650
AVERAGE MOLE WEIGHT = 157.567
SLOPE OF THE TPD CURVE = 0.000000E+00
CUBIC AVERAGE BOILING POINT (DEG K) = 463.650
MOHAL AVERAGE BOILING POINT (DEG K) = 463.650
MEAN AVERAGE BOILING POINT (DEG K) = 463.650
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SUMMARY FOR COMPONENT BI424

VOLUME AVERAGE BOILING POINT (DEG K) = 491.428
AVERAGE MOLE WEIGHT = 174.749
SLOPE OF THE TBP CURVE = 0.0000000E+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) R CHAR. FACTOR = 11.7974
API GRAVITY = 42.4000
SG GRAVITY (160/60 F) = 0.813686
PERCENT AROMATICS = 18.4543
PERCENT NAPHTHENES = 34.8047
PERCENT PARAFFINS = 46.7410
$YSOP\ SELECTED = 1.000000

PROP-DATA

COMP-LIST BI424

CVAL MW 1 1 174.7492457
CVAL TC 1 1 678.90431101
CVAL PC 1 1 2046.325455
CVAL VC 1 1 0.041023678
CVAL EC 1 1 0.233132566
CVAL OMEGA 1 1 0.1744671501

REGRESSION SUMMARY

ITERATION = 1083.0000
NUMBER OF PARMS UNFIT = 0.
SUM OF SQUARES = 0.37239392E-03

CVAL PLXANT 1 1 23.32202054 / 4 0.0000000000E+00
3 -35.62503664 0.0000000000E+00
5 0.0000000000E+00 0.0000000000E+00
7 0.0000000000E+00 104.9000000
9 464.9000000

REGRESSION SUMMARY

ITERATION = 1083.0000
NUMBER OF PARMS UNFIT = 0.
SUM OF SQUARES = 0.51398002E-15

CVAL CPG 1 1 -1.87760000 / 2 960.0819410
3 -0.1964763064 0.0000000000E+00
5 0.0000000000E+00 0.0000000000E+00
7 255.3722222 922.0380869
9 1059.37178010 848.0705904
11 2.06000000

CVAL DHFORM 1 1 -215691379.6
CVAL DGFORM 1 1 83612056.42
CVAL TB 1 1 351.1277776
CVAL VH 1 1 0.257068872
CVAL RHVINT 1 1 133108275.13 / 2 961.4277778
3 0.3806000000 / 4 0.0000000000E+00
5 0.0000000000E+00

REGRESSION SUMMARY

ITERATION = 9.0000000
NUMBER OF PARMS UNFIT = 0.
SUM OF SQUARES = 0.21607444E-03

CVAL RKTZA 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
UDP (WATSON) K CHAR. FACTOR = 11.8115
API GRAVITY = 39.4400
SG GRAVITY (60/60 F) = 0.827776
PERCENT AROMATICS = 10.4490
PERCENT NAPHTHENES = 35.5597
PERCENT PARAFLNS = 45.9912
SYNAP SELECTED = 4.00000

PROP-DATA

COMP-LIST BP475

CVAL MW 1 1 194.0446714
CVAL TC 1 1 205.0792314
CVAL PC 1 1 1874283.634
CVAL VC 1 1 0.7243595772
CVAL ZC 1 1 0.2315101225
CVAL OMEGA 1 1 0.52/4e+36183

REGRESSION SUMMARY

ITERATION = 2853.0000
NUMBER OF PARMS UNFIT: = 0.
SUM OF SQUARES = 0.30849307E-03

CVAL PXANT 1 1 21.37752016 /2 -4395.994140 /3 -83.21176104 /4 0.0000000000E+00 /5 0.0000000000E+00 /6 0.0000000000E+00 /7 0.0000000000E+00 /8 0.0000000000E+00 /9 0.0000000000

REGRESSION SUMMARY

ITERATION = 126.0000
SUM OF SQUARES = 0.52661271E-15

CVAL CPIG 1 1 -13511.21313 /2 1055.09×321 /3 -0.4007784155 /4 0.0000000000E+06 /5 0.0000000000E+06 /6 0.0000000000E+06 /7 0.0000000000E+06 /8 0.0000000000E+06 /9 0.0000000000E+06 /10 0.0000000000E+06

CVAL DIMFORM 1 1 -2152.3761.0
CVAL DGFORM 1 1 103716630.8
CVAL TR 1 1 519.2111111
CVAL VB 1 1 0.2620122×19
CVAL DFAIL 1 1 451311247.18 /2 519.2611111 /3 0.3880000000 /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 RTHRA 1 1 0.2415432282
CVAL MUP 1 1 0.0000000000E+00

REGRESSION SUMMARY
ITERATION = 31.000000
NUMBER OF PARS UNFIT = 0.
SUM OF SQUARES = 0.2666666666E-02

CVAL MULAND 1 1 144.14422313 /2 -11437.15050 /
3 -23.98095836 /4 536.3152250 /
5 691.5656586

SUMMARY FOR COMPONENT BP525
VOLUME AVERAGE BOILING POINT (DEG K) = 547.0
AVERAGE MOLAR WEIGHT = 215.8
SLOPE OF THE TEP CURVE = 0.0000000000E+00
CUBIC AVERAGE BOILING POINT (DEG K) = 547.0
HOMO AVERAGE BOILING POINT (DEG K) = 547.0
MEAN AVERAGE BOILING POINT (DEG K) = 517.8

PROP DATA
CVAL NH 1 1 215.3536473
CVAL TC 1 1 712.00027723
CVAL PC 1 1 1726024.936
CVAL WC 1 1 0.7982679251
CVAL ZC 1 1 0.3260392255
CVAL OMEGA 1 1 0.5807696660

REGRESSION SUMMARY
ITERATION = 2223.0000
NUMBER OF PARS UNFIT = 0.
SUM OF SQUARES = 0.368445076-03

CVAL FLEXANT 1 1 215.31843597 /2 -4577.493817 /
3 -85.03146066 /4 0.0000000000E+00/
5 0.0000000000E+00 /6 0.0000000000E+00 /
7 0.0000000000E+00 /8 925.100000 /
9 565.100000

REGRESSION SUMMARY
ITERATION = 140.0000
NUMBER OF PARS UNFIT = 0.
SUM OF SQUARES = 0.742812493E-15

CVAL CG 1 1 -110563.51615 /3 -1153.508129 /
3 -0.0430912707 /4 0.0000000000E+00 /
5 0.0000000000E+00 /6 0.0000000000E+00 /
7 255.37472272 /8 922.0388889 /
9 55141.14646 /10 777.6476633 /
11 1.0000000000

CVAL DHEF 1 1 -18651718.7
CVAL DGF 1 1 113525607.2
CVAL TG 1 1 547.0944444
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CVAL DHEF 1 1 4896419.83 /2 547.0944444 /
3 0.3800000000 /4 0.0000000000E+00
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| CVAL KETRA | 1 | 0.2377557794 |
| CVAL MUP | 1 | 0.0000000000E+00 |

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| CVAL MULAND | 1 | 153.63059211 /2 | -125.0426428 /3 |
| CVAL 3 | 3 | -25.13270850 /4 | 556.3222070 /5 |
| CVAL 4 | 5 | 717.3427149 |

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| CVAL PIRAT | 1 | 21.65416311 /2 | -853.946714 |
| CVAL 3 | 3 | -94.15447758 /4 | 0.0000000000E+00 /4 |
| CVAL 5 | 5 | 0.0000000000E+00 /6 | 0.0000000000E+00 /6 |
| CVAL 7 | 7 | 0.0000000000E+00 /6 | 535.1600000 /6 |
| CVAL 9 | 9 | 815.1000000 |

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| CVAL CPF | 1 | -9620.64864 /2 | 1255.871869 |
| CVAL 3 | 3 | -0.9853028171 /4 | 0.0000000000E+00 /4 |
| CVAL 5 | 5 | 0.0000000000E+00 /6 | 0.0000000000E+00 /6 |
| CVAL 7 | 7 | 255.3722222 /8 | 922.038888 |
| CVAL 9 | 9 | 63339.31856 /10 | 846.2385199 |
| CVAL 11 | 11 | 1.0000000000 |
CVAL DHFORM 1 1 -154323072.6
CVAL DGFORM 1 1 125169908.9
CVAL TB 1 1 574.9722222
CVAL VB 1 1 0.3528859529
CVAL DHVLMT 1 1 51811255.89 /2 574.8722222 /3 0.3800000000 /4 0.0000000000E+00 /5 0.0000000000E+00

REGRESSION SUMMARY
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NUMBER OF TERMS UNIT: = 0.
SUM OF SQUARES = 0.53100048E-03

CVAL HRTZRA 1 1 0.2742167825
CVAL HUP 1 1 0.006060600000E+00

REGRESSION SUMMARY
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NUMBER OF TERMS UNIT: = 0.
SUM OF SQUARES = 0.37192264E-02

CVAL HULARD 1 1 161.9558236 /2 -13618.07707 /3 26.350872133 /4 575.9657870 /5 742.6153581

DEF-STREAMS HEAT H01
PROPERTIES SYSDP GLOBAL
PROP-SOURCES
GLOBAL ASPENPCD COMPS=ALL

BLOCK INPUT

FLOWSHEET
BLOCK FIA1 IN=501 OUT=502 503 H01

FEED STREAMS & RECycles

FEED STREAMS
STREAM 501 TEMP=100 PRES=14.656
FLOW FIA2 22.6 / FIA2 23.5 /
FIA3 22.4 / FIA3 20.0 /
FIA4 17.4 / FIA4 15.8 /
FIA5 14.7 / FIA5 13.0 /
50.56 VAP. LIQ. SPLIT

BLOCK FIA1 FLUSH
PARAM PRES=-1 V=0.5
Figure C.5

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

SO2 (Vapor)

Separator

Temp = Calculated
Press = 13.696 psia

SO1 (Feed)
Temp = 400°F
Press = 14.696 psia

SO3 (Liquid)
Figure C.6
ASPEN report summary for 50/50 split simulation using SYSOP4
ASPDEN(VER D) ALLIED SIGNAL CORP - SCIENTIFIC COMPUTATION
 DATE: 3/14/89 PAGE I

ASPDEN RUN OF ASPIC.INP
DESCRIPTION

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

RUN CONTROL INFORMATION

TYPE OF RUN: NEW

INPUT FILE NAME: ASPIC

INPUT PROBLEM DATA FILE NAME: MSIC UPDATE NO. 0

MAIN CALLING PROGRAM NAME: MSIC

CPU TIME USED DURING SIMULATION STEP: 1.54 SECONDS
SIMULATION REQUESTED FOR ENTIRE FLOWSHEET
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<td>FLOWSHEET CONNECTIVITY BY STREAMS 1</td>
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<td>FLOWSHEET CONNECTIVITY BY BLOCKS 1</td>
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<td>COMPUTATIONAL SEQUENCE 1</td>
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<td>OVERALL FLOWSHEET BALANCE 1</td>
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<td>PHYSICAL PROPERTIES SECTION 2</td>
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<td>COMPONENTS 2</td>
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<td>OPTION SETS 2</td>
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<td>MAJOR AND SUBORDINATE PROPERTY ROUTES 3</td>
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<td>PARAMETER SOURCES 7</td>
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<td>UNIT OPERATIONS BLOCK SECTION 13</td>
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ASPINALLD SIGNAL CORP - SCIENTIFIC COMPUTATION DATE: 3/14/89 PAGE 1
ASPIN RUN OF ASPiC.INP
FLOWSHEET SECTION

FLOWSHEET CONNECTIVITY BY STREAMS

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FLOWSHEET CONNECTIVITY BY BLOCKS

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COMPUTATIONAL SEQUENCE

SEQUENCE USED WAS:

FLA1

OVERALL FLOWSHEET BALANCE

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*** MASS AND ENERGY BALANCE ***
**COMPONENTS**

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**OPTION SETS**

KEY TO OPTION SET TABLES:

- OPTION SET ID
- MP KEYWORD
- MP ROUTE ID
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### MAJOR AND SUBORDINATE PROPERTY ROUTES

**KEY TO ROUTE TABLES:**

**ROUTE 15**  KEYWORD  METHOD CODE  MP  EP  
**ASSOCIATED MODELS:**  NAME  PROPERTY  DATA SET  OPTION CODES  
**ASSOCIATED MAJOR  SUBORDINATE PROPERTIES:**  KEYWORD  ROUTE 16

| PHILMX00 | PHILMX 2 | MP |
MAJOR AND SUBORDINATE PROPERTY ROUTES (CONTINUED)

ASSOC. MP'S: PHIL PHIX00

HVMMX00 HVMX 3 MP

HMNX00 HLMX 3 MP
ASSOC. SP'S: DHLNX DHLNX00

GLMX00 GVMX 3 MP
ASSOC. SP'S: DGVMX DGVMX00

SMX00 SVMX 2 MP
ASSOC. SP'S: DSVMX DSVMX00

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

VVMX00 VVMX 1 MP
ASSOC. MODELS: VV21G VVNX 1

VLNX01 VLMX 1 MP
ASSOC. MODELS: VL2KNT VLMX 1

MVVMX01 MVVMX 1 MP
ASSOC. MODELS: MVV2BOK MVVMX 1

MULNX01 MULMX 1 MP
ASSOC. MODELS: MULX2AN MULNX 1

KVMX01 KVMX 1 MP
ASSOC. MODELS: KVJWNS KVMX 1

KLNX01 KLNX 1 MP
ASSOC. MODELS: KLMXVW KLMX 1

DLVNX01 DLVNX 1 MP
ASSOC. MODELS: DLVCEWL DLVNX 1

SLGMX01 SLGMX 1 MP
ASSOC. MODELS: SLMXVSW SLGMX 1

PHIVX00 PHIV 1 MP
ASSOC. MODELS: PHIVUSH PHIV 1

PHILX00 PHIL 2 MP
ASSOC. MODELS: PLOXANT PLX 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:  VV01G VV 1

VL01  VL 1 MP
ASSOC. MODELS:  VL01G VL 1

HUV01 HUV 1 MP
ASSOC. MODELS:  HUV0HUGK HUV 1

HUL01 HUL 1 MP
ASSOC. MODELS:  HUL0HUGK HUL 1

K01  KU 1 MP
ASSOC. MODELS:  KV0STLTH KV 1

KL01  KL 1 MP
ASSOC. MODELS:  KL0U9KL KL 1

SIGL01 SIGL 1 MP
ASSOC. MODELS:  SIG0KSS SIGL 1

PHISMX02 PHISMX 2 MP
ASSOC. MODELS:  PHIS0LS PHISMX 1
ASSOC. MP'S:  PH15 PH1502

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

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

SSMX01 SSMX 1 MP
ASSOC. MP'S:  SSMX SSMX02 / GSMX GSMX02

VSX02 VSX 2 MP
ASSOC. MODELS:  VS01G VSX 1
ASSOC. MP'S:  VS VS01
MAJOR AND SUBORDINATE PROPERTY ROUTES (CONTINUED)

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

PHIS02  PHIS 2 MP
ASSOC. MODELS:  P90ANT PS 1

HS02  HS 1 MP
ASSOC. MODELS:  HSOPOLI HS 1

GS02  GS 1 MP
ASSOC. MODELS:  GSOPOLI GS 1

SS02  SS 1 MP
ASSOC. MODELS:  SSOPOLI SS 1

VS01  VS 1 MP
ASSOC. MODELS:  VSOPOLY VS 1

KS01  KS 1 MP
ASSOC. MODELS:  KSOPOLY 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

MUVHX02  MUVHX 1 MP
ASSOC. MODELS:  MUV2DNST MUVHX 1
MAJOR AND SUBORDINATE PROPERTY ROUTES (CONTINUED)

MULLMX02 MULLMX 1 MP
ASSOC. MODELS: MULZLEST MULLMX 1

KVMX02 KVMX 1 MP
ASSOC. MODELS: KV2STLTH KVMX 1

DVMX02 DVMX 1 MP
ASSOC. MODELS: DVIDMIX DSMX 1

DILMX00 DILMX 2 SP
ASSOC. SP’S: DIL DILMX00

DGVMX00 DGVMX 1 SP
ASSOC. MODELS: ESI E0S 1

DGLMX00 DGLMX 2 SP
ASSOC. SP’S: DGL DGLMX00

DSVMX00 DSVMX 1 SP
ASSOC. MODELS: EDIC E0S 1

DSLMX00 DSLMX 2 SP
ASSOC. SP’S: DILMX DSLMX00 / DGLMX DGLMX00

DHL00 DHL 3 SP
ASSOC. MODELS: DHLVLTVSN DHLV 1

DGVMX00 DGVMX 2 SP

DGL00 DGL 2 SP
ASSOC. SP’S: PHI PHI00

DHVMX01 DHVMX 1 SP
ASSOC. MODELS: ESI E0S 1

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PARAMETER SOURCES

GLOBAL
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### STREAMLIED SIGNAL CORP - SCIENTIFIC COMPUTATION DATE: 3/14/89 PAGE 10

**ASPN RUN OF ASPIC.INP**

**PHYSICAL PROPERTIES SECTION**

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PROPERTY OPTION SET SYSOP4

*** MASS AND ENERGY BALANCE ***

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TOTAL BALANCE

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*** INPUT DATA ***

| PRESSURE DROP (PSIA) | 1.0000 |
| VAPOR FRACTION      | 0.5000 |
| MAXIMUM ITERATION NO. | 36 |
| CONVERGENCE TOLERANCE | 0.10000E-03 |
| LIQUID ENTRAINMENT  | 0.60000E+00 |

SOLID SPLIT FRACTIONS:
- MIXED SUBSTREAM, NO SOLID SPLITS.

*** RESULTS ***

| OUTPUT TEMPERATURE (F) | 375.19 |
| OUTPUT PRESSURE (PSIA) | 11.696 |
| HEAT DUTY (BTU/HR)     | -0.67318E+06 |
| VAPOR FRACTION         | 0.50000 |

V-L PHASE EQUILIBRIUM:

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<th>Y(I)</th>
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STREAM CLASS : HEAT
STREAM ATTN : HEAT

DESCRIPTION OF STREAM CLASS CONVEN

STREAM CLASS : CONVEN
SUBSTREAMS : MIXED
SUBSTRM CLASS: MIXED
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**ASPN(VER D)ALLIED SIGNAL CORP - SCIENTIFIC COMPUTATION DATE: 3/14/89 PAGE 16**

**STREAM ID**

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**VFRAC**

| 1.0000 |
| 0.0000 |
| 0.6314 |

**LFRAC**

| 0.0000 |
| 1.0000 |
| 0.3685 |

**ENTROPY**

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**AVG MW**

| 141.8196 | 161.7052 | 161.2624 |
H01

STREAM ID  H01
FROM : FLA1
TO : HEAT

STREAM ATTRIBUTES:
HEAT
Q  BTU/HR  .67418E+06
# S02 S03 S01

## STREAM SECTION

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## STRUCTURE: CONVENTIONAL

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## Fجو

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## VFRAC |

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## ENTHALPY BTU/LB |

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## ENTHALPY BTU/LB-R |

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## DENSITY LB/CUFT |

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</table>
Figure C.7
PROCESS listing for 50/50 split simulation using PR
**TITLE**
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

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**STREAM DATA**
PROP STRM=S01, TEMPERATURE=100.0, PRESSURE=14.696,  
COMD=22.6/13.5/22.4/20.0/17.4/15.8/14.7/13.8

**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
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"
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 - DYN
FORM FOR ENTERING COMPONENT LIQUID DENSITIES - API

4 TOLERANCES

PRODUCT CONVERGENCE ON COMPONENTS WITH X GT 0.0100 0.01000
TEMPERATURE
PRESSURE -1.000

TOWER ENTHALPY BALANCES 0.00500
Bubble Point Relations 0.00100
Component Balances

SPECIFICATIONS ON TEMPERATURE -0.10000
PRESSURE 0.00500
Stream Rate/Property 0.01000
Purity/Recovery 0.01000
Heater/Chiller Duty 0.00100
Others 0.00100

7 CALCULATIONAL OPTIONS

NUMBER OF TRIALS
10

compute water properties assuming saturated conditions
## Defined Components

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<th>COMP NO</th>
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III THERMODYNAMIC AND TRANSPORT DATA

1 SUMMARY

SET 1

KVALUE PENG-ROBINSON

" LIQUID "
ENTHALPY PENG-ROBINSON
ENTROPY PENG-ROBINSON
DENSITY API

" VAPOR "
ENTHALPY PENG-ROBINSON
ENTROPY PENG-ROBINSON
DENSITY PENG-ROBINSON
IV STREAM DATA

1 STREAM 501, IS OF MIXED PHASE

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TOTAL RATE, LB HOLS/HR 150.2000
TEMPERATURE, DEG F 400.0000
PRESSURE, PSIA 14.6560
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
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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**

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**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 |
| M FT3/HR | 36.508 | 56.099 | 0.000 |
| ACTUAL M FT3/HR | 56.145 | 102.848 | 0.000 |
| LBS/M FT3 | 232.889 | 232.770 | 0.000 |
| Z | 0.96293 | 0.96298 | 0.00000 |
| CP,BTU /LB MOLE | 7.6646E+01 | 9.0278E+01 | 0.0000E+00 |

**LIQUID**

| M LBS/HR | 10.399 | 0.000 | 0.214 |
| MOLECULAR WEIGHT | 192.600 | 0.000 | 213.641 |
| STD LIQ FT3/HR | 201.671 | 0.000 | 4.088 |
| ACTUAL GPM | 30.0549 | 0.0000 | 0.6203 |
| FT3/HR | 241.066 | 0.000 | 4.976 |
| LBS/FT3 | 42.137 | 0.000 | 42.937 |
| Z | 0.00711 | 0.00000 | 0.00700 |
| CP,BTU /LB MOLE | 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 PSEUODOCRITICALS 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
Figure C.9
50/50 Composition simulation result for liquid stream S03

Relative err. diff. in Composition

Pseudocomponent

BP225 BP275 BP325 BP375 BP425 BP475 BP525 BP575

TYPE *** Ideal *** SRK O--O PR

S.E.S. 3/89
APPENDIX D

ASTM standards
Pages 327-386 have been redacted for online presentation due to copyright concerns
Index

1967 ASME water correlations (11)

ACE
   ASPEN Cooperative Enhancement Group (56)

Antoine (25), (34)
   vapor pressure (16)

API
   American Petroleum Institute (3)
   API= (62)
   gravity (6)
   Procedure 5A1.13 (32)
   Report 1-77 (39)

ASPEN
   input language (61)
   pure component data bank (25)
   pure component data bank enhancements (25)
   reference conditions (29)

ASPEN major properties (9)

ASTM
   D86 (58)
   D86,D216,D1160 (3)
   slope of ASTMD86 (62)

Benedict-Webb-Rubin
   EOS (11)

Boiling point
   for petroleum (48)

Boiling Points
   (4)

Cavett
   enthalpy (11), (20), (42)
   vapor pressure (17), (34)

Chao-Seider (10)

Crude petroleum
   composition (1)

DFMS (25), (64)
   data file management system (4)
   translator (59)

Distillation curve (3)
   gas chromatograph (4)

Documentation
   Fortran (56)

Error/warning information (60)

ESTPRO (56), (57), (59), (61)
   program execution (66)

Flowsheet simulator
   component based (1)

Fraction
   or petroleum cut (3)

Gunn Yamada (39), (47), (49)
Saturated liquid densities (37)
Marquardt method (29)
Mathias
   Redlich Kwong Soave EOS (11)
Maximum number of estimations (56)
Maxwell Bonnell
   vapor pressure correlation (32)
NRTL
   activity coef. (11)
Parameters
   for 12 sysops (15)
   Table (13)
   universal and model specific (12)
Peng-Robinson
   EOS (11)
   interaction parameters (12)
PROCESS (67)
   Trademark (67)
Rackett (37), (76)
   equation (20)
   parameter (37)
Radius of Gyration
   estimation (50)
Redlich-Kwong (11)
Riazi Daubert method
   definition (31)
Scatchard-Hildebrand (10), (47)
Soave
   Redlich Kwong EOS (11)
SYSOP (8), (15), (28), (65)
   SYSOP's (9)
   SYSOP-1 (65)
   SYSOP0 (10), (15), (44), (53), (59)
   SYSOP1 (10), (15)
   SYSOP10 (11)
   SYSOP12 (11), (48)
   SYSOP14 (10), (11)
   SYSOP2 (10), (15)
   SYSOP3 (10), (11)
   SYSOP4 (10), (11)
   SYSOP5 (10), (11)
   SYSOP8 (11)
   SYSOP9 (11)
   SYSOPs (8), (10)
Tia Juana light (58), (64)
UNIQUAC
   activity coef. (11)
Universal parameters
   definition (15)
UOP
   K factor (4), (6)
Universal Oil Products (3)
Van Laar
  activity coef. (11)
Watson (10), (39)
  enthalpy of vaporization (42)
  heat of vaporization (19)
Wilson
  activity coef. (11)