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DEVELOPMENT OF EQUATIONS OF STATE FOR FLUIDS-CORRELATION METHODOLOGY FOR THERMODYNAMIC AND PVT PROPERTIES, INCLUDING A CASE STUDY FOR WATER.

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GRADUATE COLLEGE

DEVELOPMENT OF EQUATIONS OF STATE FOR FLUIDS-CORRELATION METHODOLOGY FOR THERMODYNAMIC AND PVT PROPERTIES, INCLUDING A CASE STUDY FOR WATER

A DISSERTATION

SUBMITTED TO THE GRADUATE FACULTY

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By

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Norman, Oklahoma

1978

DEVELOPMENT OF EQUATIONS OF STATE FOR FLUIDS-CORRELATION METHODOLOGY FOR THERMODYNAMIC AND PVT PROPERTIES, INCLUDING A CASE STUDY FOR WATER

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ABSTRACT

A correlation methodology for the development of equations of state containing large numbers of parameters is presented herein, with the development of a forty-three parameter equation of state for water presented as a case study. The methodology consists of six steps: (1) experimental data collection and selection of a working data set (subset), (2) determination of initial values of model parameters by regression on pressure, (3) parameter value improvement by regression on density, (4) development of base equation by multiproperty analysis of density, vapor pressure and enthalpy departure data, (5) model improvement by systematic removal of unnecessary terms, and (6) model validity check using the complete set of available thermodynamic data.

This method was used to develop an equation of state for water covering the extensive range from the triple point, 491.67°R, 0.089 psia (271.15°K, 0.614 KPa) to 2859.67°R and 20,305 psia (1588.7°K, 140,000 KPa). A model of 48 parameters was developed and then improved to a model of 43 parameters which predicted thermodynamic properties with the following average absolute deviations: 0.58% for 1459 density

points, 0.12% for 53 vapor pressure points and 1.59 BTU/lbm (3.70 J/g) for 263 enthalpy points. Continued application of the method should allow even more improvement, especially in the high pressure region.

This methodology will allow the researcher to systematically evaluate and develop complex models for which intuition becomes inadequate.

DEVELOPMENT OF EQUATIONS OF STATE FOR FLUIDS-CORRELATION METHODOLOGY FOR THERMODYNAMIC AND PVT PROPERTIES, INCLUDING A CASE STUDY FOR WATER

CHAPTER I

INTRODUCTION AND METHODOLOGY

Equations of state are now being developed that are extremely accurate and are generalized to many fluids. This has led to equations having 40 or more parameters. Insight and intuition developed even by many years experience with equations of state often are inadequate in developing such massive models. This work presents a systematic method to develop such models.

Equations of state are basically either empirical or theoretical. Until recently the theory was not very well developed so that the most accurate equations were highly empirical. Most empirical equations are developed from isochoric data by choosing an empirical temperature dependence and then making the constants a function of density. This method was used in the Beattie-Bridgman [2], Martin-Hou [19], BWR [3], and Vennix [27] equations. Since its development in 1940 the BWR equation has received several modifications

to improve its high density, low temperature prediction. The most popular modification of the BWR equation is the form developed by Starling and Han [24] which was used in a massive correlation work by Hopke and Lin [18].

The van der Waals equation was one of the earliest to have a theoretic foundation. In it deviations from the ideal gas law were accounted for by two effects, one due to the excluded volume a molecule occupies (repulsive forces) and the other due to attractive forces. Redlick and Kwong modified the attractive term to get the R-K equation [21]. As with the BWR equation, many modifications were made to improve the R-K and are reviewed by Tsonopoulos and Prausnitz [26]. The most popular form now used in industry was developed by Soave [23], in which the equation parameters were made functions of temperature and accentric factor, omega. This equation along with the Starling-Han BWR was reviewed by West and Erbar [30].

With the development of high speed digital computers, idealized systems of particles were studied by Monte Carlo and molecular dynamics simulations. From this developed the theory for the properties of a system of hard spheres. This led to equations [19] based on the van der Waals and R-K equations in which the repulsive term is replaced by that for hard spheres developed by Carnahan and Starling [4]. The well-developed hard sphere theory led to the study of more realistic fluids by using hard spheres as a reference

for a perturbation expansion. Since argon was known to be accurately represented by a Lennard-Jones potential, Lennard-Jones fluids were thoroughly studied. The accuracy of perturbation theories for such fluids was studied by comparing predictions with computer simulations. This led to the well developed perturbation theories of Weeks, Chandler and Anderson (WCA) [29] and Verlet and Weiss [28]. The success of perturbation theories encouraged the use of this technique for other molecular effects such as those due to dispersion, overlap and multipole forces.

The accuracy desired and the number of fluids that are to be represented have led to equations of state that have many parameters. When working with many parameters, as the 50 of the Keenan and Keyes [15] equation of state for water, a systematic approach is needed. This work presents a method developed to logically handle large models. It consists of a regression package EZFIT and a set of guidelines.

The steps of the method are:

1. Collect data sets and selection of a working data set (subset).
2. Get initial parameters by a pressure regression.
3. Improve the density regression.
4. Develop a base equation by multi-property analysis.

5. Improve the model by eliminating terms.
6. Check validity of the equation by predicting more data.

This method was used to develop a 43 parameter equation of state for water as a case study in the present work.

CHAPTER II

REGRESSION METHODS

The heart of developing any model is finding the values of the parameters. This leads to the use of linear and nonlinear regression methods.

Our fitting function for the ith point of the random sample is y_i,

$$Y_i(x_1, x_2, \ldots x_i, a_1, a_2, \ldots a_\ell) = Y_i(\{x\}_n; \{a\}_\ell) \quad (1)$$

where the x_i's are the independent variables (in this case temperature and density) and the a_i's are the parameters whose values are desired. The functional form of Y is dependent upon whether the sample point is density, enthalpy departure or vapor pressure. The parameters we desire are those which maximize the joint probability distribution for the sample. With the assumption the data points are normally distributed with known variance σ_i^2 and mean $Y_i(\{x\}_n; \{a\}_\ell)$, maximizing the probability corresponds to minimizing the function χ^2

$$\chi^2 = \sum_i 1/\sigma_i^2 [Y_i - Y_i(\{x\}_n; \{a\}_\ell)]^2$$

$$= \sum_i \omega_i [Y_i - Y_i(\{x\}_n; \{a\}_\ell)]^2 \quad (2)$$

where Y_i is the experimental value for the ith sample point and ω_i is the weight for that point. The condition for a minimum is the ℓ normal equations

$$\frac{\partial \chi^2}{\partial a_j} = \partial/\partial a_j \sum_i \omega_i [Y_i - Y_i(\{x\}_n; \{a\}_\ell)]^2 = 0$$

$$j=1,2,\ldots\ell \qquad (3)$$

Since our fitting function is in general nonlinear and implicit in the parameters a linearization technique is used [4]. The fitting function when expanded about estimates of the parameters, $\{a_0\}_\ell$, and truncated to first order in the corrections Δa_j becomes

$$Y_i(\{x\}_n; \{a\}_\ell) = Y_{i0}(\{x_i\}_n; \{a_0\}_\ell) + \sum_{j=1}^{\ell} \frac{\partial Y_{i0}}{\partial a_j} \Delta a_j \qquad (4)$$

To the first order approximation, χ^2 can be expressed as

$$\chi^2 = \sum_i \omega_i \{Y_i - [Y_{i0} + \sum_j \frac{\partial Y_{i0}}{\partial a_j} \Delta a_j]\}^2 \qquad (5)$$

where the variables of Y_{i0} have been dropped for convenience. The normal equations are then

$$\frac{\partial \chi^2}{\partial \Delta a_k} = -2 \sum_i \omega_i \{Y_i - Y_{i0} - \sum_j \frac{\partial Y_{i0}}{\partial a_j} \Delta a_j\} \frac{\partial Y_{i0}}{\partial a_k}$$

$$= 0 \qquad k = 1,2, \ldots,\ell \qquad (6)$$

In matrix form these equations are then

$$\beta_k = \overline{\Delta a}\ \underline{\alpha} = \sum_j \Delta a_j \alpha_{jk} \tag{7}$$

where

$$\beta_k = \sum_i \omega_i [Y_i - Y_{i0}] \frac{\partial Y_{i0}}{\partial a_k} \tag{8}$$

and

$$\alpha_{jk} = \sum_i \omega_i \frac{\partial Y_{i0}}{\partial a_j} \frac{\partial Y_{i0}}{\partial a_k} \tag{9}$$

The equations are solved for $\overline{\Delta a}$ and the new estimates of the parameters are

$$\bar{a} = \bar{a}_0 + \overline{\Delta a}. \tag{10}$$

This direct solution of equation 7 is the Gauss-Newton method for nonlinear regression.

To solve these equations, the gradient expansion method of Marquardt [4] is used, in which the diagonal elements of the curvature matrix $\underline{\alpha}$ are increased by a factor λ. The matrix equations are then

$$\beta = \overline{\Delta a}\ \underline{\alpha}', \tag{11}$$

$$[\alpha'_{jk}] = \alpha_{jk}(1+\lambda), \text{ for } j=k$$

$$\alpha_{jk} \quad , \text{ for } j \neq k \tag{12}$$

The factor λ is optimized to reduce χ^2.

After the vector $\overline{\Delta a}$ is calculated, the parameters are updated. This process of updating the parameters is continued until the minimum of χ^2 is reached.

When the function is linear in the parameters $\{a_j\}_\ell$

$$Y_i(\{x_i\}_n;\ \{a_j\}_\ell) = \sum_j a_j X_j(\{x_i\}_n) \tag{13}$$

where $X_j(\{x_i\}_n)$ are functions of the x_i set of x, the normal equations can be obtained directly from 6 as

$$\frac{\partial \chi^2}{\partial a_k} = -2 \sum_i w_i (Y_i - Y_i(\{x_i\}_n;\ \{a\}_\ell)) X_k(\{x_i\}_n) = 0$$

$$k = 1, 2, \ldots, \ell \tag{14}$$

This gives rise to the equivalent matrix equations as 7 through 9 in which $Y_{i0} = 0$ and $\partial Y_{i0}/\partial a_k = X_k$

$$\beta_k = \sum_i w_i [Y_i] \frac{\partial Y_{i0}}{\partial a_k} = \sum_i w_i\ Y_i\ X_k\{x_i\}_n \tag{15}$$

and

$$\alpha_{jk} = \sum_i w_i \frac{\partial Y_{i0}}{\partial a_j} \frac{\partial Y_{i0}}{\partial a_k} = \sum_i w_i\ X_j X_k \tag{16}$$

The derivatives with respect to the parameters were approximated by the finite difference method, i.e.

$$\frac{\partial f(x)}{\partial x} = \frac{f(x+h) - f(x-h)}{2h} . \tag{17}$$

Also by assuming the percentage error is constant the weight, ω_i, becomes

$$\omega_i = 1/Y_i^2 \ . \tag{18}$$

CHAPTER III

SOLUTION METHODS FOR NORMAL EQUATIONS

In derivation of the least squares problem a set of simultaneous equations called the normal equations must be solved. These equations have similar forms for the linear least squares method and the various expansion methods such as Gauss-Newton and Marquart for nonlinear functions. As shown previously, these equations are symmetric and semi-positive definite. Because of this symmetry, specialized solution techniques for symmetric systems such as the Crout algorithm and the more general methods such as the Gauss-Jordan elimination can be used. The details of these algorithms can be found in books on matrix methods [25]. For most regression work, a method is desired that will not only return the solution vector but also the inverse matrix, which is then used to obtain the variances and covariances for statistical analysis.

Because of the large number of parameters determined in equation of state regression work, stringent requirements are laid upon the solution method. Round off errors in accumulating the sums for the normal equations can lead to loss of the semi-positive definite attribute of the normal

equations and the Crout algorithm can become unstable. Although requiring more storage, the Gauss-Jordan elimination with maximum pivoting strategy is unconditionally stable. By modifying the traditional algorithms to generate the inverse in place of the coefficient matrix, storage requirements can be reduced. Because of its stability, this method was selected for EZFIT. This allowed working with larger numbers of parameters with less calculation instability as indicated by underflows and overflows in the solution. There is a time penalty for using full pivoting in that the matrix must be transformed and the reverse transformation performed upon the inverse at the end of the solution. For models with fewer parameters, the calculation requirements are not as stringent and the method of straight pivoting can be used. This option is also available in EZFIT. It is recommended that the full pivoting method be used when more than 30 parameters are being regressed. The details of the matrix inversion routine, GJEL, are given in appendix B.

One of the problems of working with a large number of parameters in a model is that many of the parameters may be highly correlated, giving rise to nearly equal rows in the normal equations. This problem is indicated when the variances, i.e., the diagonal elements of the inverse, are negative. There are several methods for reducing this problem. The most fundamental approach is to examine the

model with the purpose of eliminating parameters with high correlation or performing a transformation which will reduce the correlation. In polynomials more independence among parameters can be obtained by selecting an appropriate set of orthogonal polynomials. Typically Tchebycheff polynomials are selected for not only their orthogonality but also their ability to reduce the number of terms needed for a desired accuracy [6, 12]. This method was selected for the development of the equation of state for water. Another means to improve the independence of the normal equations is to select more data to be included, which will have the desired effect.

Numerical difficulties also arise when the effects of the parameters vary widely. The parameters with the stronger effects will tend to cause the values of the weaker ones to lose significance. This problem can be minimized by judicious choices for scaling for the parameters. To help this trouble, the regression routine CURFIT scales the normal equations so that the diagonals are unity.

Even when these various precautions have been taken there is sometimes difficulty in the generation of the normal equations. The data points which the parameters least effect are sometimes swamped by the other data points. Since the normal equations are formed as a summation of terms for each data point, the accumulations are done in double precision so that more information from all points will be used.

These accumulations also can be helped by ordering the data points so that the points with the least contribution to chi-squared are summed first.

CHAPTER IV

DATA SELECTION FOR THE CASE STUDY OF WATER

In equation of state development there exists a multitude of possible thermodynamic data that can be used in multiproperty regression. Fundamentally, all thermodynamic properties are related to the equation of state by classical thermodynamics. Some of the property types are $P_\rho T$, enthalpy, vapor pressure, speed of sound, Joule Thomson coefficient, and specific heats, C_v and C_p. These vary greatly in accuracy even among measurements of the same type from different investigators. They also vary greatly in the calculation needed to determine the property from the equation of state. To keep track of these various types of data as well as data for other compounds (this regression method is presently being used for studies of many other fluids at the University of Oklahoma), a data base system called BANKED was developed. BANKED is a card based system that identifies each data point as to the reference from which it was taken, fluid, and data type. It handles both mixture and pure fluid data. The details of BANKED are given in appendix C.

It is important that the data selected covers the range that is desired for the equation in a uniform manner so that there are not any regions that are empty. This is especially important for very flexible equations with many parameters. For this reason, an even grid of data was generated from the Keenan and Keyes [13] equation for water which was then supplemented by experimental data. The working density set is given in Figure 1. This consists of 382 points covering a temperature range of 491.67-2859.67°R (273.15-1588.7°K) and a pressure range of .66-20,305 psia (4.6-140,000 KPa). The saturated liquid densities of Osborne, Stimson, and Ginnings [20] were used to better define the saturation curve. If the saturation curve is accurate the vapor pressure and heat of vaporization will be more accurate without using these properties in regression. It is important to have high temperature isotherms that go from low densities to well above the critical density without crossing the two phase region in order to have appropriate trends in the two phase region.

In spite of these precautions in selection of density data, behavior for isotherms crossing the two phase region is not well defined because there is no physical behavior that matches the required behavior of an equation of state in this region. Where physically the pressure is constant at a given temperature for a range of densities in the two phase region, the equation of state typically exhibits the

DENSITY WORKING DATA SET

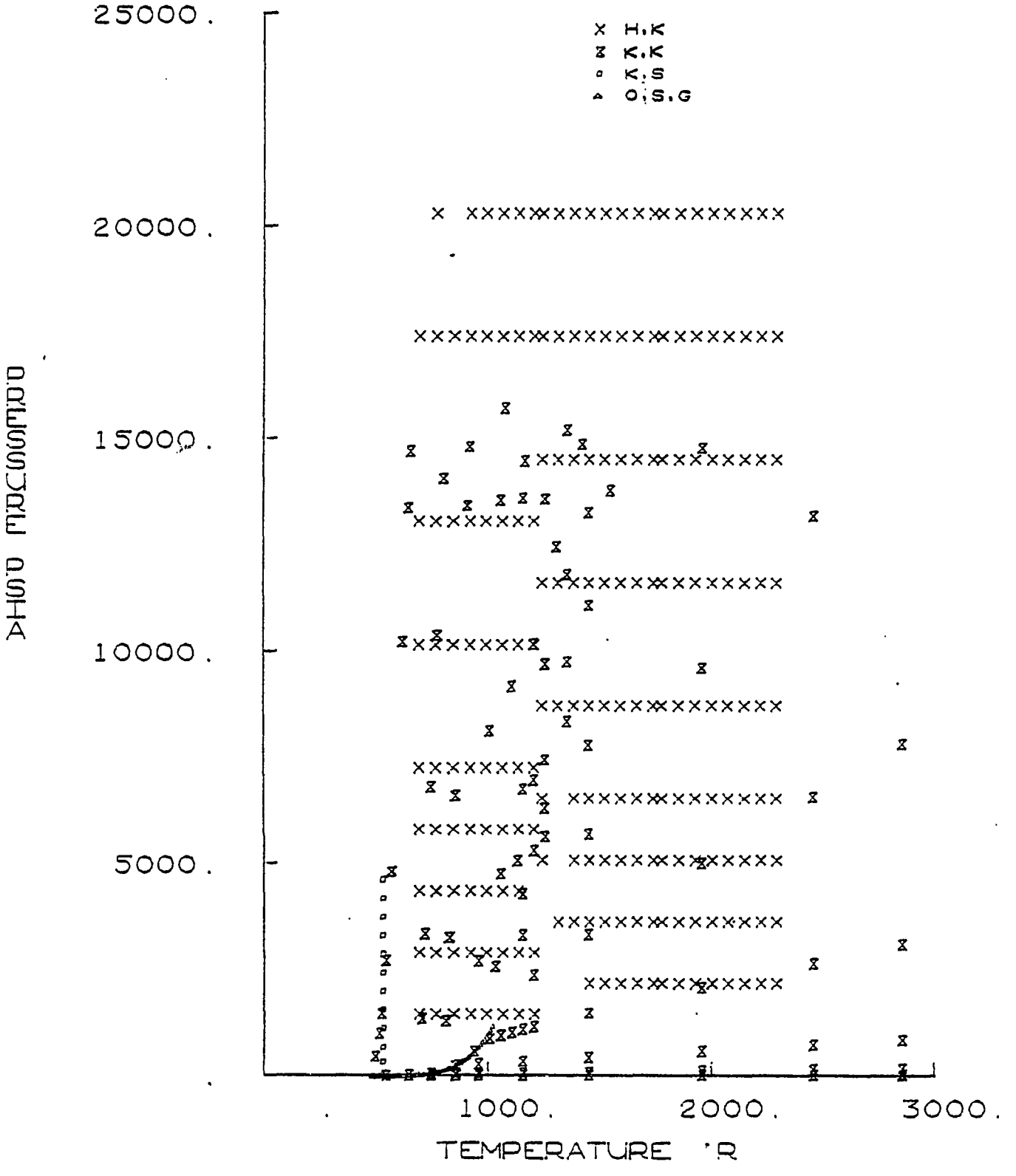


FIGURE 1. Working Density Data Set.

so-called van der Waals loop. Typical behavior of an equation of state is plotted in Figure 2. Information can be augmented for this region by including properties that are calculated as integrals across this region. This includes vapor pressure and enthalpy departure. Therefore, data were included of these types for the water equation. The enthalpy departure data consisted of 113 points generated from the Keenan and Keyes equation in a range of 509.67-2859.67°R (283.15-1588.7°K) and .66-14,694 psia (4.6-101,310 KPa). Since these were derived from an equation of state and not data (although a very accurate equation) they were not given as much importance as experimental data. For vapor pressure, the data of Osborne, Stimson and Ginnings [20] was used. The 53 points covered a range 491.67-1159.7°R (273.15-644.28°K) and 0.089-3090 psia (0.61-21,305 KPa). This covers the saturation curve from the triple point to within 5% of the critical point. The critical point was not covered because calculation algorithms used for vapor pressure and density have trouble in this region due to the flatness of the isotherms and because there is greater numerical uncertainty in the data in the critical region. The enthalpy and vapor pressure data used are plotted in Figures 3 and 4.

While obtaining a working data set, as much data as available were prepared. These data would be used to test the accuracy of both the data and the model. If a specific reference has errors exceeding those for other data sets in

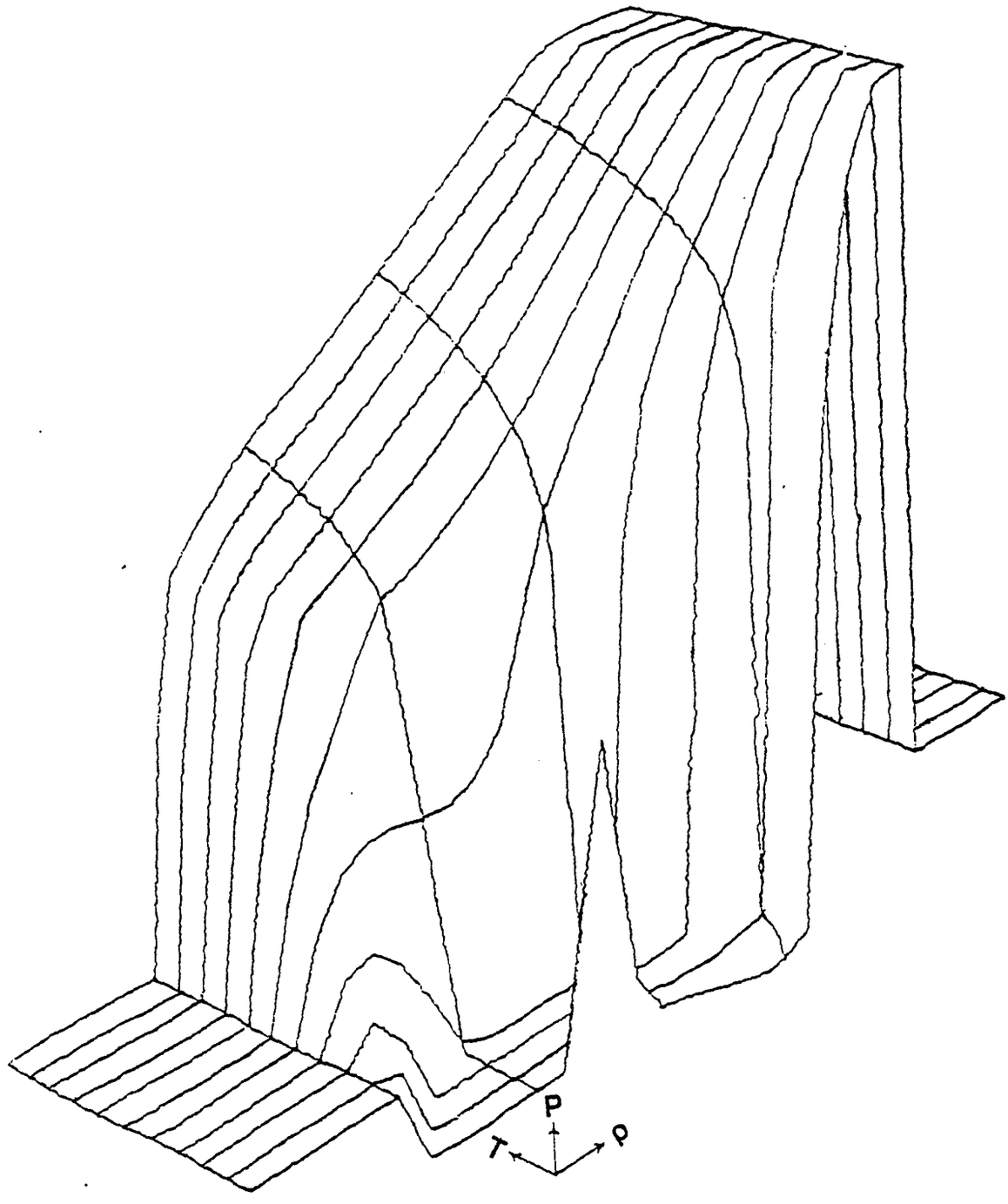


FIGURE 2A. A Three-Dimensional PρT plot of the Typical Behavior of an Equation of State.

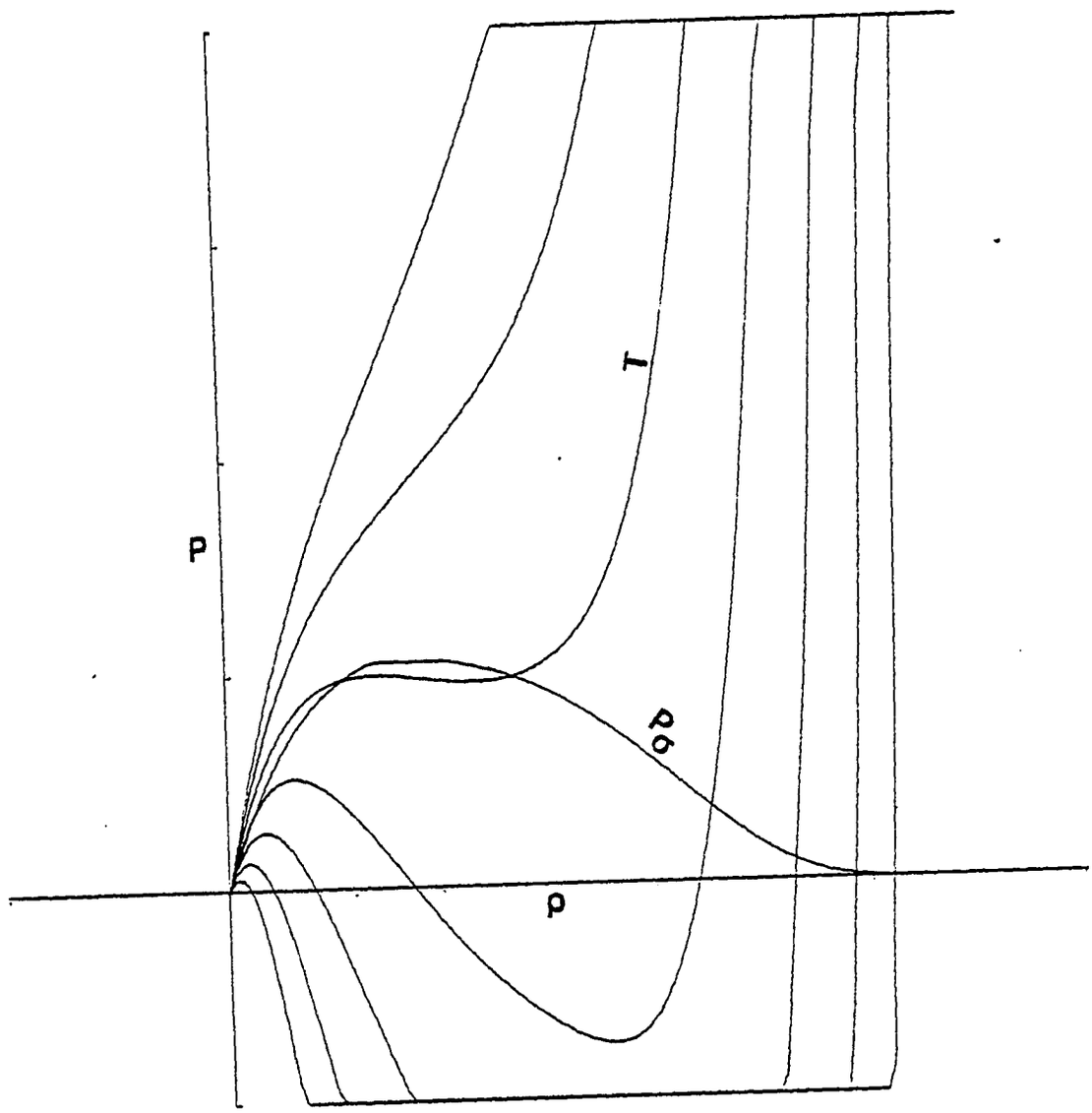


FIGURE 2B. Isotherms of a Typical Equation of State.

ENTHALPY KEENAN, KEYES, ET AL.

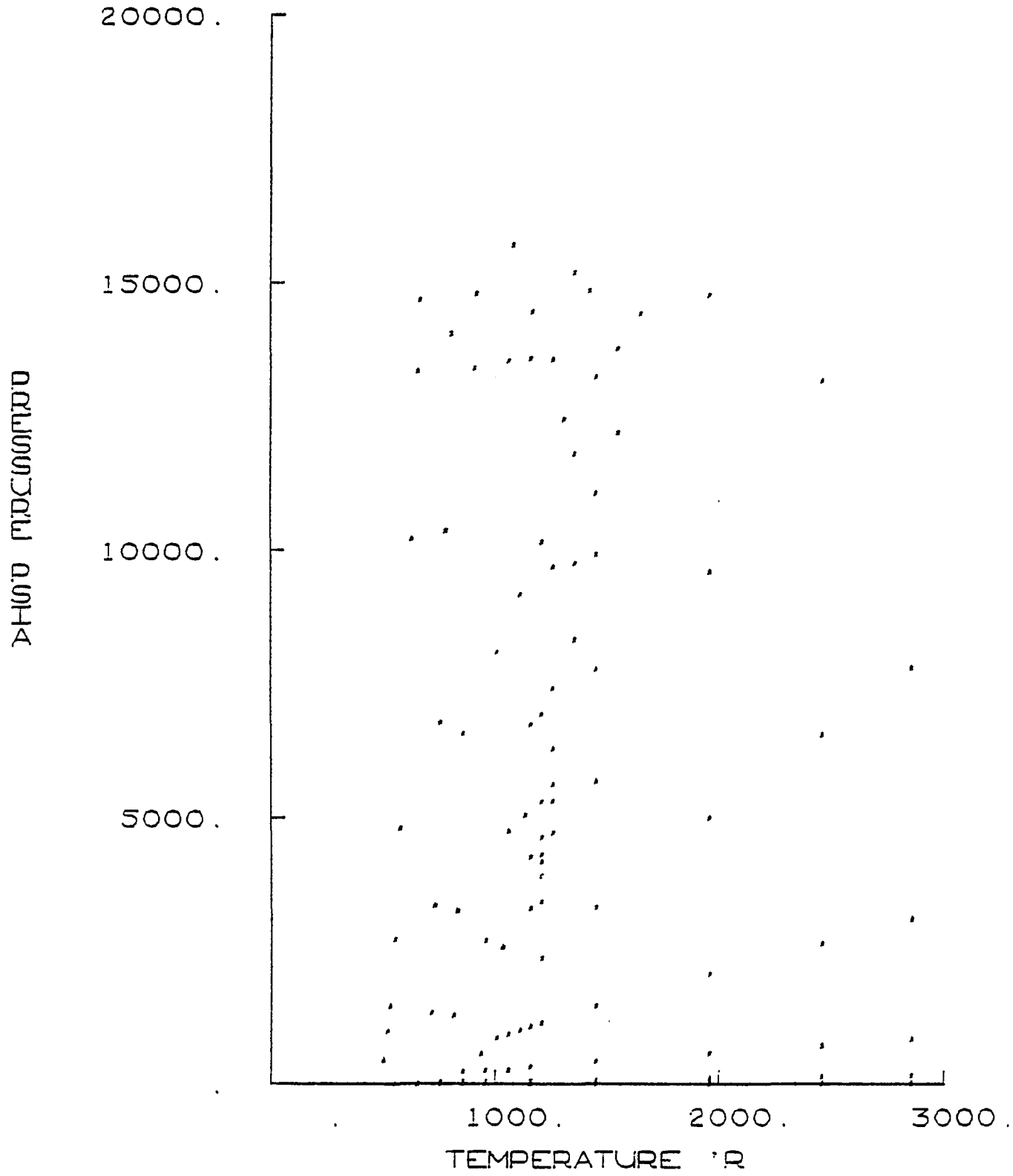


FIGURE 3. Working Enthalpy Data Set.

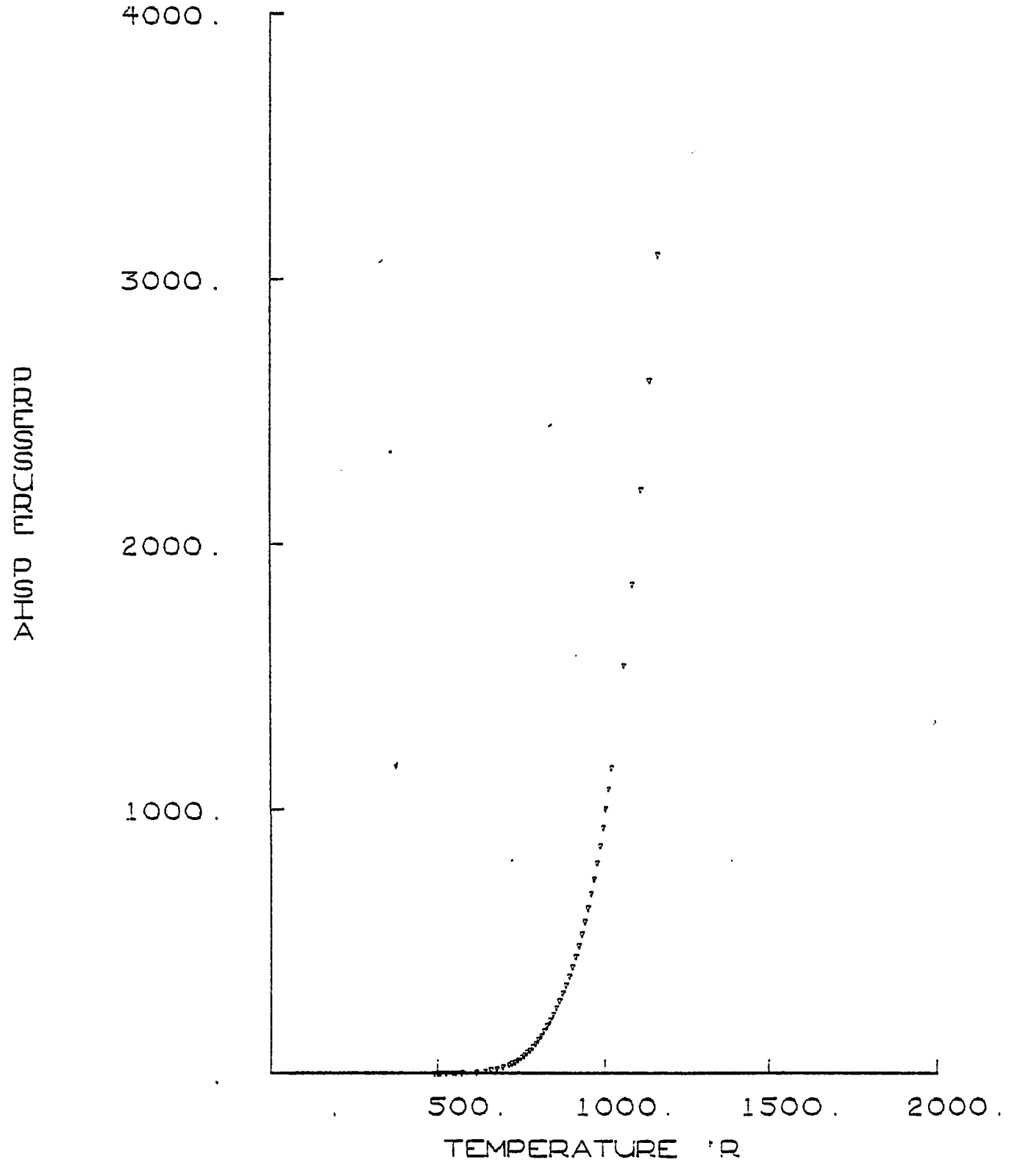


FIGURE 4. Vapor Pressure Data Set.

the region, it would signal the need for an evaluation of the data in that it might be less precise than the rest. For water, besides the working data set, density and enthalpy data were obtained from seven references. For the more massive tabulations only a representative number of points were prepared in BANKED. The data sets used are plotted in Figures 5 to 13. The regions of the pressure-temperature surface that were covered by the various data references for density are shown on Figure 14.

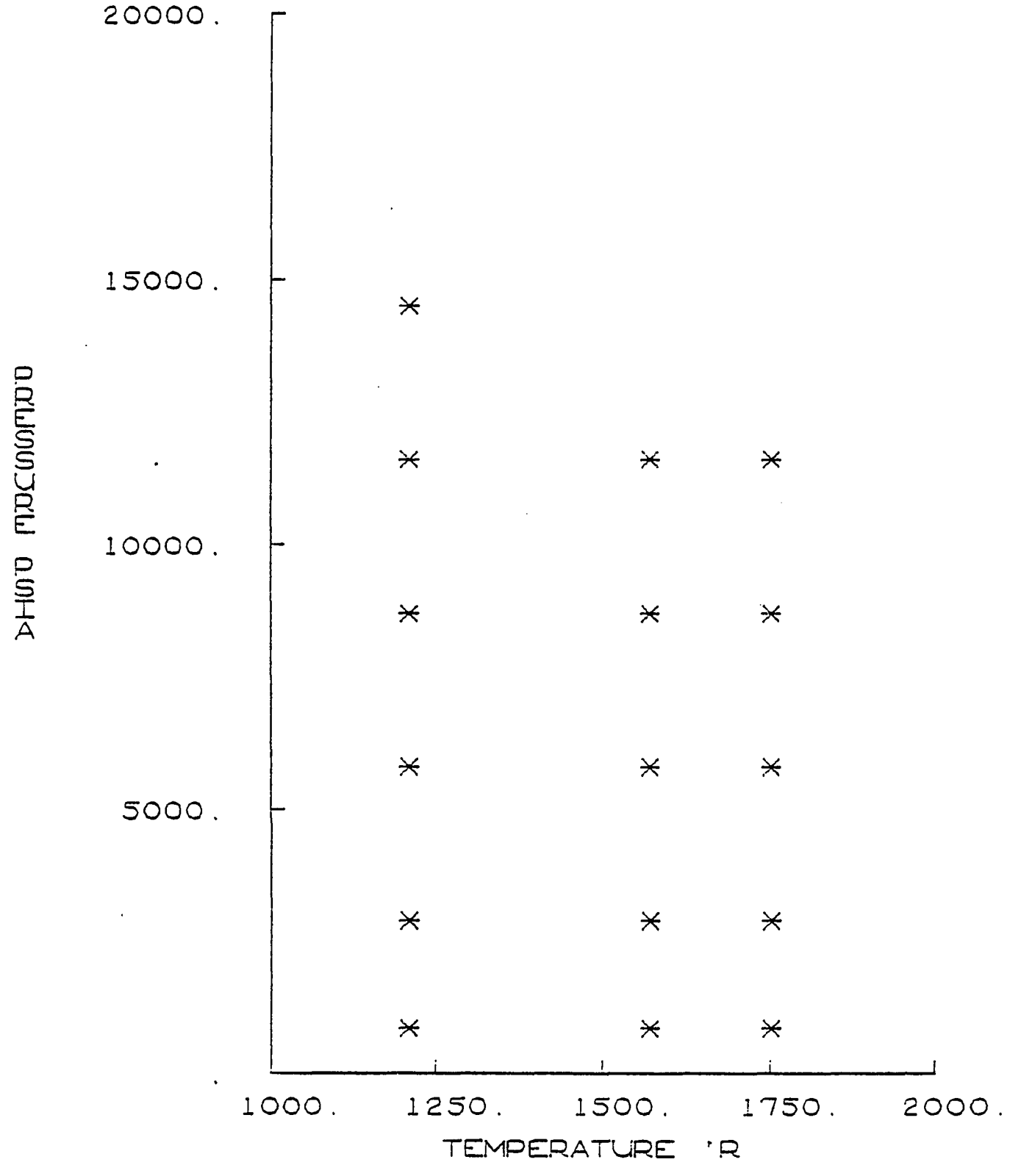


FIGURE 5. Enthalpy, Angus and Newitt

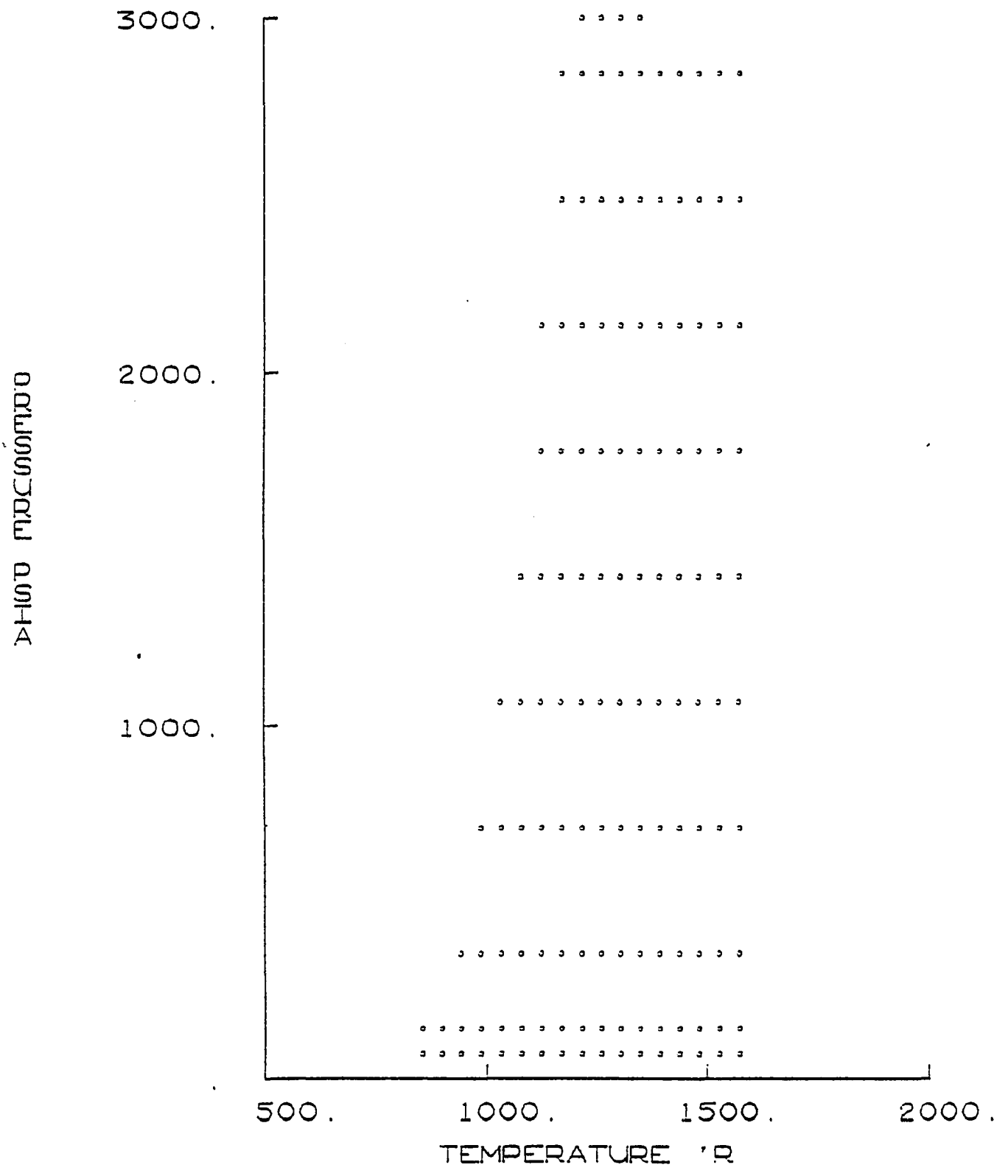


FIGURE 6. Enthalpy, Callendar and Egerton

HOLSER, KENNEDY

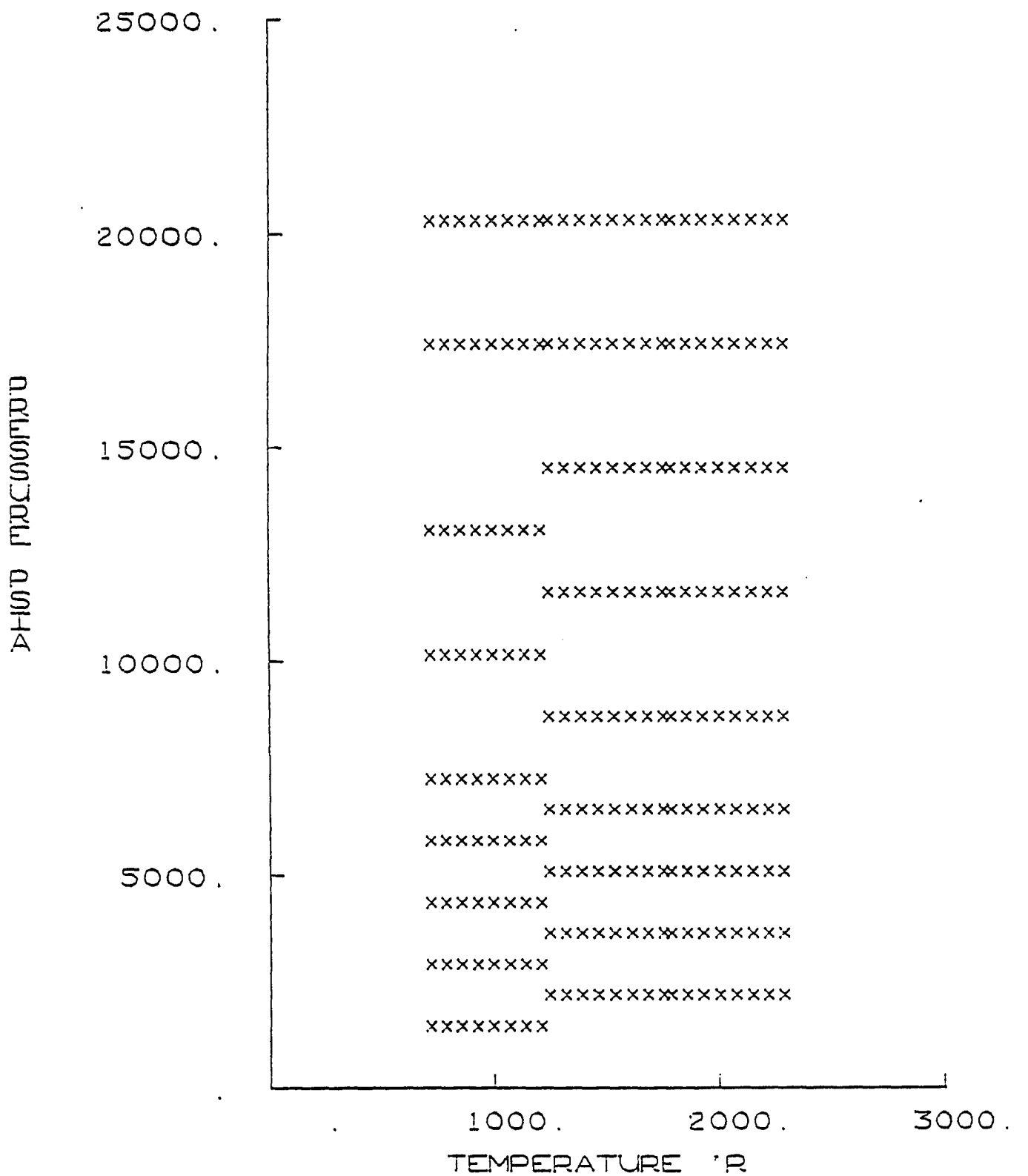


FIGURE 7 Density, Holser and Kennedy

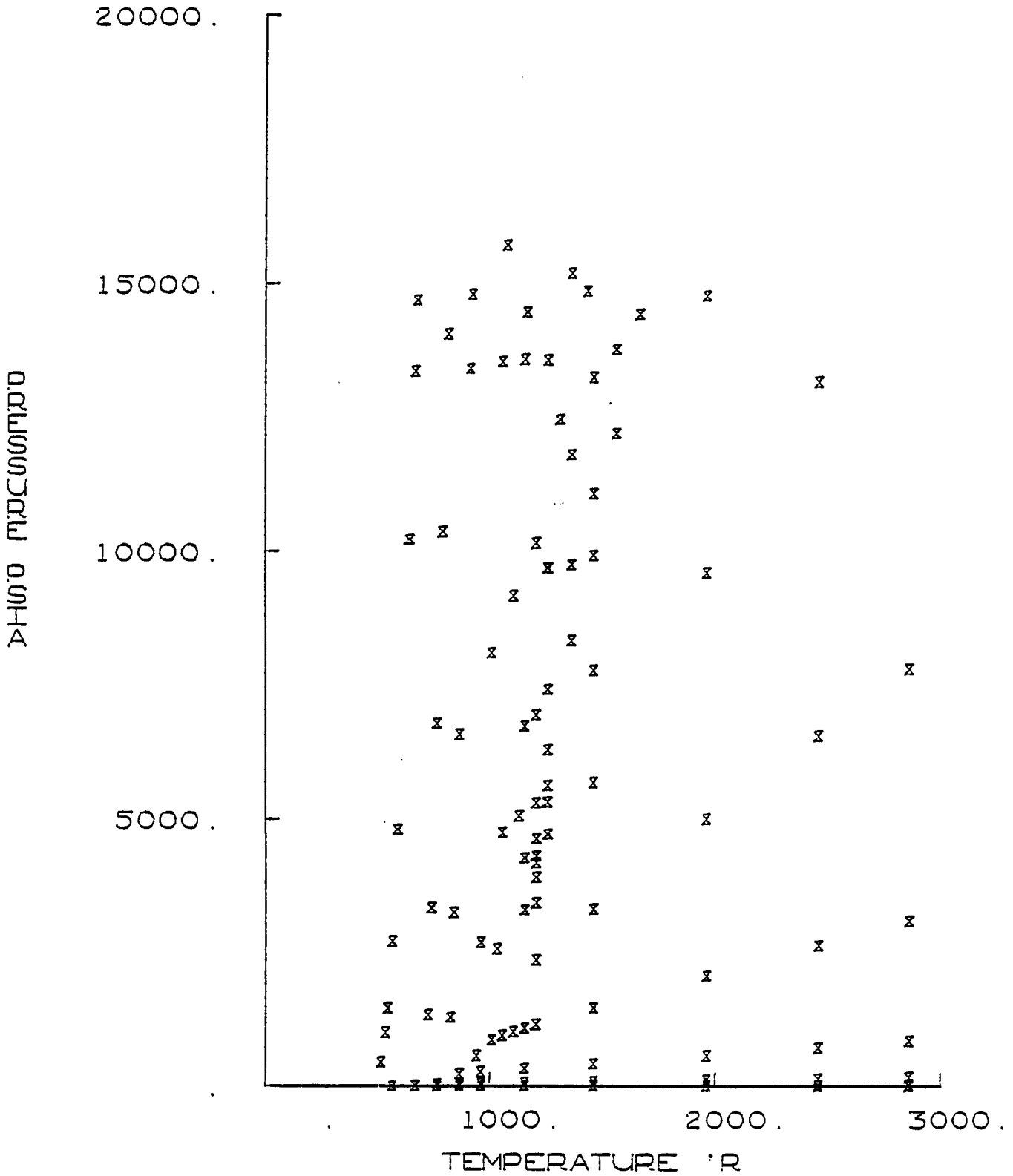


FIGURE 8. Density, Keenan and Keyes

KELL, WALLEY

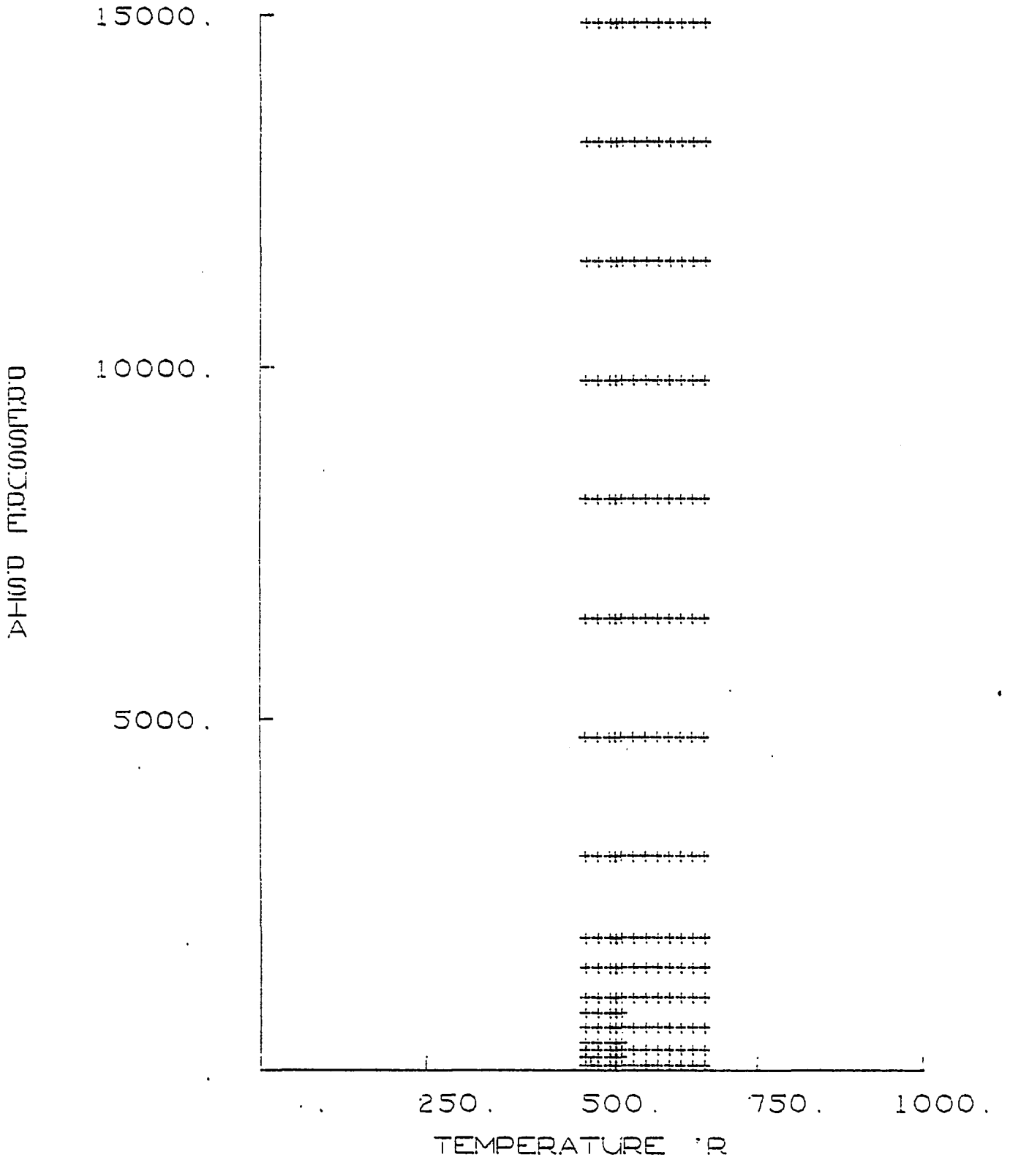


FIGURE 9, Density, Kell and Whalley

KENNEDY

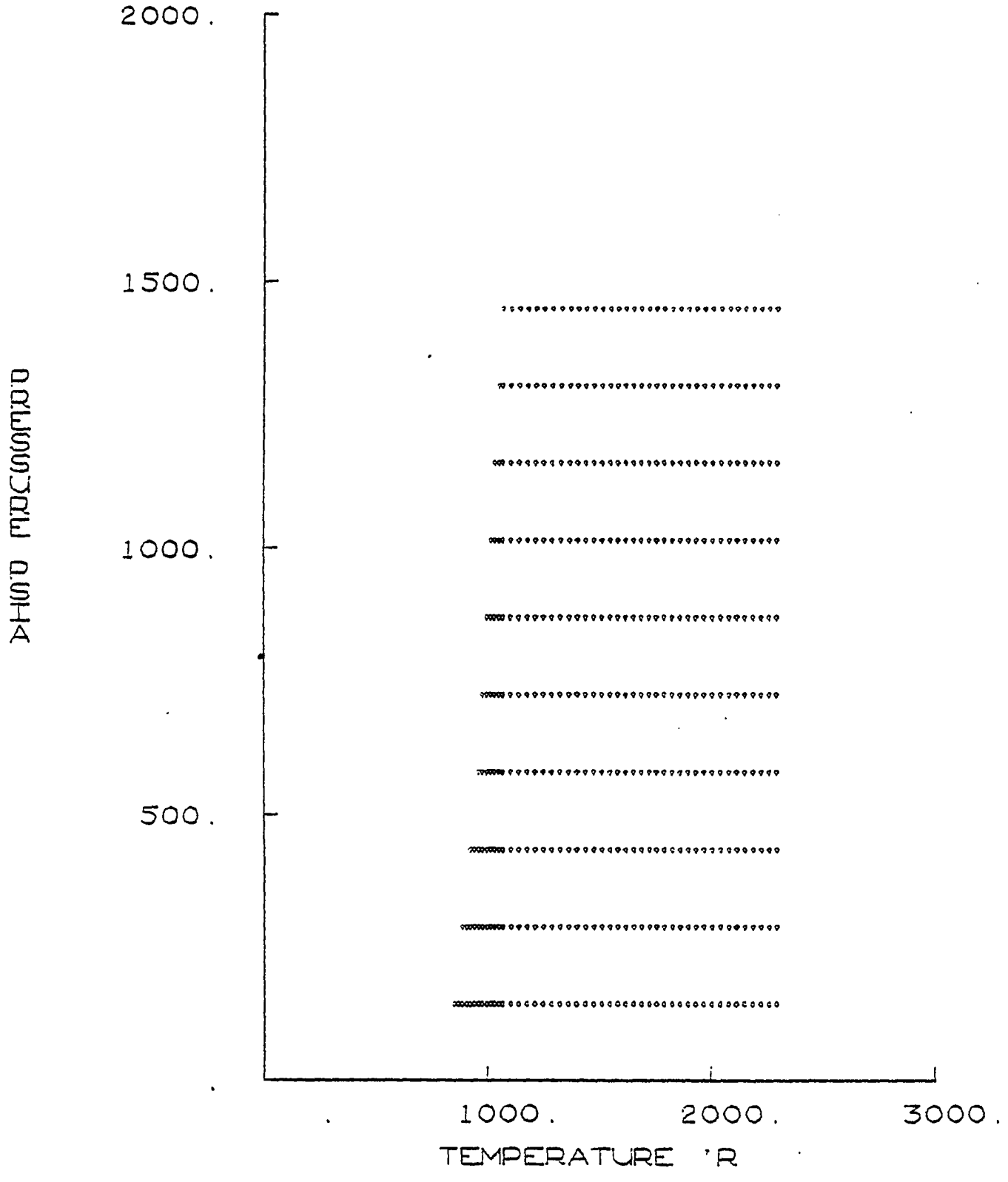


FIGURE 10. Density, Kennedy

KEYES, SMITH

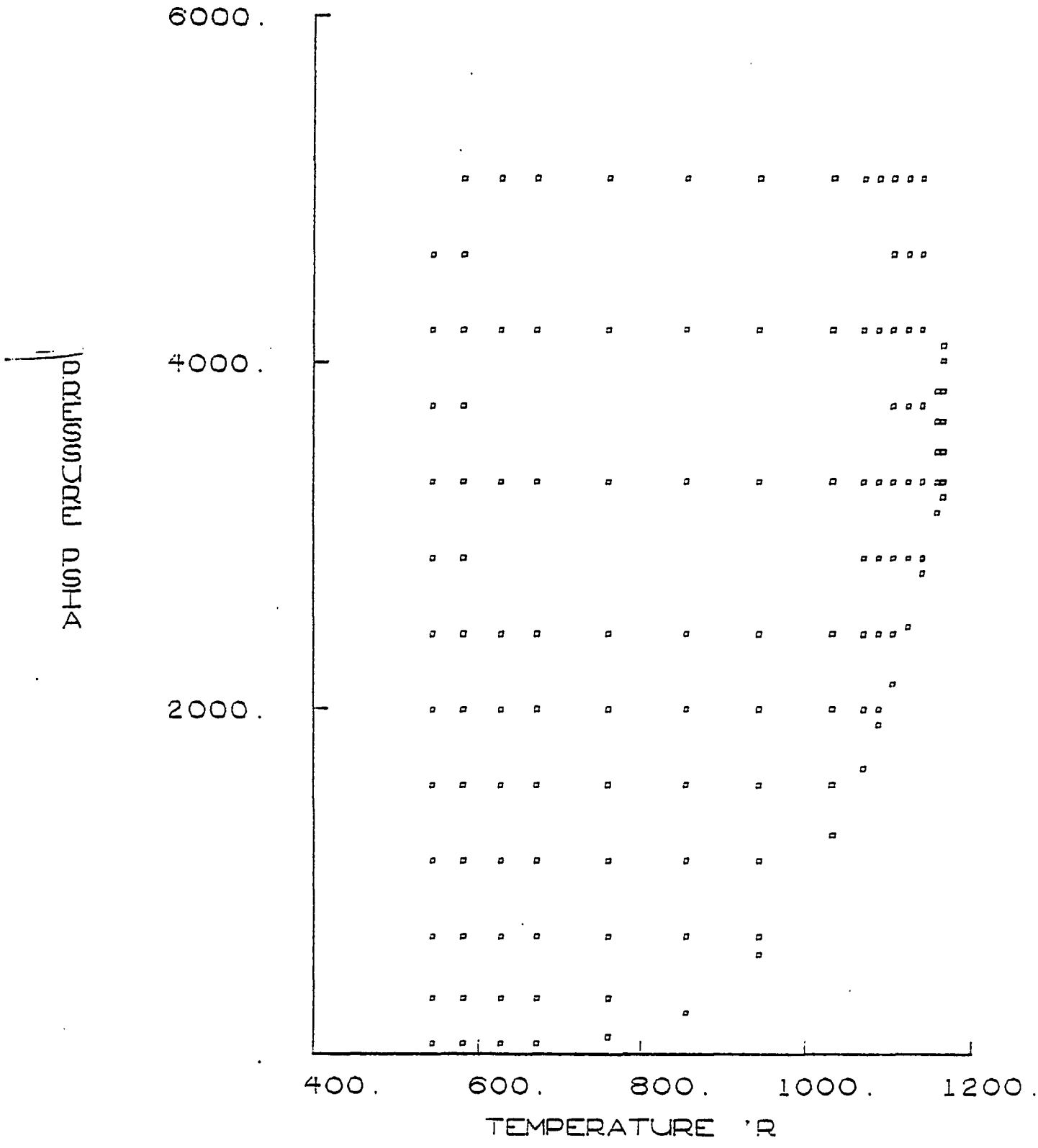


FIGURE 11. Density, Keyes and Smith

KEYES, SMITH, GERRY

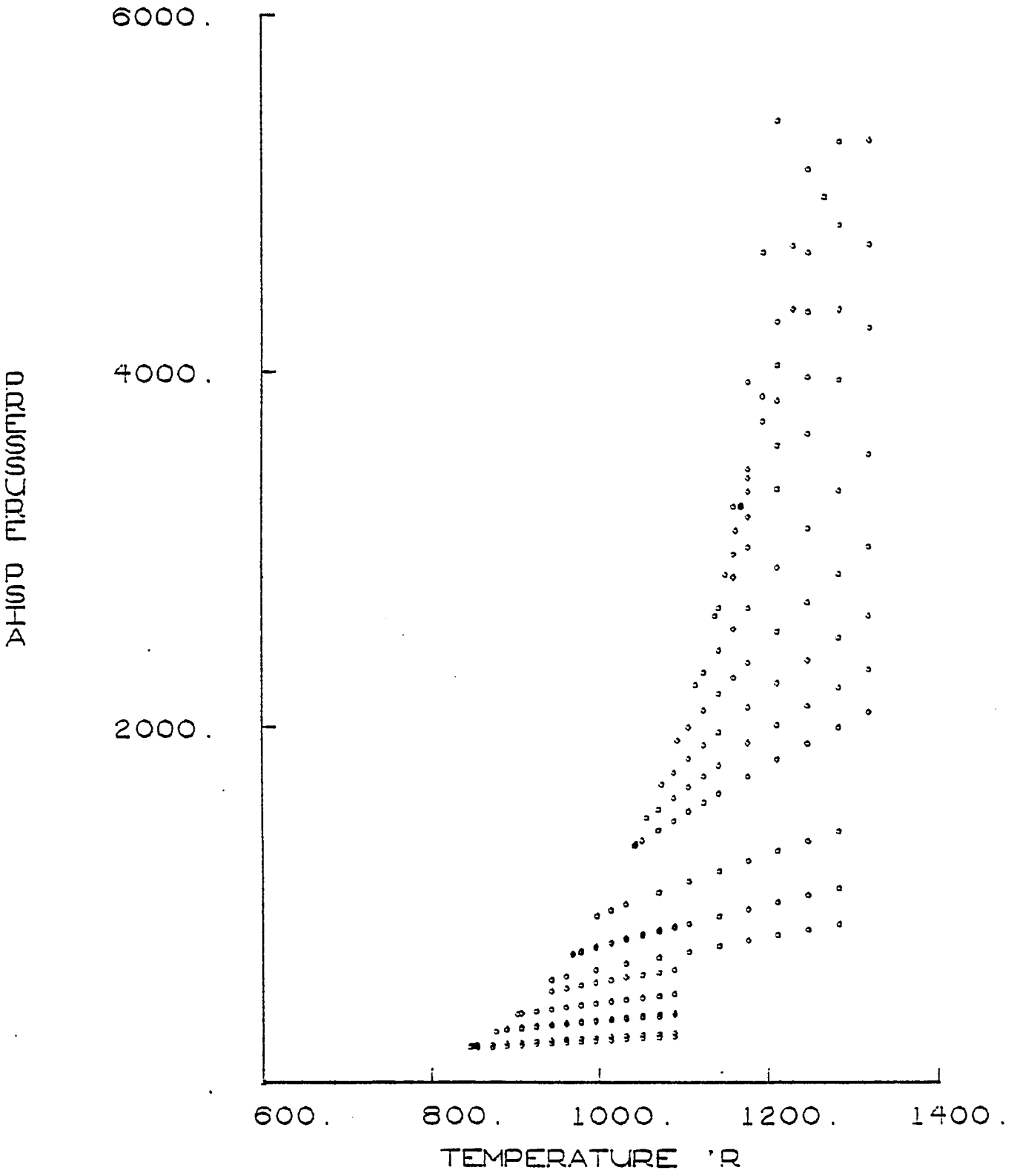


FIGURE 12. Density, Keyes, Smith and Gerry

OSBORNE, STIMSON, GINNINGS

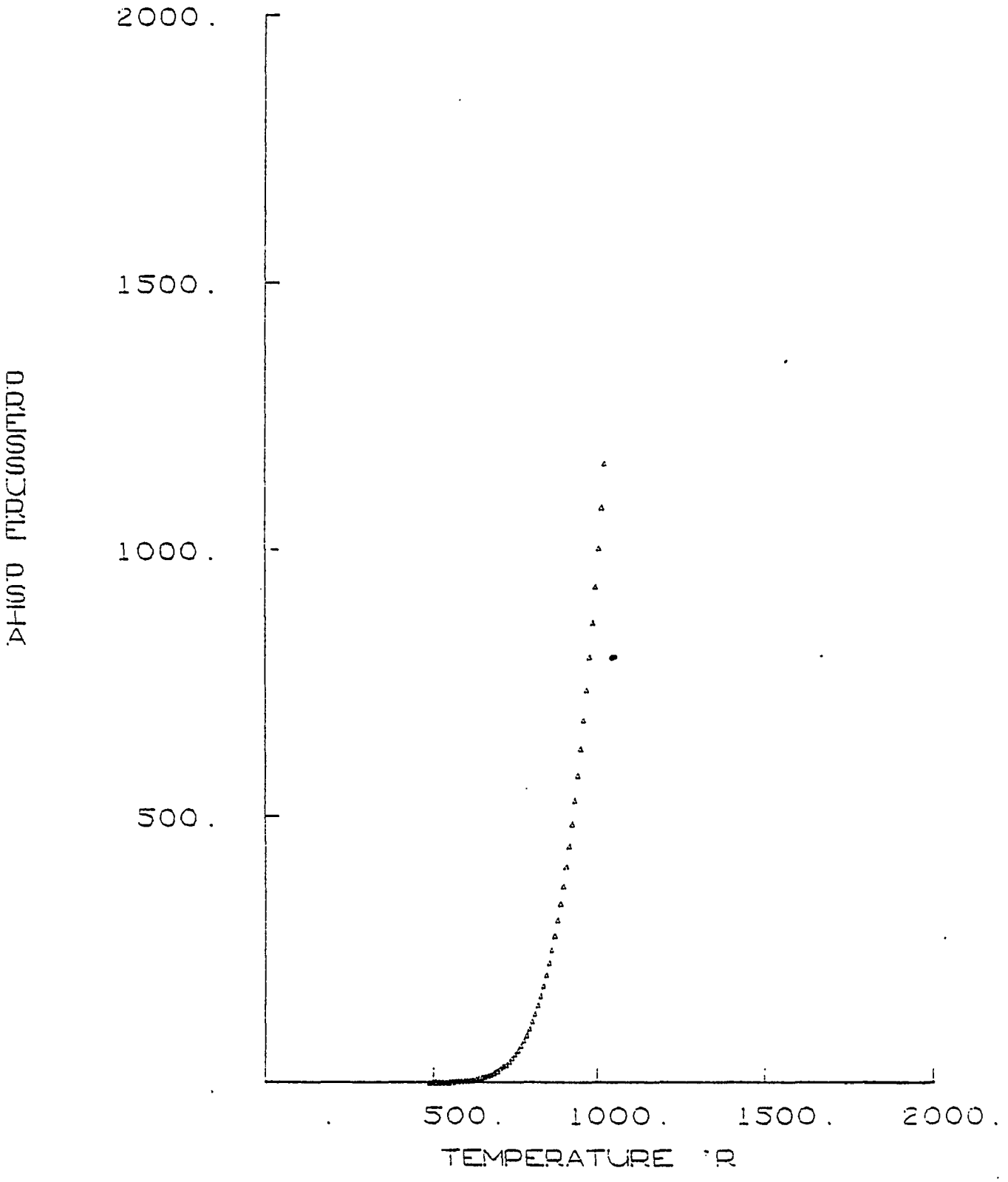


FIGURE 13. Density, Osborne, Stimson and Ginnings

DENSITY

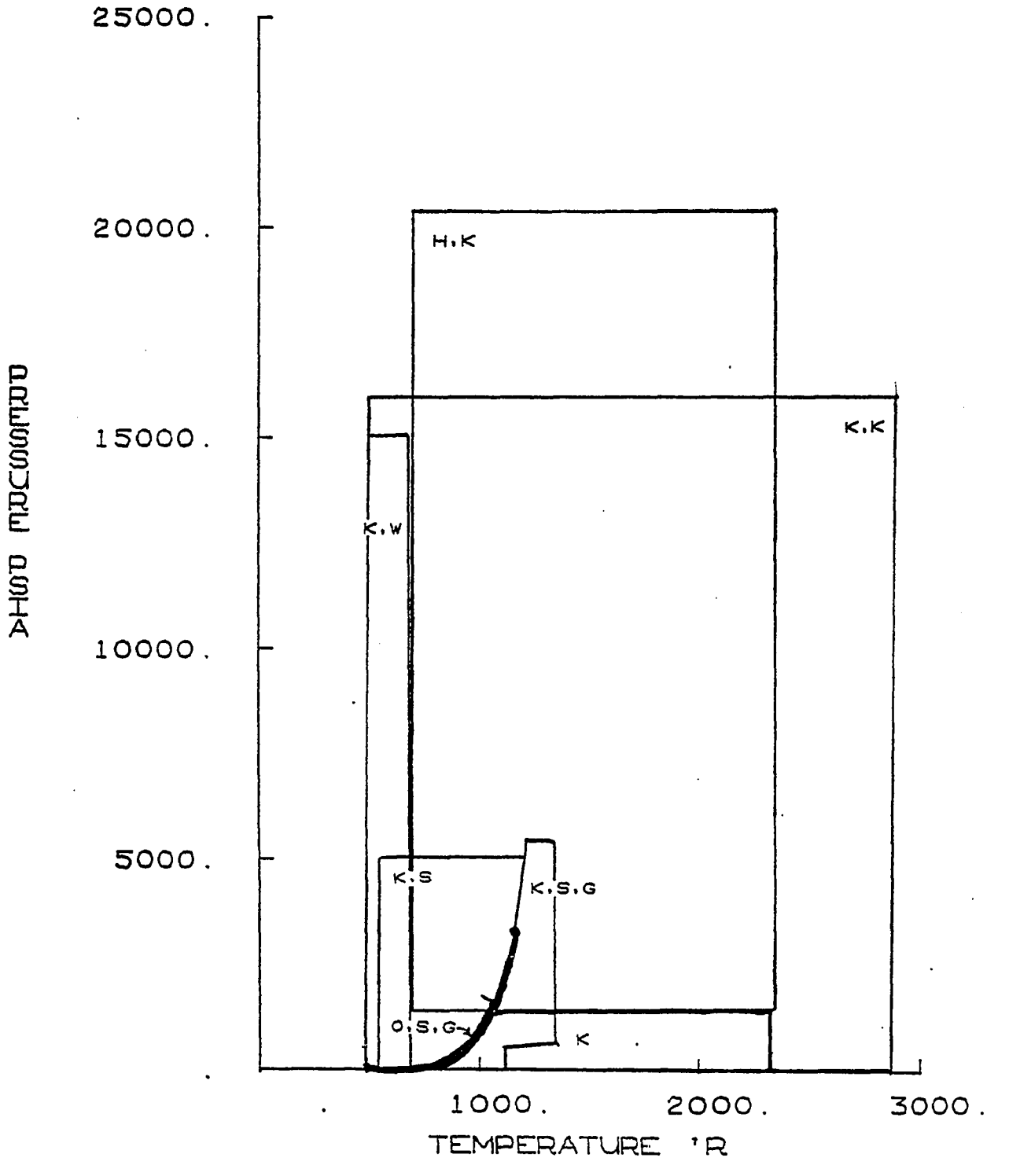


FIGURE 14. Density Data Set Ranges

CHAPTER V

MODEL SELECTION FOR CASE STUDY OF WATER

The compressibility model used for the development of water is linear in the parameters with each term consisting of a monomial of reciprocal temperature and a Tchebycheff polynomial in density. The temperature was reduced by

$$T^* = \alpha T/T_c \tag{19}$$

where α is a scaling parameter used as 1 for water and T_c is the critical temperature. The density was similarly reduced as

$$\rho^* = \beta\rho/\rho_c \tag{20}$$

where $\beta = 1$ and ρ_c is the critical density. The properties for the critical region and other properties used in the equation are given in Table IV.

The Tchebycheff polynomials, T_j, were chosen for their orthogonality, which should improve the calculation stability of the regression program. Another feature of the Tchebycheff polynomials is that they separate into even and odd polynomials. Since they are orthogonal on the

interval (-1,1), the reduced density was divided by 4 to make the largest density be within that range. Since the even polynomials go to 1 at zero but the terms should go to zero when the ideal gas limit one is explicitly given, the terms consist of density times the polynomial.

The terms in the model are then

$$A_{ij}T^{*-1}yT_j(y) \tag{21}$$

where y is the density reduced according to the relation

$$y = \beta\rho/4\rho_c. \tag{22}$$

The full 72 parameter model which was used then is

$$Z = 1 + \sum_{i=o}^{7} \sum_{j=o}^{8} A_{ij}T^{*-1}yT_j(y). \tag{23}$$

This equation was implemented in the subroutine PRES using a single subscript on the parameters. The listings of PRES and FI1 and FI2, routines used for derived properties are given in appendix C. The Tchebycheff polynomials are given in Table I. A table of the parameter indices corresponding to each term is given in Table II.

Derived Properties. Given an equation of state, the relationships of classical thermodynamics allow the derivation of the other properties. If one starts with a model equation for the Helmholtz free energy, the properties are derived from derivatives. This is the method used by Keenan

TABLE I

The first eight Tchebycheff polynomials

$$T_0(y) = 1$$

$$T_1(y) = y$$

$$T_2(y) = 2y^2 - 1$$

$$T_3(y) = 4y^3 - 3y$$

$$T_4(y) = 8y^4 - 8y^2 + 1$$

$$T_5(y) = 16y^5 - 20y^3 + 5y$$

$$T_6(y) = 32y^6 - 48y^4 + 18y^2 - 1$$

$$T_7(y) = 64y^7 - 112y^5 + 56y^3 - 7y$$

$$T_8(y) = 128y^8 - 256y^6 + 160y^4 - 32y^2 + 1$$

Recursion relation:

$$T_{n+1} - 2yT_n + T_{n-1} = 0$$

TABLE II

Table of the parameter index corresponding to a term of the type $T^{*-i}\ yT_j(y)$ in the equation of state. The numbers in parenthesis are the indices of AXTN as implemented in EZFIT.

	yT_0	yT_1	yT_2	yT_3	yT_4	yT_5	yT_6	yT_7	yT_8
T^{*0}	1	7	13	19	25	29	33	37	41(1)
T^{*-1}	2	8	14	20	26	30	34	38	42(2)
T^{*-2}	3	9	15	21	27	31	35	39	43(3)
T^{*-3}	4	10	16	22	28	32	36	40	44(4)
T^{*-4}	5	11	17	23	53(13)	57(17)	61(21)	65(25)	69(29)
T^{*-5}	6	12	18	24	54(14)	58(18)	62(22)	66(26)	70(30)
T^{*-6}	45(5)	47(7)	49(9)	51(11)	55(15)	59(19)	63(23)	67(27)	71(31)
T^{*-7}	46(6)	48(8)	50(10)	52(12)	56(16)	60(20)	64(24)	68(28)	72(32)

and Keyes for their study of water [13]. Alternatively, one can start with the pressure or compressibility formulation and derive the other properties by integration. This method was used by Starling and Han [24] in their work on the modified Benedict, Webb, Rubin equation of state. In each method, one can work with the base model and two derived relations from which all other properties are obtained. When the free energy is used, the derived relations are the temperature and density derivatives. For this work and the EZFIT physical properties package, the three relations are the compressibility and two integrals,

$$Z = P/\rho RT = 1 + \sum_{i=o}^{7} \sum_{j=o}^{8} A_{ij} T^{*-1} y T_j(y) \qquad (24)$$

$$FI_1 = \int_o^{\rho^*} (Z-1) d \ln \rho^* \qquad (25)$$

$$FI_2 = \int_o^{\rho^*} \partial Z/\partial T^* \; d \ln \rho^* \qquad (26)$$

and the reference condition

$$FI_3 = \ln(\rho RT) \qquad (27)$$

Using the definition of the compressibility, FI1 and FI2 are then given as

$$FI_1 = \sum_{i=o}^{7} \sum_{j=o}^{8} A_{ij} T^{*-1} \int_o^y T_j(y) d y \qquad (28)$$

$$FI_2 = \sum_{i=1}^{7} \sum_{j=o}^{8} A_{ij}(-i)T^{*-(i+1)} \int_o^y T_j(y)d\,y \qquad (29)$$

The integrals of the Tchebycheff polynomials are given in Table III. The physical properties used are given in Table IV.

The reduced departures as derived in appendix A are given as

$$A^* = T^* FI_1 + T^* FI_3 \qquad (30)$$

$$U^* = -T^* FI_2 \qquad (31)$$

$$H^* = -T^{*2} FI_2 + T^*(Z-1) \qquad (32)$$

$$S^* = -FI_1 + T^* FI_2 - FI_3 \qquad (33)$$

$$G^* = T^* FI_1 + T^* FI_3 + T^*(Z-1) \qquad (34)$$

$$f/f^o = \exp(FI_3 + FI_1 + Z-1) \qquad (35)$$

These relations allow the computation of the derived properties for the water model. The values of the parameters for the model were then determined by regression. For the 48 parameter model which was the base equation, the density terms were used only up to j=5.

TABLE III

The integrals of the Tchebycheff polynomials on the interval (O,y).

$$\int T_0 = y$$

$$\int T_1 = y^2/2$$

$$\int T_2 = 2/3\ y^3 - y$$

$$\int T_3 = y^4 - 3/2\ y^2$$

$$\int T_4 = 8/5\ y^5 - 8/3\ y^3 + y$$

$$\int T_5 = 8/3\ y^6 - 5\ y^4 + 5/2\ y^2$$

$$\int T_6 = 32/7\ y^7 - 48/5\ y^5 + 6\ y^3 - y$$

$$\int T_7 = 8\ y^8 - 56/3\ y^6 + 14\ y^4 - 7/2\ y^2$$

$$\int T_8 = 128/9\ y^9 - 256/7\ y^7 + 32\ y^5 - 32/3\ y^3 + y$$

TABLE IV

The physical and critical properties of water

Critical temperature	1165.3°R
Critical pressure	3208.0 psia
Critical density	1.1102 lb moles/ft^3
Molecular weight	18.015
Pitzer Accentric factor	0.348
Universal gas constant	10.7315 psia ft^3/lb moles °R
	0.110308 BTU/lbm °R

CHAPTER VI

INITIAL VALUE SELECTION

In most equation of state models, the equation reduces to the ideal gas equation when the parameters are zero. This is the easiest and most common choice. The problem with the ideal gas as the initial model is that it does so poorly in the high density region that a regression on a full range density set is unable to improve the liquid points. Information is not transmitted appropriately to the parameters. The enthalpy departure will be quite bad and the vapor pressure calculation will not converge. It is therefore usual to make some kind of quick regression for a function of the temperature and density, thereby eliminating any search techniques, to get a preliminary set of parameters. Two applicable functions are the compressibility and the pressure. The compressibility, $Z = P/\rho RT$, is commonly used and gives good results. It was used for the development of the Leonard-Jones perturbation model which was then applied to the prediction of methane [9]. Use of the pressure, on the other hand, has some problems in that in the high density region the large value of the derivative

$\partial P/\partial \rho$ controls the regression. This makes the equation over constrained in this region with a corresponding loss in accuracy in the low density region. This problem can be solved by the selection of appropriate weights for the individual pressure points instead of the usual method of selecting the weight to be $1/P^2$, i.e. the maximum likelihood weight. The weight of the point is proportional to the variance [4] and is theoretically given as

$$w_i = 1/(\sigma_p^2 + \sigma_\rho^2 \frac{\partial P}{\partial \rho}^2 + \sigma_T^2 \frac{\partial P}{\partial T}^2) \qquad (36)$$

The problem with this method is the evaluation of the derivatives. Since the function has no other parameters yet, the derivatives, if evaluated from the model, would be those of the ideal gas and inaccurate.

In development of the water equation of state, a tabular function was developed for the weight based upon the density. The weighting function is given in Table V. This function was used to perform the regression on just the parameter portion of the model, that is the ideal gas portion was subtracted from the pressure. Good results were obtained. For the 48 parameter equation these pressure terms were able to predict density to 1.08% for 335 points. This set of parameters is quite adequate for starting density and multi-property regression.

TABLE V

WEIGHTING FUNCTION FOR PRESSURE

DEPARTURE REGRESSIONS

Reduced Density	Weight
4.0-3.0	0.009
3.0-2.5	0.001
2.5-1.2	0.10
1.2-0.5	10.0
0.5-0.1	1.00
0.1-0.001	$10.0(T_r > 1.2)$
0.001-0.0	$100.0(T_r > 1.2)$
0.1-0.0	$100.0(T_r < 1.2)$

CHAPTER VII

MODEL IMPROVEMENT BY REMOVAL OF INSIGNIFICANT PARAMETERS

In working on large models, that is models with over 30 parameters, some logical method is needed to determine if a parameter is significant to model the data. If it is not significant the result will not be as accurate as possible because information was used to determine values for this parameter which should not have been included in the regression. Statistical analysis of the variance σ_a^2, of the parameters can give the needed guides. For a single parameter the standard way to check is to test the hypothesis that the parameter is zero. This leads to the standard T-test,[4] that the parameter should be zero if the relation is satisfied

$$|a| < t_\alpha \sigma_a \tag{37}$$

where t_α is the Student's t statistic at the α level, σ_a is the standard error, which is the square root of the variance for the parameter.

For linear functions the model can be generated stepwise by only adding terms that have the highest correlation coefficient with the data. This method has been used to develop equations for oxygen and nitrogen [11]. Since this is only applicable to linear regressions, another method was developed. This method investigates the contribution that each parameter gives to the reduction of the sum of squared errors [8]. The contribution for the parameter a is approximated as

$$SSE_a = \left(\frac{a}{\sigma_a}\right)^2 \tag{38}$$

The parameters with the smallest contributions can many times be eliminated with little effect on the results. When the new parameter set is regressed with the low SSE terms set to zero, improvement over the previous regression is obtained. EZFIT outputs the variance, standard error and the SSE for each parameter allowing easy evaluation of the significance of the parameters.

This method was used to develop the equation of state for water. Using the method, it was possible to reduce the number of parameters from 48 to 43 and to improve the prediction. With the continued application of the method even more improvement would be possible. It was decided to stop at this stage because the method was sufficiently exposited. The procedure was initiated using the previously

mentioned method for getting preliminary parameters for density, that is, a density regression was performed to get the best density results for the 48 parameter version. Using these results, a multiproperty regression of density, enthalpy departure, and vapor pressure was performed to get the base equation from which to work for improvement. Average absolute deviations for properties (also referred to as errors) for this base equation were 0.66% for 382 density points, 1.04% for 53 vapor pressure points and 1.09 BTU/lbm (2.53 J/g) for 113 enthalpy departure points. This is the standard data set plotted in Figures 1, 3 and 4 which was used for the equation development.

The six least significant parameters as determined by the SSE criterion were then studied to see the effect their removal from the model would have upon the results. The details of this study are given in Table VI. As shown in Table VI, the parameters have little effect upon density with the most effect caused by parameter 59, which increased the density deviation to 1.12%. On the other hand, enthalpy departure and vapor pressure are more sensitive. The enthalpy deviation was increased to 27.9 BTU/lbm and vapor pressure deviation to 49.1% with the elimination parameter 59. It was decided to remove the three parameters with the least effect, 22, 46, and 60. This set of parameters when removed increased the errors to 0.73% for density, 2.57% for vapor pressure, and 5.12 BTU/lbm (11.9 J/g) for enthalpy departure.

TABLE VI

Effects of removing parameters by setting to zero in the 48 parameter equation

Parameters Set to Zero	Errors		
	Density(%)	Vapor pressure(1%)	Enthalpy Departure(BTU/lbm)
None	0.66	1.09	1.09
46	0.68	2.65	2.53
60	0.66	3.18	2.94
22	0.76	6.29	6.43
48	0.88	18.8	26.3
5	0.89	27.6	18.6
59	1.12	49.1	27.9
22, 46, 60	0.73	2.56	5.12

When the reduced set of 45 parameters were regressed there was improvement over the 48 parameter base equation in both density and vapor pressure and slightly less accurate results for enthalpy departure. The average absolute deviations were 0.62% for density, 0.98% for vapor pressure and 1.12 BTU/lbm (2.60 J/g) for enthalpy departure. The method was once again applied to this equation to try for further improvement and reduction in the number of parameters. The three parameters with the lowest SSE this time were 20, 26, and 5, of which only 5 had been in the previous set to be considered. When parameter 20 was removed, there was a remarkable improvement in the vapor pressure prediction; the average absolute deviation was reduced to 0.13%. Only the removal of parameter 5 caused an unacceptable error increase in the enthalpy and vapor pressure predictions. This time parameters 20 and 26 were eliminated. The details of the effects of these parameters are given in Table VII.

When the 43 parameters were regressed it was found that the enthalpy controlled the regression and the improvement in vapor pressure was lost. This was remedied by adjusting the group weights for each data type so that each group contributed about the same amount to chi-squared. This led to the final 43 parameter equation. The resultant average absolute deviations were 0.42% for density, 0.12% for vapor pressure and 1.58 BTU/lbm (3.67 J/g) for enthalpy

TABLE VII

Effects of removing parameters by setting to zero in the 45 parameter equation

Parameters Set to Zero	Errors		
	Density(%)	Vapor Pressure(%)	Enthalpy Departure(BTU/lbm)
None	0.62	0.98	1.12
20	0.67	0.13	1.87
26	0.63	1.01	1.12
5	0.72	8.20	8.31
20, 26	0.68	0.12	1.84

departure. This is a marked improvement over the 48 parameter equation for density and vapor pressure, which are the most accurate experimental data. The enthalpy departure predictions are acceptable, especially since the enthalpy departures were totally derived data and not measured.

CHAPTER VIII

SUMMARY OF METHODOLOGY AND RESULTS FOR CASE STUDY

Using the method outlined in this work, an equation of state was developed for water as a case study. The steps of the method are:

1. Collect data sets and selection of a working data set (subset).
2. Get initial parameters by a pressure regression.
3. Improve the density regression.
4. Develop a base equation by multi-property analysis.
5. Improve the model by eliminating terms.
6. Check validity of the equation by predicting more data.

This method was used to develop a 43 parameter equation of state of the form

$$Z = 1 + \sum_{i=o}^{7} \sum_{j=o}^{5} A_{ij} T^{*-i} \, yT_j(y) \qquad (39)$$

where $y = \beta\rho/4\rho_c$, $T^* = \alpha T/T_c$ and T_j is the Tchebycheff polynomial. The parameters for the equation are given in Table VIII.

Data Sets. Data from 9 references were collected as well as uniform data sets generated from the high precision equation of Keenan and Keyes. This led to a collection of 1459 density points, 263 enthalpy departure points, and 53 vapor pressure points covering the pressure range 0.089-20,305 psia (0.61-140,000 KPa) and the temperature range 491.67-2859.67°R (273.15-1588.7°K). A working data set was selected from these data points, consisting of 382 density points, 113 enthalpy points and 53 vapor pressure points.

Initial parameters and density regression. The initial values of the 48 parameters were determined by performing regression on the density data set. The data were converted to pressure departure by subtracting the ideal gas pressure and were then fit (using pressure as the objective) using the tabulated weighting function given in Table V. This let to an average absolute error in density of 1.08% for the 382 density points. A regression with the density as the objective was then performed. This led to the prediction of density with 0.50% average absolute error.

Multiproperty base equation. The density results were used to predict enthalpy departure and vapor pressure. As usually happens with equation of state parameters determined from density data alone, several of the low temperature

TABLE VIII

Values of the parameters for the 43 parameter Tchebycheff polynomial equation of state for water

Index	(I,J)	Value	Index	(I,J)	Value
1	00	0.489078	25	04	0.644619
2	10	-1.33375	27	24	2.89299
3	20	0.0447899	28	34	0.0472269
4	30	-0.0433729	29	05	-0.537426
5	40	0.026460	30	15	-0.697395
6	50	-0.189002	31	25	0.366763
7	01	4.90720	32	35	0.713576
8	11	0.294431	45	60	-0.0773029
9	21	0.439805	47	61	-0.071481
10	31	1.14694	48	71	0.00894616
11	41	0.634109	49	62	0.121502
12	51	0.0938234	50	72	0.0768117
13	02	-0.334176	51	63	-0.258435
14	12	1.48579	52	73	-0.0697795
15	22	4.77029	53	44	-0.141785
16	32	1.49032	54	54	-0.124966
17	42	1.00340	55	64	0.369510
18	52	0.217828	56	74	-0.0548949
19	03	-0.714156	57	45	0.513778
21	23	0.117546	58	55	0.538242
23	43	-0.580674	59	65	-0.127041
24	53	-0.208757			

vapor pressure points did not converge. The lowest temperature enthalpy points also had errors in excess of 5 BTU/lbm (12 J/g). For the first few iterations of the multiproperty regression, the nonconverging vapor pressure points were removed and the weight for the enthalpy points with large errors was reduced. As the results improved with increased iterations, the complete working data set was used. This resulted in the 48 parameter base equation. This equation predicted density to 0.56%, enthalpy departure to 1.09 BTU/lbm (2.53 J/g) and vapor pressure to 1.04%.

Model Improvement. The results for the base equation were improved by eliminating the least significance parameters. An estimate of each parameter's significance was determined as the contribution to the sum of squares, $SSE_j = A_j^2/\sigma_j^2$, which is the ratio of the parameter squared to its variance. This method was used to eliminate 5 parameters in two steps. This final 43 parameter equation predicted the 382 density points to 0.43%, the 113 enthalpy departure points to 1.58 BTU/lbm (3.67 J/g) and the 53 vapor pressure points to 0.12%. The 43 parameters for the equation of state are given in Table VIII.

Data predictions. This 43 parameter equation was then tested for 1775 data points. The results are summarized in Table IX, see Appendix D for complete tabulation. For the 1459 density points the average error was 0.58%. The high pressure and low temperature compressed liquid region

TABLE IX

Results for the 43 parameter equation of state for water

Reference	Number of Data Points	Pressure Range		Temperature Range	Average Absolute Deviation
DENSITY					
Working set*	382	0.66-20,305	psia	491.67-2859.67 °R	0.43%
Subsets	265	0.66-10,000	psia	491.67-2859.67 °R	0.31%
	117	10.000-20,305	psia	634.67-2459.67 °R	0.68%
Holser, Kennedy[10]	216	1450.38-20,305	psia	707.67-2291.67 °R	0.50%
Keenan, Keyes[13]	108	0.66-14694	psia	509.67-2859.67 °R	0.4 %
Kennedy[15]	401	145.038-1450.48	psia	851.67-2291.67 °R	0.31%
Keyes, Smith[16]	129	61.96-5066.71	psia	545.67-1139.67 °R	0.58%
Keyes, Smith, Gerry[17]	283	194.28-5403.28	psia	842.67-1319.67 °R	0.73%
Kell, Whalley[14]	217	76.87-14,886.5	psia	491.67-671.67 °R	1.03%
Osborne, Stimson, Ginnings[20]	60	0.089-1160.667	psia	491.67-1022.67 °R	0.36%
TOTAL	1459	0.089-20,305	psia	491.67-2859.67 °R	0.58%
ENTHALPY					
Working set					
Keenan, Keyes[13]	113	0.66-14,694	psia	509.67-2859.67 °R	1.58 BTU/lbm
Angus, Newitt[1]	16	870.2-14,503	psia	1211.67-1751.67 °R	2.90 BTU/lbm
Callendar, Egerton[5]	134	71.5-2842.	psia	851.67-1571.67 °R	1.45 BTU/lbm
TOTAL	263	0.66-14503	psia	509-67-2859.67 °R	1.59 BTU/lbm
VAPOR PRESSURE					
Osborne, Stimson, Ginnings[20]	53	0.089-3090	psia	491.67-1159.67 °R	0.12%

*Included in individual density data sets also.

have the largest errors. As shown in Table IX, the largest density error, 1.03% occurs for the liquid data of Kell and Whalley [14]. Gas densities are predicted quite accurately as shown by the data of Kennedy [15], for which the error is 0.31%. The trouble with the high pressure region is more apparent when the test data set is separated into pressures below and above 10,000 psia (69,000 KPa). For the low pressure set, the error is only 0.32%, while for the high pressure set, the error more than doubles, to 0.68%.

Predictions for the enthalpy departure set of 263 points have an average absolute error of 1.59 BTU/lbm (3.70 J/g). The prediction errors for the gas phase data of Callendar and Egerton [5] were comparable to the errors of the working set, i.e., 1.45 BTU/lbm (3.37 J/g) as compared to 1.58 BTU/lbm (3.67 J/g). The only experimental liquid and high pressure points available were the 16 points of Angus and Newitt [1]. Because of the increased errors in this region for density, it is not surprising that the prediction errors for this set has higher errors, 2.90 BTU/lbm (6.74 J/g).

The vapor pressure data were included totally in the regression. Predicted vapor pressures have an average absolute error of 0.12% from the triple point to within 0.4% of the critical pressure.

CHAPTER IX

CONCLUSIONS

The six step method outlined in this work will allow systematic development of a high precision equation of state. The method gives a logical way of handling the large number of parameters required by complex models. The success of this method was shown by its use to develop the 43 parameter equation for water. This equation was not pushed to its ultimate because of the restriction of time and expense. By using the embodiment of this method in the regression package EZFIT and the guidelines outlined herein, it is now possible for the researcher to quickly and systematically develop as complex a model as needed to represent the data to an accuracy approaching the experimental uncertainty.

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APPENDIX A

Derivation of Reduced Residual Thermodynamic Properties

From classical thermodynamics relationships are obtained for the various thermodynamic properties of a fluid. These are required to obtain the thermodynamic properties used in design from an equation of state. The basic relations for bulk properties are[1]

$$A = U - T \cdot S \tag{1-a}$$

$$H = U + P \cdot V \tag{1-b}$$

$$G = U + P \cdot V - T \cdot S \tag{1-c}$$

$$\mu_i = (\partial A / \partial n_i)_{T,V,n_j} \tag{1-d}$$

where A is the Helmholtz free energy, U the internal energy, T the absolute temperature, S the entropy, H the enthalpy, P the pressure, V the volume, and μ_i the chemical potential of a system of n moles of which there are n_i moles of the ith component.

The molar quantities are obtained by dividing by n to get the following relations in which the tilde (~) represents a molar quantity

$$\tilde{A} = \tilde{U} - T \cdot \tilde{S} \tag{2-a}$$

$$\tilde{H} = \tilde{U} + P/\rho \qquad (2\text{-b})$$

$$\tilde{G} = \tilde{U} + P/\rho - T\cdot\tilde{S} \qquad (2\text{-c})$$

$$\mu_i = (\partial\tilde{A}/n_i)_{T,V,n_j} \qquad (2\text{-d})$$

where [n_i is the number of moles of the ith component and] ρ is the molar density, $\rho=n/V$.

A modified excess property is defined as the difference between the quantity at the temperature and density of the system and the sum of the product of the mole fraction and the value of the property as an ideal gas at the temperature and unit pressure. For internal energy the modified excess property is

$$\Delta\tilde{U} = \tilde{U} - \Sigma X_i U_i^o \qquad (3)$$

in which the superscript ^{o} represents the ideal gas condition of the same temperature and unit pressure. Similarly, equations 2 become

$$\Delta\tilde{A} = \tilde{U} - T\cdot\tilde{S} - (\Sigma X_i U_i^o - T\Sigma X_i S_i^o) = \Delta\tilde{U} - T\Delta\tilde{S} \qquad (4\text{-a})$$

$$\Delta\tilde{H} = \tilde{U} + P/\rho - (\Sigma X_i U_i^o + \Sigma X_i RT) = \Delta\tilde{U} + R\cdot T(Z-1) \qquad (4\text{-b})$$

$$\Delta\tilde{G} = \tilde{U} + P/\rho - T\,\tilde{S} - (\Sigma X_i U_i^o + RT - T\Sigma X_i S_i^o)$$

$$= \Delta\tilde{U} - T\Delta\tilde{S} + RT(Z-1) \qquad (4\text{-c})$$

$$\Delta\mu = (\partial\tilde{A}/\partial n_i)_{T,V,n_j} - (U_i^o - T\cdot S_i^o) = (\partial\Delta\tilde{A}/\partial n_i)_{T,V,n_j} \qquad (4\text{-d})$$

where R is the universal gas constant and Z is the compressibility $Z = P/\rho RT$.

By defining a dimensionless temperature, $T^* = \alpha T/T_c$, where α is a scaling parameter and T_c is the critical temperature and using the universal gas constant, dimensionless properties are given as

$$A^* = \alpha\Delta\tilde{A}/RT_c \tag{5-a}$$

$$U^* = \alpha\Delta\tilde{U}/RT_c \tag{5-b}$$

$$H^* = \alpha\Delta\tilde{H}/RT_c = U^* + T^*(Z-1) \tag{5-c}$$

$$S^* = \Delta\tilde{S}/R = (U^*-A^*)/T^* \tag{5-d}$$

$$G^* = \alpha\Delta\tilde{G}/RT_c = U^* - T^* S^* + T^*(Z-1) \tag{5-e}$$

$$\mu_i^* = \alpha\Delta\mu_i/RT_c = (\partial A^*/\partial n_i)_{T,V,n_j} \tag{5-f}$$

The fugacity f, which is defined as

$$RT \ln f_i = \mu_i \tag{6}$$

then is

$$T^* \ln f_i/f_i^o = \mu_i^* \tag{7}$$

where f_i^o is the fugacity of the ith component in an ideal gas mixture at the same temperature and unit pressure.

The Helmholtz free energy is derived from a pressure explicit equation of state as[1]

$$A = \int_V^\infty (P-nRT/V)dV - RT\Sigma n_i \ln(V/n_iRT) + \Sigma n_i(U_i^o - TS_i^o) \tag{8}$$

As in equation 2-a, A is given in molar form as

$$\tilde{A} = \int_v^\infty (P-RT/v)dv - RT\Sigma X_i \ln(v/X_iRT) + \Sigma X_i(U_i^o - TS_i^o) \tag{9}$$

The modified excess form (4-a) then is

$$A^* = \alpha/RT_c \int_v^\infty (P-RT/v)dv - T^*\Sigma X_i \ln(v/X_i RT) \qquad (10)$$

By using the relationships $P = Z\rho RT$, $dv = -d\rho/\rho^2$, and $\rho^* = \beta\rho/\rho_c$, where β is a scaling factor and ρ_c is the critical density, 10 is further reduced to

$$A^* = \alpha/RT_c \int_\rho^o (Z\rho RT-\rho RT)(-d\rho/\rho^2) + T^*\Sigma X_i \ln(X_i\rho RT)$$

$$= T^* \{\int_o^{\rho^*} (Z-1)d \ln \rho^* + \Sigma X_i \ln X_i\rho^* T^* + \ln(R\rho_c T_c/\beta\alpha)\} \qquad (11)$$

In a similar fashion, the internal energy is given as

$$U = \int_v^\infty (P-T(\partial P/\partial T)_{V,n})dV + \Sigma n_i U_i^o \qquad (12\text{-a})$$

$$U^* = \alpha/RT_c \int_v^\infty (P-T(\partial P/\partial T)_{V,n})dv \qquad (12\text{-b})$$

$$U^* = \alpha/RT_c \int_\rho^o (Z\rho RT - \rho RT(Z+T\partial Z/\partial T))(-d\rho/\rho^2)$$

$$= -T^{*2} \int_o^{\rho^*} \partial Z/\partial T^* \; d \ln\rho^* \qquad (12\text{-c})$$

By defining the following terms

$$FI_1 = \int_o^{\rho^*} (z-1) \; d \ln\rho^* \qquad (13\text{-a})$$

$$FI_2 = \int_o^{\rho^*} \partial Z/\partial T^* \; d \ln\rho^* \qquad (13\text{-b})$$

$$FI_3 = \Sigma X_i \ln(X_i\rho^* T^*) + \ln(R\rho_c T_c/\beta\alpha) \qquad (13\text{-c})$$

and using the previous results the thermodynamic properties are given from an equation of state as

$$A^* = T^* FI_1 + T^* FI_3 \tag{14-a}$$

$$U^* = -T^{*2} FI_2 \tag{14-b}$$

$$H^* = -T^{*2} FI_2 + T^*(Z-1) \tag{14-c}$$

$$S^* = -FI_1 + T^* FI_2 - FI_3 \tag{14-d}$$

$$G^* = T^* FI_1 + T^* FI_3 + T^*(Z-1) \tag{14-e}$$

$$\ln f_i/f_i^o = 1/T^*(\partial A^*/\partial X_i)_{T,V,X_j} \tag{14-f}$$

For a pure fluid the fugacity reduces to

$$\ln f_i/f_i^o = FI_3 + FI_1 + Z-1 \tag{15}$$

[1]Prausnitz, J.M., "Molecular Thermodynamics of Fluid-phase Equilibria", Prentice-Hall, Englewood Cliffs, New Jersey, 1969.

APPENDIX B

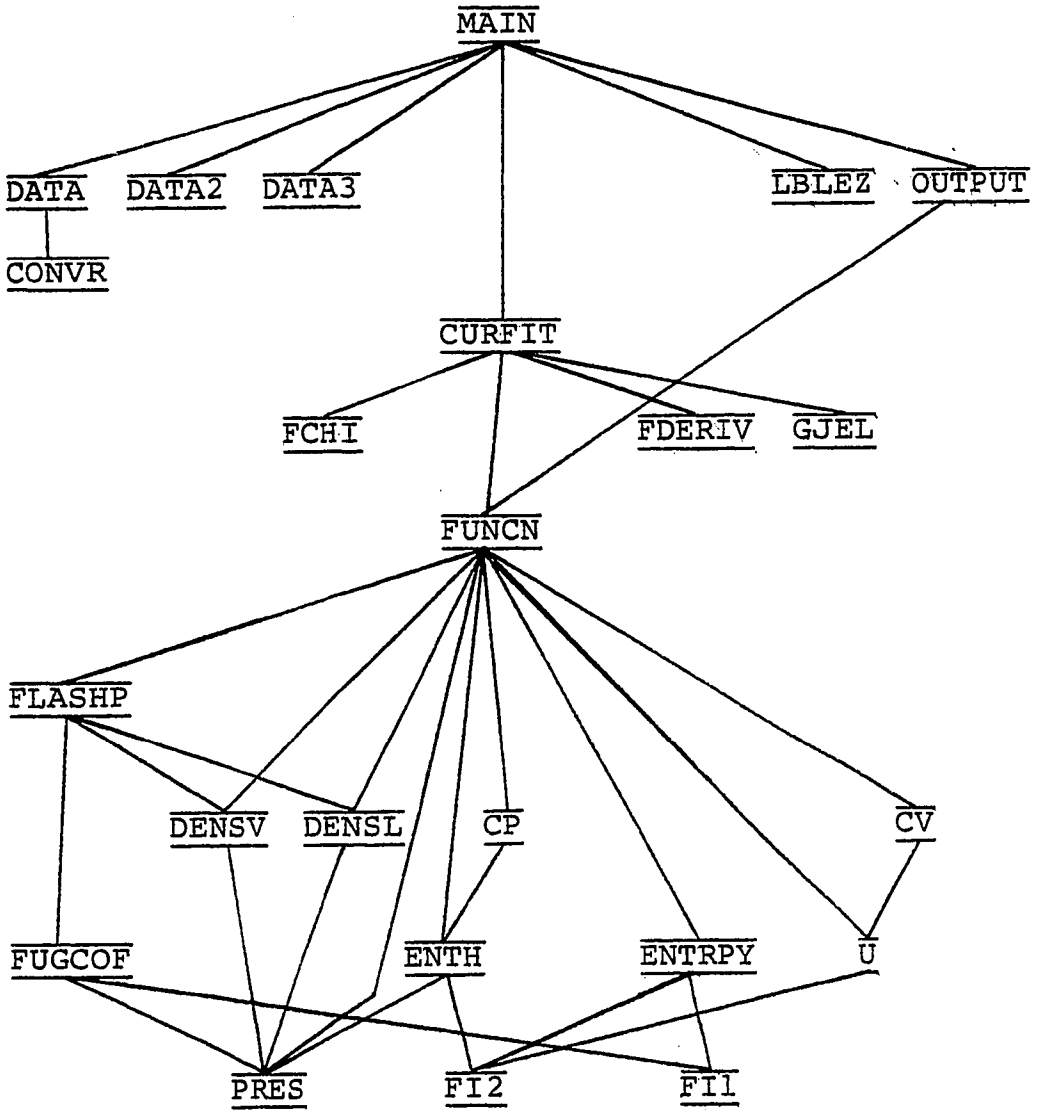
EZFIT USERS GUIDE

EZFIT is a flexible nonlinear regression program designed specifically for equation of state development. By its nature, though, it is easily adapted for any nonlinear regression. Two methods for regression are available by appropriate selection of control variables, the simpler Gauss-Newton and the Marquart[1]. EZFIT features the selection of three data input routines that can be tailored to various formats, as standard, the ability to pass 40 parameters and fit 30 and to use any combination of independent variables and data points so long as their product is less than 3000 (such as 10 independent variables and 300 data points). Specific parameters from the maximum of 40 can be selected for regression in any order while the rest are fixed. The program can also do successive regressions with adding a term to the result of the previous regression.

The following sections explain in detail the method of EZFIT. Figure 1 shows the overall organization of the program subroutines. The first section explains the details

[1]Bevington, Phillip R., "Data Reduction and Error Analysis for the Physical Sciences", McGraw-Hill, New York, 1969.

Program Organization



of the main program. The second section describes the common blocks used to pass property and control information among the routines. The third section gives detailed descriptions of the subroutines. The fourth sections tells how to adapt EZFIT to fit any function. The last section gives a listing of the FORTRAN source. In these descriptions, card input is detailed as which columns the numbers are in,y i.e., cc $1\text{-}5_y$, etc. If the variable inputed is an integer as noted by its first letter being I-N, the value is right justified with no periods. Other variables are real numbers and must include periods. In describing the algorithms the level of logic is shown by indentations with the major sections being at the first level.

EZFIT MAIN PROGRAM

The EZFIT main program controls the calculations to be performed. Through the input of 22 control cards the various calculation options of Gauss-Newton, Marquart and linear regression can be selected. The control selects the input method for data points, selection of parameters to be used in the regression, and initial values of the parameters. The main program controls convergence and of the algorithms and checks time limits. Details of the various options of the control cards are given in the following section. The algorithm used is in the succeeding section.

Control Cards for EZFIT

Card Control Functions and Format

1 cc. 1-5; IOUT; Program code control selects various calculations performed as given below:
- 1 Full regression, echo print of input data as received from data input routines, for each iteration a table of Y, Y_{calc}, and % error, regression summary statistics, output tables of calculated properties and correlation coefficients.
- 3 The echo print is omitted from the features of type 1.
- 4 Correlation coefficients is omitted.
- 5 Full regression, regression summary statistics, output tables of calculations.
- 8 Same as 9 but with table of correlation coefficients added.
- 9 Calculation of statistics with no parameter update for regression summary statistics, output tables of calculations.
- 10 No regression, output tables of results.

2 cc. 1-5; idata; Selection of data input routines as:
- 1 DATA; Compound cards, then preBANKED data.
- 2 DATA2; Blocked, BWR original data format.
- 3 DATA3; Blocked form of data in BANKED format.

3 cc. 1-10; DFLMDA: Selection of regression method as:
- .001 Marquart
- 0.00 Gauss-Newton
- <0 Linear regression

4 cc. 1-10; TMAS; Maximum time allowed for regression without the time for calculation of the output tables. It is used to end the regression nearly when convergence is not possible in the time allotted for the job.

5 cc. 1-5; ISTATE(3); Parameter constraint mode for allowance of sign change as:
- 0 Unconstrained
- 1 Constrained against sign changes

cc. 6-10; ISTATE(5); Selection of derivative calculation mode:
- 0 Numeric derivative with precision test
- 1 Numeric derivative with delta of .01 of parameter.

6 cc. 1-5; ISTATE(4); Selection of error message mode:
0 Full messages
5 Minimum of error messages

7 cc. 1-5; NUMB; Dummy passed to calculation routines for their use.

8 cc. 1-5; NFPARM; Number of parameters not entering to regression but passed to the calculation routines.
cc. 6-10; FPARM; Initial number of parameters to be fitted in a series of regressions.

9 cc. 1-5; NNTERM: dummy

10 cc. 1-5; NU1FR; Initial number of parameters to be fitted in a series of regressions.
cc. 6-10; NU1TO; Final number of parameters to be fitted.

11-13 16I5; ITERM(40); Parameter numbers in order to be fitted. As standard 40 may be supplied but no more than 30 can be fitted.

14-18 8F10.0; A1(40); Initial values of parameters in ascending order form parameter 1.

19 cc. 1-5; NCODE: Weighting mode selected as
1 Weights supplied by data input routine.
0 Equal weights
-1 Weight as $1/y_{exp}$

20 cc. 1-10; RGAS; Universal gas constant used to select equation units.

21 cc. 1-5; N; Maximum number of independent variables per data point. (not used in module GOINE as restricted to 3 variables).

22 cc. 1-5; NPTS; Number of data points.

23 Control cards as specified by the selected data input routine

COMPOUND CODE CARD

Short Form

1 cc. 1-8; Eight character acronym for compound.
cc. 9-10; Two digit compound code.
cc. 11-20; TCRIT; critical temperature in Rankine.
cc. 21-20; PCRIT; critical pressure in psia.
cc. 31-40; RHOC; critical density in $lbmole/ft^3$.
cc. 41-50; XMW; molecular weight.
cc. 51-60; W; Pitzer acentric factor.
cc. 61-70; ALPHA; reduced temperature scaling factor.
cc. 71-80; BETA; reduced density scaling factor.

Common Block Definitions

Common Block PRM

```
Common/PRM/RGAS,RENRGY,TCRIT,PCRIT,RHOC,W,ALPHA,BETA,XMW,
1   A(40),B(7),NTERMS,NPARM,NUMB,RTOP,RMIDL,RMIDV
```

Common block, PRM, properties management, contains the control variables, scaling parameters, and other things needed by the physical properties package. It contains the parameters for the equation of state. The variables and their usage are:

RGAS	The universal gas constant used to determine the pressure units used by the system.
RENRGY	The universal gas constant used to determine the energy units used by the system.
TCRIT	The critical temperature in consistent absolute units.
PCRIT	The critical pressure in consistent units.
RHOC	The critical density in consistent units.
W	Pitzer acentric factor.
ALPHA	Reduced temperature scaling parameter, $T^* =$ ALPHA*T/TCRIT
BETA	Reduced density scaling parameter, $RHO^* =$ BETA*RHO/RHOC
XMW	The molecular weight.
A(40)	Parameters for the equation of state.
B(7)	Parameters for the ideal gas function.
NTERMS	Used by some equations; defined as parameters fitted minus NNTERM, see control variable definitions.
NPARM	The number of parameters in the equation of state.

NUMB	Used in do-loop control in some equations.
RTOP	The maximum liquid density allowed in DENSL.
RMIDL	The minimum liquid density allowed in DENSL.
RMIDV	The maximum vapor density allowed in DENSV.

Algorithm for MAIN Program

1. Initialization
    1. Set CPU clock
    2. Zero ICOMP, ISTATE
2. Data Input
    1. Input control variables: IOUT,IDATA,DFLAMDA,EPS,TMAX, ISTATE(3,4&5),NUMB,NFPARM,FPARM,NTERM, NUIFR, NUITO, ITERM,A1,NCODE,RGAS, N, NPTS
    2. Print summary of program status
    3. Input data points
        1. If IDATA=1, Call DATA
        2. If IDATA=2, Call DATA2
        3. If IDATA=3, Call DATA3
    4. Echo data points if desired.
       If IOUT<3, Print DATAID and X
3. Initialize regression: IPRES=0, NPART=1, CHI=1
4. Do series of regressions
   For NU1=NU1FR to NU1TO
    1. Initialize;
       NTERMS=NU1-NNTERM
       NPARM=NU1+NFPARM
       DF=NPTS-NU1
       CHI=10^{60}
    2. Store parameters; STORE(LL)=A1(LL)
    3. Check for output only
        1. If IOUT<10 Go to 4.4
        2. Move parameters to COMMON; $A=A1_{1=40}$, $AXTN=A1_{41-100}$
        3. Go to 1110
    4. Initialize for regression
        1. FLAMDA=DFLAMDA
        2. STORE(1)=CHI
        3. STORE(1+L)=A1(L)

5. Perform regression iterations
   For I=1 to 20
   1. Do one iteration; Call CURFIT

   2. Calculate and output relative change in parameters; STORED(L)= (STORED(L+1)-A1(L))/A1(L)

   3. Calculate and output length of change as SSQ= Σ(STORED(L+1)-A1(L))^2

   4. If first iterations store variances; STORE(1+NPARM+L)= SIGMAA(L)

   5. Evaluate results of iteration
      1. If chi-squared increased, CHI<CHISQR, Print message and go to 4.6.

      2. If change less than EPS, Print convergence message and go to 7.6.

      3. If no improvement on initial values of parameters, i.e. FLAMDA>100 and CHI>10^{50}, Print message and go to 8.

      4. Output results at valid improvement
         1. Print new parameters A1, new chi-squared CHI, and variances SIGMAA(1).

         2. Store new parameters and variances; STORE(1)=CHI, STORE(1+L)=A1(L), STORE(1+NPARM+L)=SIGMAA(L)

      5. Check for exceeding time limit,
         1. Call CPUTIM(TIME,ST2) and print elasped time, ST2.

         2. If no regression to be made, ISTATE(2)>5, print message and go to 4.6.

         3. If time limits exceeded print message and go to 4.6.

   6. Output results
      1. Retrieve parameters and variances from STORE.

      2. Output tabled parameter index, ITERM(J), parameter, A1, standard error, SE= SIGMAA*CHISQR, variance, SIGMAA, and contributions to chi-squared, ASE=(A1/SE)^2.

3. Print statistics: CHISQR,chi-squared; DF,degrees of freedom; FR, F-statistic for correlation, FCH1, F-statistic for adding term to regression.

4. Store unreduced chi-squared for next FCH1, CHI1=CHIN

5. Output results for points; call OUTPUT

5. Stop program with regression series complete.

Common Block DAT

```
COMMON/DAT/IPRES,ISTATE(20)
```

Common block DAT, control data, contains status and control variables for both the curvefitting and physical properties package. The variables and their usage are:

IPRES	The number of times the pressure routine, PRES, has been called.
ISTATE(1)	Number of the data point being evaluated.
ISTATE(2)	Calculation mode control.
ISTATE(3)	Parameter constraint control.
ISTATE(4)	Error message control.
ISTATE(5)	Derivative precision control.
ISTATE(6)	Program control bits.
ISTATE(7)	Program status bits.
ISTATE(8)	Subroutine status bits.
ISTATE(9)	Derivative status indicator.
ISTATE(10-20)	are not presently used.

Common Block PRP

```
COMMON/PRP/ICOMP(20),CPC(20),CRC(20)CMW(20),CW(20),CTC(20),
1    CA(20),CB(20),CNAME(20,2)
```

Common block PRP, properties package, contains identification codes, names, and physical properties for twenty substances used by the calculation routines. The variables and their usage are:

ICOMP(20)	The BANKED compound identification code.
CPC(20)	The critical pressure for the compound in consistent units.
CRC(20)	The critical density in consistent units.
CMW(20)	The molecular weight.
CW(20)	The Pitzer acentric factor.
CTC(20)	The critical temperature in consistent units.
CA(20)	The reduced temperature scaling parameter.
CB(20)	The reduced density scaling parameter.
CNAME(20,2)	An eight character compound acronym.

Documentation of Subroutines

Subroutine CONVR

1. Hierarchy: Called by: DATA
   Calls: -

2. Functional Description:

This subroutine converts a positive integer INUM, less than 9999 into its EBCDIC representation and returns it in a real, CHAR, and an integer, ICHAR, variable.

3. Variables:

   a. Input:

      1. Argument: INUM,

   b. Output:

      1. Arguments: ICHAR, CHAR.

   c. Intermediate:

      1. IFACT power of 256 place keeper.

      2. I10 working variable.

      3. I, working variable.

      4. J, do-loop parameter.

      5. IDUM, DUM equivalenced variable for changing type specification.

4. Algorithm:

   1. Initialize: ICHAR = 0, IFACT = 1,

   2. Transfer number to working area, I = INUM

   3. For J = 1 to 4

      1. Isolate character, multiply by place value and add to character variable:

```
I10 =I/10
ICHAR = (I-I10*10+240)*IFACT+ICHAR
```

      2. Prepare for next digit:

```
I = I10
```

3. Prepare next place value: IFACT = IFACT*256.

4. Move bit pattern to real variable:

   1. IDUM=ICHAR

   2. CHAR=DUM

Subroutine CP

1. Hierarchy: Called By: FUNCN
   Calls: ENTH

2. Functional Description:

This subroutine calculates the specific heat at constant pressure C_p by numerical derivative of the enthalpy as

$$C_p = (\partial H/\partial T)_p$$

The method of finite differences is used with the interval adjusted to obtain the precision desired by an internal testing algorithm.

3. Variables:

   a. Input:

      1. Arguments:

         T, absolute temperature.
         RHO, density.

   b. Output:

      1. CP, the calculated specific heat.

   c. Intermediate:

      1. The same as FDERIV.

4. Algorithm:

The algorithm is the same as that used in FDERIV with the appearances of FUNCN replaced by ENTH.

Subroutine CV

1. Hierarchy: Called By: FUNCN
   Calls: U

2. Functional Description:

This subroutine calculates the specific heat at constant volume, C_v, by numerical derivative of the internal energy as

$$C_v = (\partial U/\partial T)_v$$

The method of finite differences is used with the interval adjusted to obtain the precision desired by an internal testing algorithm.

3. Variables:

   a. Input:

      1. Arguments:

         T, absolute temperature.
         RHO, density.

   b. Output:

      1. CV, the calculated specific heat.

   c. Intermediate:

      1. The same as FDERIV.

4. Algorithm:

The algorithm is the same as that used in FDERIV with the appearances of FUNCN replaced by U.

Subroutine DATA

1. Hierarchy: Called By: MAIN
   Calls: -

2. Functional Description:

This subroutine inputs data in pre-BANKED format, generates weights, mean and variance. It may be custom programmed to fit the users needs.

3. Variables:

   a. Input:

      1. Arguments:

         N, number of independent variables.
         NPTS, number of data points to be read.
         NCODE, code for weighting method

      2. Card Input:
         Card 1; NCOMP, number of components.
         Card 2-NCOMP+1; NCOMP physical properties cards
                BANKED short form: CNAME, IWHOLE, CTC,
                CPC, CRC, CMW, CW, CA, CB
         Cards NCOMP+2-; NPTS cards in pre-BANKED format.
                CONTROL, T,P,Y,DATAID(2X,4F10.0,26X,3A4)

   b. Output:

      1. Arguments:

         X,array of independent variables for data points
         Y, dependent variables for data points
         WEIGHT, weights for data points
         YBAR, mean of Y's
         YVAR, variance of Y's
         NPTRHO, number of density data points
         NPTH, number of enthalpy departure data points
         NPTVP, number of vapor pressure points
         DATAID, array of data identifications for points

      2. COMMON/PRP/ICOMP(20),. . . CNAME(20,2)

   c. Intermediate

      1. I,J,L, do-loop parameters

      2. SUM, accumulator for weighted mean

      3. SUMW, sum of the weights

4. SUMY, accumulator for the variances

5. IFRACT, fraction portion of control variable

4. Algorithm:

1. Initialize counters to 0; NPTRHO, NPTH, NPTVP=0

2. Input and echo print NCOMP

3. Input physical property cards;
For L=1 to NCOMP;
1. Read the Lth CNAME,ICOMP,CTC,CPC,CRC,CMW,CW, CA,CB

4. Input data cards;
For I=1 to NPTS

5. 1. Read the Ith X's, Y, and DATAID

2. Prepare weight; WEIGHT(I)=Y(I)

3. Separate control variables;
IWHOLE=|X(I,1)|+.005
IFRACT=|X(I,1)-IWHOLE+.005|*100

4. Calculate subtotal for data types;
If IFRACT=0, NPTRHO=NPTRHO+1
If IFRACT=10, NPTH=NPTH+1
If IFRACT=20, NPTVP=NPTVP+1

6. Initialize accumulators for mean and variance;
SUM=0, SUMW=0

7. For I=1 to NPTS

1. Evaluate weights;
1. If NCODE<0, and Y≠0, WEIGHT(I)=1/|Y(I)|

2. If NCODE<0, and Y(I)=0, WEIGHT(I)=1

3. If NCODE=0, WEIGHT(I)=1

4. If NCODE>0, WEIGHT(I)=1/WEIGHT(I)**2

2. Accumulate sum of weights and weighted Y's;
SUM=SUM+WEIGHT(I)*Y(I)
SUMW=SUMW+WEIGHT(I)

8. Calculate weighted mean;
   SUM=SUM/SUMW; YBAR=SUM

9. Calculate weighted variance;

   1. Initialize accumulator; SUMY=0

   2. For I=1 to NPTS,
      SUMY=SUMY+WEIGHT(I)*(Y(I)-SUM)**2

   3. YVAR=SUMY*NPTS/(SUMW*(NPTS-1))

Subroutine DATA2

1. Hierarchy: Called By: MAIN
   Calls: CONVR

2. Functional Description:

This subroutine inputs data in the pre-BANKED and original Han format, generates weights, data point identification, and means and variance. It may be custom programmed to fit the users needs.

3. Variables:

a. Input:

1. Arguments:

N, number of independent variables.
NPTS, number of data points to be read
NCODE, code for weighting method

2. Card input
Card 1; NCOMP number of data blocks
Card 2; Physical properties in BANKED short form
CNAME, IWHOLE, CTC, CPC, CRC, CMW, CW, CA, CB
Card 3; Data block control: NPTHRL- number of density points, NPTHL-number of enthalpy points, NPTVPL-number of vapor pressure points, NPTA-total number of points pre-BANKED format. SCALE-weight for group.
Card 4- a: NPTA cards in pre-BANKED format. Control, T,P,Y,DATAID (2X,4F10.0,26X,3A4)
b: NPTRHL cards in Han density format (T,P,ρ,CODE-3F10.0,20X,I5)
c: NPTHL cards in Han enthalpy format (T,P,ΔH,CODE-3F10.0,20X,I5)
d: NPTVPL cards in Han vapor pressure format (T,P-F5.0,F10.0)
Repeat from Card 2 NCOMP times.

b. Output:

1. Arguments:

X, array of independent variables for data points
Y, dependent variables for data points
WEIGHT, weights for data points
YBAR, mean of Y's.
YVAR, variance of Y's
NPTRHO, number of density data points
NPTH, number of enthalpy departure data points
NPTVP, number of vapor pressure points
DATAID, array of data identifications for points

2. COMMON/PRP/ICOMP(20). . . CNAME(20,2)

c. Intermediate

1. COMMON/PRM/RHOC
2. I, do-loop and index parameter
3. J, L, JA, do-loop parameters
4. P, inputed pressure
5. T, inputed temperature
6. D1, D2, Characters for identification code
7. SUM, accumulator for weighted mean
8. CODE, inputed phase code
9. NPTL, number of points read in previous groups.
10. SUMW, sum of the weights
11. SUMY, accumulator for the variances
12. IFRACT, fraction portion of control variable
13. IWHOLE, whole portion of control variable

4. Algorithm

1. Initialize counters to 0; NPTL, NPTRHO, NPTH, NPTVP=0
2. Input and echo print NCOMP
3. Input blocks of data;

For L=1 to NCOMP

1. Read Lth physical property card into COMMON/PRP/
2. Read number of each type of data; NPTRHL, NPTHL, NPTVPL, NPTA, SCALE
3. Calculate group weight;
   If SCALE=0, SCALE=1.
   SCALE=SQRT(SCALE)
4. Read in any data in pre-BANKED form;
   1. If NPTA=0 go to 3.5
   2. For JA=1 to NPTA
      1. Read Ith data point; I=JA+NPTL
      2. Calculate WEIGHT=Y/SCALE

```
      3.  Calculate subtotal for data types;
          IWHOLE=|X(I,1)|+.005
          IFRACT=|X(I,1)-IWHOLE+.005|*100
          If IFRACT=0 NPTRHO=NPTRHO+1
          If IFRACT=10, NPTH=NPTVP+1
          If IFRACT+20, NPTVP=NPTVP+1
   3. Update index offset; NPTL=NPTL+NPTA

5. Read in any density data;

   1. If NPTRHL=0, go to 3.6

   2. For J=1 to NPTRHL
      1. Read the Ith data point; I=J+NPTL
         DATAID(I,1)=D1, DATAID(I,2)=D2
      2. Convert to pre-BANKED form;
         T=T+460, CODE=-1
         If RHO<RHOC, CODE=1
         If CODE<0 X(I,1)=-IWHOLE
         If CODE<0, X(I,1)=IWHOLE
         X(I,3)=P, X(I,2)=T, Y(I)=RHO
      3. Prepare weight; WEIGHT=Y(I)/SCALE

   3. Update counters;
      NPTRHO=NPTL+NPTRHL

6. Read in any enthalpy departure data;

   1. If NPTHL=0, go to 3.7

   2. For J=1 to NPTHL
      1. Read the Ith data point; I=J+NPTL
         DATAID(I,1)=D1, DATAID(I,2)=D2
      2. Convert to pre-BANKED form;
         T=T+460,
         If CODE<0, X(I,1)=-(IWHOLE+.10)
         If CODE>0, X(I,1)=IWHOLE=.10
         X(I,2)=T, X(I,3)=P, Y(I)=DELH
      3. Prepare weight; WEIGHT=Y(I)/SCALE

   3. Update counters;
      NPTH=NPTH+NPTHL
      NPTL=NPTL+NPTHL

7. Read in any vapor pressure data;

   1. If NPTVPL=0, go to 3.8

   2. For J=1 to NPTVPL
      1. Read the Ith data point; I=J+NPTL
         DATAID(I,1)=D1, DATAID(I,2)=D2
      2. Convert to pre-BANKED form;
         T=T+460;X(I,1)=IWHOLE+.2; X(I,2)=T;
         X(I,3)=P; Y(I)=P
```

3. Prepare weight; WEIGHT=Y(I)/SCALE

3. Update counters;
NPTVP=NPTVP+NPTVPL
NPTV=NPTL+NPTVPL

8. Continue read loop

4. Initialize accumulators for mean and variance;
SUM=0, SUMW=0

5. For I=1 to NPTS

1. Make character id number for data in Han's format;
If DATAID(I,1)=D1 and DATA(I,2)=D2, Call
CONVR(I,ICHAR,DATAID(I,3)

2. Evaluate weights;

1. If NCODE<0, and Y(I)≠0, WEIGHT(I)=1/|Y(I)|

2. If NCODE<0, and Y(I)=0, WEIGHT(I)=1.

3. If NCODE=0, WEIGHT(I)=1

4. If NCODE>0, WEIGHT(I)=1/WEIGHT(I)**2

3. Accumulate sum of weights and weighted Y's;
SUM=SUM+WEIGHT(I)*Y(I)
SUMW=SUMW+WEIGHT(I)

6. Calculate weighted mean;
SUM=SUM/SUMW; YBAR=SUM

7. Calculate weighted variance;

1. Initialize accumulator; SUMY=0

2. For I=1 to NPTS,
SUMY=SUMY+WEIGHT(I)*(Y(I)-SUM)**2

3. YVAR=SUMY*NPTS/(SUMW*(NPTS-1))

Subroutine DATA3

1. Hierarchy: Called By: MAIN

2. Functional Description:

This subroutine inputs data in the BANKED format in blocks with individual group weights from the specified input unit. It generates individual point weights, and the mean and variance for the data set.

3. Variables:

a. Input:

1. Arguments:

N, number of independent variables.
NPTS, number of data points to be read
NCODE, code for weighting method
ND, dimension for DATAID, ND=3

2. Card input:
Card 1; NBLKS, number of data blocks
Card 2; Physical properties in BANKED short form, CNAME,IWHOLE,CTC,CPC,CRC,CMW,CW,CA,CB
Card 3; Data block control:
IFILE, unit number from which data is read
NPTA, number of points in data block
SCALE, weight for group
Card 4-; Data cards in BANKED format, X, Y, ICONT, DATAID
Repeat from Card 2 to Card 4 NBLKS times.

b. Output:

1. Arguments

X, array of independent variables for data points
Y, dependent variables for data points
WEIGHT, weights for data points
YBAR, mean of Y's
YVAR, variance of Y's
DATAID, array of data identifications for points

2. COMMON/PRP/ICOMP(20), . . . CNAME(20,2)

c. Intermediate:

1. I,JBLK,J,K,JJ,JL,JS,JJJ, do-loop parameters

2. NPTL, number of points read in previous groups.

3. SUM, accumulator for weighted mean

4. SUMW, accumulator for the weights

5. SUMY, accumulator for the variances

4. Algorithm:

1. Initialize counters and control;
NPTL=0, ICOMP(1)=0, L=1

2. Input NBLKS

3. Input blocks of data:

For JBLK=1 to NBLKS
1. Read the Lth CNAME,IWHOLE,CTC,CPC,CRC,CMW,CW,CA,CB

2. Check if properties for compound have already been read:
1. L1=L-1

3. For JL=1 to L1
1. Check if IWHOLE is already present
If ICOMP(JL)=IWHOLE go to 4.4

4. IWHOLE is not present so include in PRP
1. ICOMP(L)=IWHOLE
L=L+1

5. Check to see if there is free space in PRP
If L>20, print no more room.
ICOMP(L)=0

4. Read data control card; IFILE, NPTA, SCALE

5. Prepare group weights; IWT=0
1. If SCALE>0, go to 3.4.1.2
1. Else, Set code for equal weights for points in group;
IWT=1,
SCALE= |SCALE|
2. If SCALE=0, SCALE=1
3. SCALE=1/SCALE

6. Input cards in BANKED format
For L=1 to NPTA

1. Set storage index; I=NPTL+L

2. Read lead card from unit IFILE, if end of file go to 5; X(I,1),X(I,2),X(I,3),Y(I),ICONT,DATAID

3. Prepare to read following card for point;
   JL=3,
   If ICONT=0, go to 3.5.5, no more cards.

4. Read rest of cards for point:
   For JJ=1 to ICONT
   1. Set indices for X's;
      JS=JL+1
      JL=JS+5
      If JL>N, JL=N
   2. Read X(I,JS) to X(I,JL) from unit IFILE.

5. Check for all X's filled as read:
   1. If JL=N, go to 3.5.6
   2. Fill X(I,JL+1) to X(I,N) with 0.

6. Prepare weight for point:
   1. WEIGHT(I)=1
   2. If Y(I)≠0, WEIGHT(I)
   3. WEIGHT(I)=WEIGHT(I)/SCALE
   4. If IWT=1, WEIGHT(I)=1/SCALE

7. Update offset for indices;
   NPTL=NPTL+NPTA

5. Update Number of points, NPTS=NPTL, and go to 6.

6. Print end of file error message and stop.

7. Initialize accumulators for mean and variance:
   SUM=0, SUMW=0

8. For I=1 to NPTS

   1. Evaluate weights;
      1. If NCODE<0, and Y≠0, WEIGHT(I)=1/|Y(I)|
      2. If NCODE<0, and Y(I)=0, WEIGHT(I)=1
      3. If NCODE=0, WEIGHT(I)=1
      4. If NCODE>0, WEIGHT(I)=1/WEIGHT(I)**2

   2. Accumulate sum of weights and weighted Y's;
      SUM=SUM+WEIGHT(I)*Y(I)
      SUMW=SUMW+WEIGHT(I)

9. Calculate weighted mean;
   SUM=SUM/SUMW; YBAR=SUM

10. Calculate weighted variance:

   1. Initialize accumulator; SUMY=0
   2. For I=1 to NPTS;
      SUMY=SUMY+WEIGHT(I)*(Y(I)-SUM)**2
   3. YVAR=SUMY*NPTS/(SUMW*(NPTS-1))

Subroutine DENSL

1. Hierarchy: Called By: FUNCN, FLASHP
   Calls: PRES

2. Functional Description:

This subroutine finds the density root of equations of state in the region between the critical density and four times it, i.e. the liquid density. It does this by a combined method of false position and successive bisections. It uses the ideal gas value as the initial approximation and has several safe guards to secure the selection of the correct root.

3. Variables:

   a. Input:

      1. Arguments:

         T, absolute temperature
         P, pressure

      2. COMMON/PRM/RGAS, TCRIT, RMIDL, RTOP

      3. COMMON/DAT/ISTATE(4), ISTATE(9)

   b. Output:

      1. Argument:

         DENSL, liquid density root

   c. Intermediate:

      1. IT, ITMAX, iteration parameters

      2. PO, local storage for P

      3. P1, P2, P3, intermediate pressures used in the search

      4. DEL, search interval

      5. CODE, status variable

      6. EPSP, tolerance in pressure, 10^{-5}

      7. EPSR, tolerance in density, 10^{-5}

      8. PMIN, minimum pressure in secondary search.

9. RHOMIN, density corresponding to PMIN

10. RHO1, RHO2, RHO3, intermediate densities used in search.

11. SRHO, SP, results of previous calculation used for start when called from FDERIV

4. Algorithm:

a. Basis;

The density is found by a false position search. If this fails by not meeting convergence criteria or the root having a negative derivative, a search from RTOP is made down to RMIDL by step DEL until the root is bounded. When it is bounded successive bisection is performed until the convergence criteria are satisfied. If the root was unable to be bounded the density corresponding to the minimum pressure is used. If the routine is called from FDERIV the results from the previous calculation are used for the initial locations saving some time in that they were for the same T and P conditions.

b. Procedure:

1. Initialize:
ITMAX=20, set maximum iterations for false position
PO=P, move P to local storage
PMIN=10^{60}, initialize minimum search pressure.
CODE=0, initialize minimum search pointer.
DEL=RTOP/20, delta as twentieth of top bound
IT=1, start counter

2. Check if T is so small that false position will be skipped
If T/TCRIT<.4 go to 7

3. Check if in derivative routine and if so use last result to start;
If ISTATE(9)≠0, RHO1=RHO2

4. Set up initial values for false position;
RHO2=1.01*RHO1
P1=PRES(T,RHO1)-PO
P2=PRES(T,RHO2)-PO

```
5.  Start false position iteration:
    1. Check for convergence;
       If |P1-P2|<EPSP*PO or |RHO1-RHO2|<|RHO2|*EPSR
       go to 6
    2. Check if exceeded
    2. Check if exceeded 20 iterations;
       If IT>ITMAX, go to 7

    3. Project by false position;
       RHO3=(RHO1*P2-RHO2*P1)/(P2-P1)

    4. If RHO3 is out of bounds randomize start
       1.  If RHO3>RTOP or RHO3<RMIDL, RHO3=RTOP*(50+IT)/50

       2.  Select pair with positive slope to continue
           1.  If RHO1<RHO2 and P1>P2 go to 5.5
           2.  Make start:
               RHO2=RHO1
               RHO1=RHO3
               P2=P1
               IT=IT+1
               P1=PRES(T,RHO1)-PO
               go to 5.1

    5. Update for next iteration
       RHO1=RHO2
       RHO2=RHO3
       P1=P2
       P2=PRES(T,RHO2)-PO

    6. Go to 5.1

6.  Check for positive slope for correct root;
    RHO1=.99*RHO2
    P1=PRES(T,RHO1)-PO
    If RHO2<RMIDL it is out of range, go to 7
    If P1<P2, go to 11.

7.  Initialize for search to bound root;
    ITMAX = 40
    RHO1=RTOP
    P1=PRES(T,RHO1)

8.  Check for root outside top bound;
    1. If P1>PO, go to 9

    2. Check if error messages desired;
       If ISTATE(4) 5, print Root too large.

    3. Select root as bound;
       RHO2=RHO1
```

4. If not in FDERIV return;
   If ISTATE(9)=0, go to 11

5. Modify bound root so that derivative will have correct sign;
   1. P1=PRES(T,RHO2)
   2. If P1<PS, go to 8.5.3
      1. Else, RHO2=RHO2-DEL, go to 11.
   3. RHO2=RHO2+DEL, go to 11.

9. Begin search for bound;

   1. P1=PRES(T,RHO1)

   2. Check for bounded root;
      If P1<P0, go to 10

   3. Check for first minimum;
      If P2<PMIN and CODE=0, go to 9.8

   4. First minimum found; CODE=1

   5. Update iteration values;
      RHO2=RHO1
      P2=P1

   6. Check for reaching left bound;
      If RHO1<RMIDL go to 9.9

   7. Continue search;
      RHO1=RHO1-DEL
      Go to 9.1

   8. Update minimum with lower values;
      PMIN=P1
      RHOMIN=RHO1
      Go to 9.5

   9. Since out of bounds use minimum;
      1. Check if error messages desired;
         If ISTATE(4)<5, print minimum used

      2. RHO2-RHOMIN

      3. Go to 11.

   10. Begin successive bisections
      1. Calculate values at interval center;
         RHO3=(RHO1+RHO2)/2
         P3=PRES(T,RHO3)

2. Check for convergence;
   If |P1-P2|<EPSP*PO or |RHO1-RHO2|<|RHO2|*EPSR,
   go to 11.

3. Check number of iterations;
   IT=IT+1
   If IT>ITMAX, go to 10.5

4. Find interval containing root;
   1. If P3>PO, go to 10.4.3

   2. Between top and middle;
      RHO1=RHO3
      P1=P3
      Go to 10.1

   3. Between bottom and middle;
      RHO2=RHO3
      P2=P3
      Go to 10.1

5. Search failed;
   1. Check if error messages desired;
      If ISTATE(4)<5, Print, L density
      did not converge.

11. Prepare to leave;
   1. Transfer result; DENSL=RHO2

   2. If ISTATE(9)=1, return

   3. Not in derivative so store result;
      SRHO=DENSL
      SP=PRES(T,SRHO)
      Return

Subroutine DENSV

1. Hierarchy: Called By: FUNCN, FLASHP
   Calls: PRES

2. Functional Description:

This subroutine finds the density root of equations of state in the region between zero and the critical density, i.e. the vapor density. It does this by a combined method of false position and successive bisections. It uses the ideal gas value as the initial approximation and has several safeguards to secure the selection of the correct root.

3. Variables:

   a. Input:

      1. Arguments:

         T, absolute temperature
         P, pressure

      2. COMMON/PRM/RGAS,RMIDV,TCRIT

      3. COMMON/DAT/ISTATE(9),ISTATE(4)

   b. Output:

      1. Argument:

         DENSV, gas density root

   c. Intermediate:

      1. IT, ITMAX iteration parameters

      2. PO, local storage for P

      3. P1, P2, P3, intermediate pressures used in the search.

      4. DEL, search interval

      5. CODE, status variable

      6. EPSP, tolerance in pressure, 10^{-5}

      7. EPSR, tolerance in density, 10^{-5}

      8. PMAX, maximum pressure in secondary search.

      9. RHOMAX, DENSITY corresponding to PMAX.

      10. RHO1,RHO2,RHO3, intermediate densities used in search.

4. Algorithm:

a. Basis;

The density is found by a false position search. If this fails by not meeting convergence criteria or the root having a negative derivative, a search from P/2RT is made up to RMIDV by step DEL until the root is bounded. When it is bounded successive bisection is performed until the convergence criteria are satisfied. If the root was unable to be bounded the density corresponding to the maximum pressure is used.

b. Procedure;

1. Initialize
   ITMAX=20, set maximum iterations for false position
   PO=P, move X to local storage
   DEL=PO/RGAS/T/10, delta as a tenth ideal gas density
   RHO1=.5*PO/RGAS/10, first density as half ideal gas
   IT=1, start counter

2. Check if T is so small that false position will likely fail
   If T/TCRIT<.4, go to 7

3. Check if in derivative routine and if so use last result to start:
   If ISTATE(9)≠0, RHO1=RHO2

4. Set up initial values for false position;
   RHO2+.8*RHO1-L
   P1=PRES(T,RHO1)-PO
   P2=PRES(T,RHO2)-PO

5. Start false position iteration;

   1. Check for convergence;
      If |P1-P2KEPS*PO or |RHO1-RHO2|<|RHO2|*EPSR
      go to 6|

   2. Check if exceeded 20 iterations;
      If IT>ITMAX go to 7

   3. Project by false position;
      RHO3=(RHO1*P2-RHO2*P1)/(P2-P1)

   4. If RHO3 is out of bounds randomize start
      If RHO3>RMIDV or RHO3<O, RHO3=(1-IT/50)*PO/(RGAS*T)

   5. Update for next iteration;
      RHO1=RHO2
      RHO2=RHO3
      P1=P2
      P2=PRES(T,RHO2)-PO
      IT=IT+1

6. Go to 5.1

6. Check for positive slope for correct root;
RHO1=.99*RHO2
P1=PRES(T,RHO1)-PO
If RHO2<RMIDV, it is out of range, go to 7
If P1<P2 go to 11.

7. Initialize for search to bound root;
ITMAX=RMIDV/DEL+5, set limit as 5 steps past RMIDV
IT=0
Convert differences from PO into pressures;
P1=P1+PO
P2=P2+PO
RHO1=DEL

8. Begin search to bound root;

1. P1=PRES(T,RHO1)

2. Check to be sure P1 is below PO, i.e. on the left;
1. If P1<PO, go to 8.3

2. Else, not bound on left;
1. Check if error messages desired;
If ISTATE(4)<5 Print error root too small
2. RHO2=RHO1
3. Go to 11.

3. Start search;
RHO2=RHO1+DEL
PMAX=P1
RHOMAX=RHO1
CODE=0., shows start of search

4. P2=PRES(T, RHO2)

5. Check for bound;
If P2>PO, go to 9.

6. Check for first maximum;
If P2>PMAX and CODE=0, go to 8.12

7. First maximum found; CODE=1

8. Update iteration values;
IT=IT+1
RHO1=RHO2
P1=P2
RHO2=RHO2+DEL

```
      9.  Test for end of iterations;
          If IT>ITMAX, go to 8.11

     10.  Continue search if not at bound;
          If RHO1<RMIDV, go to 8.4

     11.  Since out of bounds use maximum;
          1.  Check if error messages desired;
              If ISTATE(4)<5 print maximum used
          2.  RHO2=RHOMAX
          3.  Go to 11.

     12.  Iteration exceeded without finding bound;
          1.  Check if error messages desired;
              If (ISTATE(4)<5 print V root not found
          2.  Go to 11.

     13.  Update maximum with higher values;
          PMAX=P2
          RHOMAX=RHO2
          Go to 8.8

  9.  Root bounded so initialize for bisections;
      IT=0

 10.  Begin successive bisections

      1.  Calculate values at interval center;
          RHO3=(RHO1+RHO2)/2
          P3=PRES(T, RHO3)

      2.  Check for convergence;
          If |P1-P2|<EPSP*PO or |RHO1-RHO2|<|RHO2|*EPSR
          Go to 10.5

      3.  Check number of iterations;
          IT=IT+1
          If IT>ITMAX, go to 10.6

      4.  Find interval containing root;
          1.  If P3>PO, go to 10.4.3
          2.  Between top and middle;
              RHO1=RHO3
              P1=P3
              Go to 10.1
          3.  Between bottom and middle;
              RHO2=RHO3
              P2=P3
              Go to 10.1
```

5. Transfer middle solution root for result;
   RHO2=RHO3
   Go to 11.

6. Search failed;
   1. Check if error messages desired;
      If ISTATE(4)<5, Print V density did not converge.

11. Return result;
    DENSV=RHO2
    Return

Subroutine CURFIT

1. Hierarchy: Called by MAIN
   Calls: GJEL, FUNCN, MESSG, FDERIV, LBLEZ, FCHISQ

2. Functional Description:

This subroutine calculates one iteration in a regression by the method of Marquart or Gauss-Newton for non-linear functions. It generates the normal equations, obtains their solution and evaluates the solution. It also reduces to a standard linear regression in which repeated solution of the normal equations is used to reduce round-off error.

3. Variables:

   a. Input:

      1. Arguments:

         X, Y, WEIGHT, N, NPTS, NTERMS, A, FLAMDA, ITERM

   b. Output:

      1. Arguments:

         SIGMAA, YFIT, CHISQ1

      2. COMMON/DAT/ISTATE(1), ISTATE(2), ISTATE(3)

   c. Intermediate:

4. 1. I,J,K,L, Do-loop parameters.

   2. DET, determinant from GJEL

   3. IER, error code for the results of GEJEL

   4. IBD, control code for calling LBLEZ

   5. NPN, dimension of transfer vector to FUNCN

   6. BETA, constant vector for normal equations

   7. DELM, largest delta for parameters

   8. JM, index corresponding to DELM

   9. FACT, reducing factor for constrained parameters

10. PERC, percent error in calculating Y

11. SUM1, accumulator for percent errors

12. ALPHA, triangular matrix to accumulate the normal equations

13. ARRAY, scaled coefficient matrix for normal equations

14. DERIV, array of derivatives of Y with respect to the A's

15. NFREE, degrees of freedom

16. CHISQR, trial value of chi-squared

b. Algorithm:

1. Initialize:
   IC/5/Output counter
   IBD/0/, label control saying LBLEZ not called

2. Have LBLEZ called once;
   If IBD≠1, CALL LBLEZ, IBD=1

3. Inialize Percent accumulator, SUM1=0, and FACT=.99

4. Check to see if program dimensions are exceeded;
   If NTERMS>100, NTERMS=100, print only 100 fitted

5. Calculate transfer vector dimension; NPN=NPTS+NPARM

6. Check degrees of freedom;

   1. NFREE=NPTS-NTERMS

   2. If NFREE>0, go to 7.

   3. Else, stop calculations
      Print error degrees of freedom less than 1
      FLAMDA=1000
      CHISQR=10^{55}
      Go to 24

7. Evaluate alpha and beta matrices;

   1. Zero matricies;
      For J=1 to NTERMS
      1. BETA(J)=0
      2. For K=1 to J
         1. ALPHA(J,K)=0

   2. Put parameters into transfer vector;
      For L=1 to NPARM
      1. Z(L+N)=A(L)

```
3.  Zero ARRAY

4.  Accumulate terms by data point;
    For I=1 to NPTS
    1.  Put X's for point in Z's;
        For L=1 to N, Z(L)=X(I,L)

    2.  Identify and evaluate YFIT for point
        ISTATE(1)=I
        YFIT(I)=FUNCN(Z,NPN)

    3.  Calculate and accumulate error;
        1.  If Y(I)=0, go to 7.4.3.3

        2.  PERC=100*(Y(I)-YFIT(I))/Y(I))

        3.  SUM1=SUM1+|PERC|

        4.  Check if result is to be printed;
            If ISTATE(2)>4 go to 7.4.4

        5.  If Gauss-Newton skip until 5th time;
            If IC<5 and FLAMDA=0, go to 7.4.4

        6.  Print Y,YFIT,PERC

    4.  Evaluate parameter derivatives;
        For L=1 to NTERMS
        1.  JJ=ITERM(L)+N, get index.

        2.  DERIV(L)=FDERIV(Z,JJ,NPN), calculate derivative

        3.  Accumulate derivatives for average
            ARRAY(L)=ARRAY(L)+|DERIV(L)|

        4.  Check for 0 derivative;
            If |DERIV(L)|<10^-30, DERIV(L)=0

        5.  Accumulate matricies;
            For J=1 to NTERMS
            1.  Check if Linear or Nonlinear
                1.  Nonlinear; If FLAMDA≥0,
                    BETA(J)=BETA(J)+WEIGHT*(Y-YFIT)*DERIV(J)
                2.  Linear; If FLAMDA<0,
                    BETA(J)=BETA(J)+WEIGHT*Y*DERIV(J)

            2.  For K=1 to J
                1.  ALPHA(J,K)=ALPHA(J,K)+WEIGHT*DERIV(J)*
                    DERIV(K)
```

5. Print average percent error;
SUM1=SUM1/NPTS,PRINT,SUM1

8. Update print control;
IC=IC+1
If IC>5 IC=1

9. Evaluate and print CHISQ1 as FCHISQ

10. Calculate and print average absolute derivatives as ARRAY(J)/NPTS

11. Form scaled augmented matrix;

1. DIAG=1

2. Check for Marquart; If FLAMDA<0, DIAG=DIAG+FLAMDA

3. For J=1 to NTERMS

1. Check for invalid diagonals
1. If ALPHA(J,J)$\leq$0, print error, ALPHA(J,J)=10^{-40}

2. Calculate constant term;
ARRAY(NTERMS+1,J)=BETA(J)/$\sqrt{\text{ALPHA(J,J)}}$

3. Calculate coefficients;
For K=1 to J
1. ARRAY(K,J)=ALPHA(K,J)/$\sqrt{\text{ALPHA(J,J)*ALPHA(K,K)}}$

2. ARRAY(J,K)=ARRAY(K,J)

4. ARRAY(J,J)=DIAG

12. Initialize search value for largest delta, DELM=0

13. Solve normal equations;

1. Check for special case of one parameter;
If NTERMS>1, go to 13.3

2. One term;
1. ARRAY(1)=1/ARRAY(1)
2. ARRAY(2)=ARRAY(2)*ARRAY(1)
3. Go to 14.

3. More than one term so call inversion routine, GJEL

14. Check if parameters are to be updated;
If ISTATE(2)=9, go to 20
If ISTATE(2)=8, go to 19

15. Calculate new parameters;
For J=1 to NTERMS

    1. Get index, JJ=ITERM(J)

    2. Check for largest parameter change;

        1. If |ARRAY(NTERMS+1, J)|<DELM, go to 15.3

        2. Else, save larger delta;
        DELM=|ARRAY(NTERMS+1, J)|

    3. Calculate new parameter as B_J

        1. B(J)=A(JJ)+ARRAY(NTERMS+1,J)/ $\sqrt{\text{ALPHA(J,J)}}$

        2. Check is parameter is to be constrained;
        If ISTATE(3)=0 or B(J)*A(JJ)>0, go to 15.3.4

        3. Else, constrain parameter against change in sign;

            1. Print message that parameter changed sign

            2. B(J)=A(JJ)*(1-FACT)

        4. Continue loop

16. Print largest delta and index, DELM,JM

17. Evaluate chi-squared at new parameters;

    1. Insert new parameters in transfer vector;
    For L=1 to NTERMS

        1. JJ=ITERM(L)

        2. Z(JJ+N)=B(L)

    2. Evaluate YFIT;
    For I=1 to NPTS

        1. Move X's to Z;
        For L=1 to N; Z(L)=X(I,L)

        2. Evaluate point;

            1. ISTATE(10)=I

            2. YFIT(I)=FUNCN(Z,NPN)

    3. CHISQR=FCHISQ(...)

    4. Output results;
    Print IPRES,CHISQR

18. Optimize acceleration parameter FLAMDA for reduction in chi-square;

    1. If Gauss-Newton or linear selected skip optimization; If FLAMDA≤0, go to 21

    2. If Chi-square decreased don't optimize; If (CHISQ1-CHISQR)>0, go to 21

    3. Change FLAMDA
       FLAMDA=10*FLAMDA
       FACT=FACT/2

    4. CHECK for top bound on FLAMDA
       If FLAMDA>1000, go to 23

    5. If FLAMDA is small save variances;

        1. If FLAMDA>.01, go to 11.

        2. Calculate variances in SIGMAA
           For I=1 to NTERMS

            1. SIGMAA(I)=ARRAY(I,I)/$\sqrt{\text{ALPHA(I,I)}}$

        3. go to 11

19. Output correlation coefficients;
    For I=1 to NTERMS;

    1. For J=1 to I

        1. Calculate row of correlation coefficients;
           B(J)=ARRAY(I,J)/$\sqrt{\text{ARRAY(I)*ARRAY(J)}}$

        2. Output row of coefficients; Print B, 1 to I

20. Calculate variances

    1. For J=1 to NTERMS

        1. SIGMAA(J)=ARRAY(J,J)/$\sqrt{\text{ALPHA(J,J)}}$

        2. CHISQR+CHISQ1
           Return

21. Move parameters and variances for leaving;

    1. For J=1 to NTERMS

        1. Insert new parameters;
           JJ=ITERM(J)
           A(JJ)=B(J)

2. Check for invalid variances;
   If ARRAY(J,J)≤0, ARRAY(J,J)=10^{-30},
   Print variance is negative.

3. Calculate variance;
   SIGMAA(J)=ARRAY(J,J)/$\sqrt{\text{ALPHA(J,J)}}$

2. FLAMDA=FLAMDA/10

22. Output correlation coefficients;

1. Check is coefficient desired;
   If ISTATE(2) 4, go to 24

2. For I=1 to NTERMS;

   1. For J=1 to I

      1. Calculate row of correlation coefficients;
         B(J)=ARRAY(I,J)/$\sqrt{\text{ARRAY(I)*ARRAY(J)}}$

   2. Output row of coefficients; Print B, 1 to I

3. go to 24

23. Evaluate at original parameters;

1. Insert parameters in transfer vector;
   For L=1 to NPARM;

   1. Z(L+N)=A(L)

2. Evaluate YFIT;
   For I=1 to NPTS;

   1. Move X's to Z;
      For L=1 to N; Z(L)=X(I,L)

   2. Evaluate point;

      1. ISTATE(1)=I

      2. YFIT(I)=FUNCN(Z,NPN)

      3. CHISQR=CHISQ1

24. Return

Subroutine ENTH

1. Hierarchy: Called By: FUNCN, CP
   Calls: PRES, F12

2. Functional Description:

This subroutine calculates the enthalpy departure at the state condition specified by the arguments temperature and density. This value is calculated for an equation of state in EZFIT form as:

$$\Delta H = R_e T_c (-T^{*2} FI2 + T^* (Z-1))/\alpha$$

3. Variables:

   a. Input:

      1. Arguments:

         T, absolute temperature.
         RHO, density.

      2. COMMON/PRM/RENRGY, TCRIT, RGAS, ALPHA

   b. Output:

      1. ENTH, the calculated enthalpy departure

   c. Intermediate:

      1. TSTAR, reduced temperature.

      2. HDEV, reduced enthalpy departure

4. Algorithm:

   1. Reduce temperature, TSTAR=ALPHA*T/TCRIT

   2. Calculate reduced enthalpy departure;
      HDEV=(TSTAR**2)*FI2(T,RHO)+TSTAR*(PRES(T,RHO)/(RGAS*T*RHO)-1)

   3. Unreduce the departure;
      ENTH=HDEV*RENRGY*TCRIT/ALPHA

Subroutine CHISQ

1. Hierarchy: Called By: CURFIT
   Calls: -

2. Functional Description:

This subroutine calculates the reduced chi-squared used as the objective function in the nonlinear regression. The is the weighted sum of squares.

3. Variables:

   a. Input:

      1. Arguments:

         Y, the experimental values for the data points
         WEIGHT, the weights for each data point.
         NPTS, number of data points
         NFREE, the degrees of freedom
         YFIT, the calculated values for the data points.

   b. Output:

      1. FCHISQ, the calculated reduced weighted sum of the squared errors, chi-squared.

   c. Intermediate:

      1. I, do-loop parameter.

      2. CHISQ, accumulator for chi-squared.

      3. FREE, real variable for degrees of freedom.

4. Algorithm:

   a. Procedure:

      1. Initialize accumulator to zero; CHISQ=0.

      2. Check to be sure that the degrees of freedom are positive;
         If NFREE$\leq$0 FCHISQ=0 and return.

      3. Calculate chi-squared;
         For I=1 to NPTS

         1. $CHISQ=CHISQ + WEIGHT_i * (Y_i * YFIT_i)^{**2}$

Subroutine ENTRPY

1. Hierarchy: Called By: FUNCN
   Calls: FI1, FI2

2. Functional Description:

This subroutine calculates the entropy departure at the state condition specified by the arguments temperature and density. This value is calculated for an equation of state in EZFIT form as

$$S = R_e(-\ln(\rho RT)-FI1-T^* FI2)$$

3. Variables:

   a. Input:

      1. Arguments:

         T, absolute temperature.
         RHO, density.

      2. COMMON/PRM/RENRGY,TCRIT,ALPHA

   b. Output:

      1. ENTRPY, the calculated entropy departure.

   c. Intermediate:

      1. TSTAR, reduced temperature.

4. Algorithm:

   1. Reduce temperature;
      TSTAR=ALPHA*T/TCRIT

   2. Calculate the unreduced entropy departure;
      ENTRPY=RENRGY*(-ln(RHO*RGAS*T)-FI1-TSTAR*FI2)

4. Reduce chi-squared;

    1. FREE=NFREE

    2. FCHISQ=CHISQ/FREE

Subroutine FDERIV

1. Hierarchy: Called By: CURFIT
   Calls: FUNCN

2. Functional Description:

This subroutine calculates the numerical derivative for the ith variable in the function FUNCN by finite differences. The interval can optionally be adjusted to obtain the precision desired by an internal testing algorithm.

3. Variables:

   a. Input:

      1. Arguments:

         X,array of independent variables
         I, number of parameter in array of which the derivative is taken
         NDIM, number of independent variables

      2. COMMON/DAT/ISTATE(5)

   b. Output:

      1. FDERIV, the calculated derivative

      2. ISTATE(9), the state of FDERIV being active.

   c. Intermediate:

      1. EPS, Minimum size for variable for which delta is calculated as fraction of variable.

      2. IT, do-loop parameter

      3. N, Number of significant digits desired,

      4. F1, FUNCN evaluated at X-delta

      5. F2, FUNCN evaluated at X+delta

      6. DEL, the delta used for the finite difference.

      7. DFDX, trial finite difference derivative

      8. SAVE, original value of the variable of which the derivative is calculated.

4. Algorithm:

a. Basis:

A first order numerical derivative can be calculated by finite differences as

$$f' = \frac{f_1 - f_2}{\Delta x} = \frac{f_2(x+\Delta x/2) - f_1(x-\Delta x/2)}{\Delta x} \tag{1}$$

Let the two functions differ by Δb in the t^{th} least significant digit, then

$$f' = \frac{f_1 - f_2(1 \pm \Delta b \cdot 10^{-t})}{\Delta x} = f_1 \cdot (\pm \Delta b . 10^{-t})/\Delta x \tag{2}$$

where

$$0 < |\Delta b| \leq 1 \tag{3}$$

If t' is the number of significant digits the machine has and N is the number of significant digits desired in the derivative, then,

$$t = t' - N, \tag{4}$$

Therefore,

$$f' = f_1/\Delta x (\pm \Delta b \cdot 10^{-(t' - N)}) \tag{5}$$

which gives the following inequality

$$|f'| \leq |f_1/\Delta x| \cdot 10^{-t+N} \tag{6}$$

For the condition that f' will have at least N digits, it then follows

$$|f'| > |f_1/\Delta x| \cdot 10^{-t'+N} \tag{7}$$

In single precision t'=6 and for this work N=3. When the 7 inequality is not satisfied the delta is increased up to five times.

b. Procedure:

1. Initialize values; EPS=.01, N=3

2. Save x; SAVE=X(I) and indicate FDERIV is active;
   ISTATE(9)=1.

3. Determine first delta;
   If SAVE<EPS, DEL=EPS
   Else DEL=|EPS*SAVE|.

4. For IT=1 to 3

   1. Calculate upper and lower functions and derivative;
      f_2 = FUNCN(X_i+DEL)
      f_1 = FUNCN(X_i+DEL)
      DFDX=(f_2-f_1)/2DEL

   2. If derivative precision is not required, ISTATE(5)=1, indicate leaving FDERIV, and go to 6.

   3. Check for equal values;
      If $|f_1-f_2|<|f_1|10^{-5}$, $f_2=f_1$

   4. Check number of significant digits;
      If |f_1-f_2|10**(6-N)>|f_1|, go to 6.

   5. Determine new delta;
      ESP=ESP*10
      IF|SAVE|<10^{-6}, DEL=EPS
      Else DEL=|EPS*SAVE|

5. Check for 0 derivative;
   If $|f_1-f_2|<|f_1|10^{-5}$, DFDX=0

6. Indicate leaving FDERIV;
   ISTATE(9)=0
   FDERIV=DFDX
   X_i=SAVE

Subroutine FI1

1. Hierarchy: Called By; FUGCOF, ENTRPY
   Calls; -

2. Functional Description;

This subroutine calculates the integral of $\partial Z/\partial T$ d ln ρ from 0 to ρ for the equation of state, for a given temperature and density. This is used to calculate entropy properties.

3. Variables:

   a. Input:

      1. Arguments:

         T, absolute temperature.
         RHO, density.

      2. COMMON/PRM/RGAS,. . .NUMB

   b. Output:

      1. FI1; the value of the integral.

4. Algorithm:

The method is any that will calculate the integral

$$FI1 = \int_0^{\rho^*} \partial Z/\partial T \; d \ln \rho^*$$

for a given equation of state. The scaling values for temperature and density and the physical properties of the substance are given in the common block. The parameters that will be fitted in the equation of state are in A of the common block.

Subroutine FI2

1. Hierarchy: Called By: ENTH, ENTRPY, U
   Calls: -

2. Functional Description:

This subroutine calculates the integral of $(Z-1)/d \ln \rho$ from 0 to ρ for the equation of state. This is used to calculate energy properties. For a given temperature and density.

3. Variables:

   a. Input:

      1. Arguments:

         T, absolute temperature.
         RHO, density.

      2. COMMON/PRM/RGAS, . . .NUMB

   b. Output:

      1. FI2, the value of the integral.

4. Algorithm:

The method is any that will calculate the integral

$$FI2 = \int_0^{\rho^*} (Z-1) d \ln \rho^*$$

for a given equation of state. The scaling values for temperature and density and the physical properties of the substance are given in the common block. The parameters that will be fitted in the equation of state are in A of the common block.

Subroutine FLASHP

1. Hierarchy: Called By: FUNCN
   Calls: DENSV,DENSL,FUGCOF

2. Functional Description:

This subroutine performs an adiabatic flash for a pure fluid to find the saturation pressure.

3. Variables:

   a. Input:

      1. Arguments:

         T, the absolute saturation temperature.
         PO, initial estimate of saturation pressure

      2. COMMON/DAT/ISTATE(4),ISTATE(9)

   b. Output:

      1. FLASHP, the calculated saturation pressure.

   c. Intermediate:

      1. P, intermediate calculated pressure,

      2. IT, do-loop parameter.

      3. EPS, precision for convergence criteria

      4. RHOL, liquid density

      5. RHOV, vapor density

      6. ITMAX, maximum number of iterations.

      7. PCRIT, critical pressure

      8. KVALUE, equilibrium ratio.

4. Algorithm:

      1. Initialize precision and maximum iterations;
         EPS=.001
         ITMAX=20

2. If called by derivative routine FDERIV, use previous pressure for initial value;
   If ISTATE(9)≠1, P=PO

3. Calculate densities
   RHOV=DENSV(T,P)
   RHOL=DENSL(T,P)

4. Start loop, IT=1

5. KVALUE=FUGCOF(T,RHOL)/FUGCOF(T,RHOV)

6. Update pressure;
   P=P*KVALUE

7. Make sure pressure does not go too high;
   If P>1.3*P_c, P=1.3*P_c, If ISTATE(4)<4 print error, FLASHP=P return.
   Else;

8. Check for convergence;
   If |1-KVALUE|<EPS, FLASHP=P, return.
   Else;

9. Check for exceeding iteration maximum;
   IT=IT+1
   If IT>ITMAX, and if ISTATE(4)<4, print error, FLASHP=P, return.
   Else;

10. Calculate new densities:
    RHOV=DENSV(T,P)
    RHOL=DENSL(T,P)

11. Go to 5

Subroutine FUGCOF

1. Hierarchy; Called By: FLASHP
   Calls: FI1 and PRES

2. Functional Description:

This subroutine calculates the pure fluid fugacity coefficient from an equation of state in EZFIT form as

$$f/f^{o} = \exp(\ln(\rho RT)+FI1+(Z-1))$$

3. Variables,

   a. Input:

      1. Arguments:

         T, absolute temperature.
         RHO, density.

      2. COMMON/PRM/RGAS

   b. Output:

      1. FUGCOF, the calculated pure fluid fugacity.

   c. Intermediate

      1. FP, reduced chemical potential.

4. Algorithm:

   1. FP=ln(RHO*RGAS*T)+FI1+(PRES/(RHO*RGAS*T)-1)

   2. Check for overflow;
      If FP>100, FP=0

   3. FUGCOF=EXP(FP)

Subroutine FUNCN

1. Hierarchy: Called By: CURFIT, OUTPUT
   Calls: FLASHP, DENSV, DENSL, ENTH, CP, ENTRPY, U, CV, PRES

2. Functional Description:

This subroutine controls the calling of the calculation subroutines for the evaluation of the data point.

3. Variables:

   a. Input:

      1. COMMON/PRM/RGAS,. . ,RMIDV

      2. COMMON/PRP/ICOMP(20),. . .CNAME(20,2)

      3. Argument X, transfer vector, NDIM, the dimension of the transfer vector.

   b. Output:

      1. COMMON/PRM/TCRIT,PCRIT,RHOC,RENRGY,W,ALPHA,BETA, RTOP,RMIDL,RMIDV,A

   c. Intermediate:

      1. SL, save location for the compound code presently active.

      2. X1, the absolute value of the control variable

      3. IWHOLE, the whole portion of the control variable.

      4. IFRACT, the fraction portion of the control variable.

      5. LIQVAP, the sign of the control variable.

      6. L, do-loop parameter.

      7. RHOL, calculated liquid density.

      8. RHOV, calculated vapor density.

4. Algorithm:

   1. Transfer parameters to A;
      N=NDIM-NPARM
      For I=1 to NPARM

1. $A_i = X_{N+i}$

2. Separate control variables;
   X1=|X_1|
   IWHOLE=X1+.005
   IFRACT=|X1-IWHOLE+.005|*100
   LIQVAP=SIGN(1.,X_1)

3. Find index of compound;
   For L=1 to 20
   1. If $ICOMP_1$ = IWHOLE, go to 5

4. Print error message.

5. Check if properties are for right compound;
   If SL=L go to 6
   Else;
   1. Set properties for compound;
      TCRIT=CTC(L)
      PCRIT=CPC(L)
      RHOC=CRC(L)
      RENRGY=1.9872/CMW(L)
      W=CW(L)
      ALPHA=CA(L)
      BETA=CB(L)
      RTOP=4*RHOC
      RMIDL=RHOC
      RMIDV=RHOC
      SL=L

6. Calculate properties;
   If IFRACT = 30 and LIQVAP=-1, calculate DENSL
   If IFRACT = 30 and LIQVAP=1, calculate DENSV
   If IFRACT = 40 and LIQVAP=-1, calculate DENSL, ENTH
   If IFRACT = 40 and LIQVAP=1, calculate DENSV, ENTH
   If IFRACT = 75, calculate FLASHP
   If IFRACT = 60, calculate PRES
   If IFRACT = 25, and LIQVAP=-1, calculate DENSL, CV
   If IFRACT = 25, and LIQVAP=1, calculate DENSV, CV
   If IFRACT = 20, and LIQVAP=-1, calculate DENSL, CP
   If IFRACT = 20, and LIQVAP=1, calculate DENSV, CP
   If IFRACT = 12, and LIQVAP=1, calculate DENSL, U
   If IFRACT = 12, and LIQVAP=1, calculate DENSV, U
   If IFRACT = 14, and LIQVAP=-1, calculate DENSL, ENTRPY
   If IFRACT = 14, and LIQVAP=1, calculate DENSV, ENTRPY

Subroutine GJEL

1. Hierarchy: Called By: CURFIT
   Calls: -

2. Functional Description:

This subroutine finds the solution to system of simultaneous linear equations by the Gauss-Jordan elimination with optional maximum pivot selection. The inverse matrix in generated over the coefficient matrix. More than one solution vector may be obtained at one time.

3. Variables:

   a. Input:

      1. Arguments:

         A, augmented matrix of coefficients and constants.
         ND, number of rows in matrix.
         MD, number of columns in matrix.

   b. Output:

      1. Arguments:

         DETD, the determinant.
         IER, the error code;
              IER=0, successful inversion
              IER=ND+1, pivot element was zero.
              IER=I, pivot was smaller than 10^{-20}

   c. Intermediate:

      1. I,J,K,II,JJ,IR, do-loop parameters.

      2. L,LL, indicies.

      3. EPS, precision for pivot element.

      4. FACT, storage for normalizing, etc.

      5. PIVOTS, row transformation vector

      6. CPIVOT, column transformation vector.

      7. IPIVOT, LPIVOT transformation indices.

      8. N,M, local storage for arguments ND,MD respectively.

      9. DET, accumulator for determinant

4. Algorithm:

1. Initialize:
   IER=0, N=ND,M=MD,DET=1

2. Begin Elimination;
   For I=1 to N
   1. Optional maximum pivot strategy:

      1. Find largest pivot;
         If I=N go to 2.1.6

      2. Initialize search;
         LPIVOT=I, IPIVOT=I,FACT=|A(I,I)|

      3. Search;
         For II=1 to N
         1. For JJ=1 to N
            1. If A(JJ,II) FACT go to 2.1.3.1.3
            2. Else, save larger pivot;
               FACT = A(JJ,II)
               LPIVOT=JJ
               IPIVOT=II
            3. Continue loop

      4. Trade columns:
         1. record trade; CPIVOT(I)=IPIVOT

         2. For K=1 to N
            1. Trade elements
               FACT=A(K,I)
               A(K,I)=A(K,IPIVOT)
               A(K,IPIVOT)=FACT

      5. Trade rows;
         1. Record trade; PIVOTS(I)=LPIVOT

         2. For K=1 to M
            1. Trade elements;
               FACT=A(I,K)
               A(I,K)=A(LPIVOT,K)
               A(LPIVOT,K)=FACT

      6. CPIVOT(N)=N
         LPIVOT(N)=N

   2. Test for invalid pivot;
      1. If A(I,I)=0, DET=0, IER=N+1, return

      2. If |A(I,I)|<EPS,DET=0, and IER=I

   3. Generate determinant; DET=DET*A(I,I)

```
4.  Test for ill conditioned matrix;
    If |DET|<10^-60, Print error message, DET=0

5.  Normalize pivot row;
    1.  FACT=A(I,I), A(I,I)=1

    2.  For J=1 to M
        1.  A(I,J)=A(I,J)/FACT

6.  Reduce other rows;
    For J=2 to N;
    1.  Select row; L=MOD(I+J-2,N)+1

    2.  If A(L,I)=0, go to 2.6.6

    3.  Save term for reduction, FACT=A(L,I)

    4.  Insert term for inverse; A(L,I)=0

    5.  Reduce row;
        For K=1 to M
        1.  Select index; LL=MOD(I+K-2,M)+1

        2.  If A(I,LL)≠0, A(L,LL)=A(L,LL)-A(I,LL)*FACT

    6.  Continue loop.

3.  Optional maximum pivot strategy;
    1.  transfer columns of inverse;
        For IR=1 to N
        1.  Calculate index so that transformation is
            in reverse; I=N-IR+1

        2.  See if transfer was made;
            If PIVOTS(I)=I, go to 3.1.5

        3.  LPIVOT=PIVOTS(1)

        4.  For J=1 to N
            1.  Trade terms;
                FACT=A(J,I)
                A(J,I)=A(J,LPIVOT)
                A(J,LPIVOT)=FACT

        5.  Continue loop.

    2.  Transfer rows of solution and inverse;
        For IR=1 to N
        1.  Calculate index so that transformation is in
            reverse; I=N-IR+1
```

2. See if transfer was made;
   If CPIVOT(I)=I go to 3.2,5

3. JPIVOT=CPIVOT(I)

4. For J=1 to M
   1. Trade terms;
      FACT=A(I,J)
      A(I,J)=A(JPIVOT,J)
      A(JPIVOT,J)=FACT

5. Continue loop.

4. Output determinant; DETD=DET

Subroutine LBLEZ

1. Hierarchy: Called By: MAIN, CURFIT
   Calls: -

2. Functional Description:

   This subroutine prints a title page identifying the use of the package EZFIT.

3. Variables: None

4. Algorithm:

   Upon its first call it outputs a title page.

Subroutine MESSG

1. Hierarchy: Called By: MAIN CURFIT, tec.
   Calls: -

2. Functional Description:

   This subroutine prints the character string TEXT of length NCHR at the left margin.

3. Variables:

   a. Input:

      1. Arguments: TEXT, NCHR.

   b. Output:

      1. TEXT printed on stream printer.

4. Algorithm:

   1. Print TEXT after advancing one line on stream printer.

Subroutine OUTPUT

1. Hierarchy: Called By: MAIN
   Calls: FUNCN

2. Functional Description:

This subroutine forms tables of output for a set of parameters for the experimental data. It can be custom tailored to the users needs. This version makes tables of each data type with point identification, weight, errors and independent variables. At the end of each table is a summary of error statistics for that block.

3. Variables:

   a. Input:

      1. Argument X,N,Y,NPTS,NPARM,A1,WEIGHT,DATAID,ND

      2. COMMON/PRP/ICOMP(20),. . .CNAME(20,2)

      3. HEADER, Heading, and IN for use on tables.

      4. IXPRINT, variable read in for optional output control.

   b. Output:

      1. All inputs except N,NPTS,NPARM,A1, and ND.

      2. Calculated Y's, percent errors, absolute errors, headings, summary errors, optional intermediate values.

   c. Intermediate:

      1. I,J, and K used for do-loop evaluation.

      2. LF the save location for the fraction portion of the control variable

      3. LW the save location for the whole portion of the control variable.

      4. SUM1, the accumulator for average absolute percent error.

      5. SUM2, the accumulator for average absolute error.

      6. JO, counter for data block.

7. SUM, the accumulator for the average absolute percent error for the entire data set.

8. Z, the transfer vector for the parameters and variables to FUNCN.

9. YC, calculated value for data point.

10. PERC, percent error for data point

11. DIFF, difference in calculated and experimental.

12. X1, the absolute value of the control variable.

13. IWHOLE, the whole portion of the control variable for the point.

14. IFRACT, the fraction portion of the control variable for the point.

15. IRHO, fraction code for density point.

16. IDH, fraction code for enthalpy departure point.

17. IVP, code for vapor pressure point.

18. RHO, calculated density.

19. RHOL, saturated liquid density at vapor pressure point.

20. RHOV, saturated vapor density at vapor pressure point.

21. PRESC, calculated pressure for density point.

22. PERC2, percent error in calculated pressure.

4. Algorithm:

What ever is desired by the user for tables of results.

Subroutine PRES

1. Hierarchy: Called By: FUNCN, DENSL, DENSV, ENTH, FUGCOF, ENTRPY.
   Calls: -

2. Functional Description:

This subroutine calculates the pressure for a given equation of state using parameters in the common blocks for the arguments of temperature and density.

3. Variables:

   a. Input:

      1. Arguments:

         T, absolute temperature.
         RHO, density.

      2. COMMON/PRM/RGAS,. . .,NUMB

   b. Output:

      1. PRES, the calculated pressure.

4. Algorithm:

The method is any that will calculate the pressure for a given equation of state. The scaling values for temperatures and density and the physical properties of the substance are given in the common block. The parameters that will be fitted in the equation of state are in A of the common block.

Subroutine U

1. Hierarchy: Called By; FUNCN,CV
   Calls; FI2

2. Functional Description;

This subroutine calculates the internal energy departure at the state condition specified by the arguments temperature and density. This value is calculated for an equation of state in EZFIT form as

$$\Delta U = R_e T_c (-T^{*2} FI_2)/\alpha$$

3. Variables:

   a. Input:

      1. Arguments:

         T, absolute temperature.
         RHO, density.

      2. COMMON/PRM/RENRGY,TCRIT,ALPHA

   b. Output:

      1. U, the calculated internal energy departure.

   c. Intermediate:

      1. TSTAR, reduced temperature.

4. Algorithm:

   1. Reduce temperature;
      TSTAR=ALPHA*T/TCRIT

   2. Calculate the unreduced internal energy departure;
      U=RENRGY*TCRIT*(-TSTAR*TSTAR*FI2)/ALPHA

Adapting EZFIT to Any General Function

EZFIT can be adapted for fitting any general function of parameters $[A]_m$ and variables $[X]_n$, $y=f([X]_n; [A]_m)$, by changing the input and output routines and the calculation routine FUNCN. The specific requirements of the routines are given below along with an example for fitting a polynomial.

Subroutine Input DATA, DATA2, DATA3. The use of three data input routines allows each to be specialized to a specific data format. The requirements of the routines are basically the same. The form of the definition and arguments are

```
SUBROUTINE DATA3(X,N,Y,NPTS,WEIGHT,YBAR,YVAR,NCODE,DATAID,ND)
DIMENTION X(NPTS,N),Y(NPTS),WEIGHT(NPTS),DATAID(NPTS,ND)
```

The arguments are:

- X — The matrix of experimental data of NPTS points with N independent variables in each row.
- N — The number of independent variables per data point.
- Y — The vector of length NPTS of the dependent variables for each data point.
- NPTS — The number of data points inputed.
- WEIGHT — A vector of length NPTS containing the weights for each data point.
- YBAR — The weighted average of the dependent variables.
- YVAR — The variance of the independent variable.
- NCODE — The control variable selecting the method of calculation of the weights given as:
  - -1 the weighting is $1/Y_{exp}$

0 the weight is 1, or equal weights.

1 the weight is $1/(\text{WEIGHT})^2$ where WEIGHT is supplied in the input section. This is usually used for percent weighting.

DATAID A matrix of NPTS rows of ND=3 columns that contain a 12 character indentification for each data point.

ND The second dimension for DATAID, which is 3, to allow object time dimensioning.

Note that object time dimensioning is used allocating work space defined in the main program. The work space is allowed for X to have 3000 variables and therefore NPTS*N$\leq$3000.

The weighted mean is calculated as:

$$Y = \Sigma w_i \, Y_i / \Sigma w_i,$$

The variance is then given as:

$$\text{Var}(Y) = \Sigma w_i (Y_i - \bar{Y})^2,$$

A sample routine is given in Table I. It reads from a card unidentified data on which the first N are variables and the last is the experimental value of Y. The data are in F10.0 format and the program generates an identification number for each point.

Subroutine Calculation FUNCN. The subroutine FUNCN is used to calculate the function to be fitted, $y=f([x]_n; [A]_m)$. The form of the definition and the arguments are

```
FUNCTION FUNCN(X,NDIM)
DIMENSION X(NDIM)
```

The arguments are:

X A transfer vector containing N independent variables first and then NPARM parameters.

NDIM The total length of the transfer vector, i.e. N+NPARM. The maximum length of the transfer vector is set to 44 in CURFIT and OUTPUT.

FUNCN requires the common block PRM to obtain the number of parameters that are passed. It can be used to pass the parameters in the transfer vector to other calculation routines through the array A. A maximum of 40 parameters can be passed this way. The calculated independent variable, Y, is returned by assigning it to FUNCN. In the example in Table 1 FUNCN is set up to calculate the (N-1)th degree polynomial,

$$Y = A_1 + A_2X + A_3X^2 + \ldots + A_nX^{N-1}.$$

Subroutine OUTPUT. The subroutine OUTPUT is used to generate tabulated results of calculations from a set of parameters. It usually calls FUNCN for the calculation of the independent variable but can also be used to calculate auxilliary information for use in analysis. The form of the definition and the arguments are:

```
      SUBROUTINE OUTPUT(X,N,Y,NPTS,NPARM,A1,WEIGHT,DATAID,ND)
      DIMENSION X(NPTS,N),Y(NPTS),A1(NPARM),WEIGHT(NPTS),
     1  DATAID(NPTS,ND)
```

X The matrix of experimental data of NPTS points with N independent variables in each row.

N The number of independent variables per data point.

Y The vector of length NPTS of the dependent variables for each data point.

NPTS The number of data points inputted.

NPARM The number of parameters used in the calculations.

A1 The vector of length NPARM containing the parameters to be used in the calculation.

WEIGHT A vector of length NPTS containing the weights for each data point.

DATAID A matrix of NPTS rows of ND=3 columns that contain a 12 character identification for each data point.

ND The second dimension for DATAID, which is 3, to allow object time dimensioning.

The user can custom program OUTPUT to his needs. A rather general version is given in the example in Table I. It reads a header used to label the table which also has column headings. The routine prints each point's identification code, experimental value, calculated value, the percent difference, the difference, the weight, and the independent variables. It also calculates the average absolute percent deviation, A.A.P.D., and the average absolute deviation, A.A.D., as

$$A.A.P.D. = \Sigma\left|(Y_c - Y_{exp})/Y_{exp}\right| * 100/NPTS$$

$$A.A.D. = \Sigma\left|Y_c - Y_{exp}\right|/NPTS$$

where the summation is over all data points. The transfer vector Z of 44 variables is used to communicate with FUNCN.

TABLE 1

An Example of Modifying EZFIT for Polynomial Regression

Source Listing

```
//NEW EXEC FORTGCLG,LIB='S4.KGDIN.MOD',PARM.LKED='LIST,LET'                EZPL0010


C     FUNCTION FUNCN(X,NDIM)                                                EZPL0020
C                                                                           EZPL0030
C     PURPOSE                                                               EZPL0040
C        EVALUATES THE FITTED FUNCTION AT THE POINT X                       EZPL0050
C                                                                           EZPL0060
C     USUAGE                                                                EZPL0070
C       RESULT = FUNCN(X,NDIM)                                              EZPL0080
C                                                                           EZPL0090
C     DESCRIPTION OF PARAMETERS                                             EZPL0100
C       X     - ARRAY OF VALUES OF INDEPENDENT VARIABLES                    EZPL0110
C       NDIM  - NUMBER OF INDEPENDENT VARIABLES                             EZPL0120
C                                                                           EZPL0130
        FUNCTION FUNCN(X,NDIM)                                              EZPL0140
        DIMENSION X(NDIM)                                                   EZPL0150
        COMMON /PRM/RGAS,RENRGY,TCRIT,PCRIT,RHOC,W,ALPHA,BETA,XMW           EZPL0160
       1   ,A(40),B(7),NTERMS,NPARM,NUMB,RTOP,RMIDL,RMIDV                   EZPL0170
        DOUBLE PRECISION SUM                                                EZPL0180
        N=NDIM-NPARM                                                        EZPL0190
        DO 20 I=1,NPARM                                                     EZPL0200
     20 A(I)=X(N+I)                                                         EZPL0210
        SUM=0                                                               EZPL0220
C     POLYNOMIAL IN X,Y=A(1)+A(2)*X+A(3)*X2 ......                          EZPL0230
        X1=X(1)                                                             EZPL0240
        DO 30 I=1,NPARM                                                     EZPL0250
        SUM=SUM*X1+A(NPARM-I+1)                                             EZPL0260
     30 CONTINUE                                                            EZPL0270
        FUNCN=SUM                                                           EZPL0280
     40 RETURN                                                              EZPL0290
        END                                                                 EZPL0300
```

```
C    SUBROUTINE DATA3                                                    EZPL0310
C                                                                        EZPL0320
C    PURPOSE                                                             EZPL0330
C      INPUTS DATA WITH 1 X PER 10 COLUMNS AND Y LAST.                   EZPL0340
C                                                                        EZPL0350
       SUBROUTINE DATA3(X,N,Y,NPTS,WEIGHT,YBAR,YVAR,NCODE,DATAID,ND)     EZPL0360
C      MODE    - DETERMINES METHOD OF WEIGHTING LEAST-SQUARES FIT        EZPL0370
C                +1 (INSTRUMENTAL) WEIGHT(I)=1/SIGMAY(I)**2              EZPL0380
C           PERCENT ERROR CONSTANT                                       EZPL0390
C                 0 (NO WEIGHTING) WEIGHT(I)= 1                        EZPL0400
C                -1 (STATISTICAL) WEIGHT =1/Y(I)                       EZPL0410
       COMMON /PRM/RGAS,RENRGY,TCRIT,PCRIT,RHOC,W,ALPHA,BETA,XMW         EZPL0420
      1  ,A(40),B(7),NTERMS,NPARM,NUMU,RTOP,RMIDL,RMIDV                  EZPL0430
       COMMON /PRP/ICOMP(20),CPC(20),CRC(20),CMW(20),CW(20) ,CTC(20)     EZPL0440
      1 ,CA(20),CB(20),CNAME(20,2)                                       EZPL0450
   20 FORMAT(4F10.0,26X,I2,3A4)                                          EZPL0460
 1100 FORMAT(8F10.0)                                                     EZPL0470
 1200 FORMAT(16I5)                                                       EZPL0480
 1300 FORMAT(3F10.0,I10)                                                 EZPL0490
 1500 FORMAT(2A4,I2,7F10.0)                                              EZPL0500
 1600 FORMAT(6F10.0)                                                     EZPL0510
 1700 FORMAT(2I5,F10.0,I5)                                               EZPL0520
       DIMENSION X(NPTS,N),Y(NPTS),WEIGHT(NPTS)                          EZPL0530
       DIMENSION DATAID(NPTS,ND)                                         EZPL0540
       DATA D1,D2/'GEN ','    '/                                         EZPL0550
C      DATA INPUT                                                        EZPL0560
       DO 40 I=1,NPTS                                                    EZPL0570
       READ(5,1100,END=70) (X(I,J),J=1,N),Y(I)                           EZPL0580
C      PERCENT WEIGHTING. ASSUMES NCODE=1                                EZPL0590
       WEIGHT(I)=1                                                       EZPL0600
       IF(Y(I).NE.0) WEIGHT(I)=Y(I)                                      EZPL0610
       DATAID(I,2)=D2                                                    EZPL0620
       DATAID(I,1)=D1                                                    EZPL0630
       CALL CONVR(I,ICHAR,DATAID(I,3))                                   EZPL0640
   40 CONTINUE                                                           EZPL0650
       GO TO 80                                                          EZPL0660
   70 CONTINUE                                                           EZPL0670
       I=I-1                                                             EZPL0680
       PRINT 200,I                                                       EZPL0690
  200 FORMAT(///1X,'****  TO FEW DATA. N=',G14.6)                        EZPL0700
       STOP                                                              EZPL0710
   80 CONTINUE                                                           EZPL0720
C                                                                        EZPL0730
C        EVALUATE WEIGHTS                                                EZPL0740
C                                                                        EZPL0750
       DO 60 I=1,NPTS                                                    EZPL0760
       IF (NCODE) 1,2,3                                                  EZPL0770
     1 IF (Y(I).EQ.0) GO TO 2                                            EZPL0780
       WEIGHT(I)=1/ABS(Y(I))                                             EZPL0790
       GO TO 10                                                          EZPL0800
```

```
    2 WEIGHT(I)=1                                                          EZPL0810
      GO TO 10                                                             EZPL0820
    3 WEIGHT(I)=1/WEIGHT(I)**2                                             EZPL0830
   10 CONTINUE                                                             EZPL0840
      SUM=SUM+WEIGHT(I)*Y(I)                                               EZPL0850
      SUMW=SUMW+WEIGHT(I)                                                  EZPL0860
   60 CONTINUE                                                             EZPL0870
      SUM=SUM/SUMW                                                         EZPL0880
C      CALCULATE THE WEIGHTED MEAN AND VARIANCE                            EZPL0890
      YBAR=SUM                                                             EZPL0900
      SUMY=0                                                               EZPL0910
      DO 50 I=1,NPTS                                                       EZPL0920
      SUMY=SUMY+WEIGHT(I)*(Y(I)-SUM)**2                                    EZPL0930
   50 CONTINUE                                                             EZPL0940
      YVAR=SUMY                                                            EZPL0950
      RETURN                                                               EZPL0960
      END                                                                  EZPL0970
```

```
      SUBROUTINE OUTPUT(X,N,Y,NPTS,NPARM,A1,WEIGHT,DATAID,ND)              EZPL0980
      COMMON /PRM/RGAS,RENRGY,TCRIT,PCRIT,RHOC,W,ALPHA,BETA,XMW            EZPL0990
     1   ,A(40),B(7),NTERMS,NPAR1,NUMB,RTOP,RMIDL,RMIDV                   EZPL1000
      DIMENSION X(NPTS,N),Y(NPTS),A1(NPARM),WEIGHT(NPTS),DATAID(NPTS,ND)EZPL1010
      DIMENSION HEADER(20)                                                 EZPL1020
      DIMENSION Z(44)                                                      EZPL1030
  100 FORMAT(1X,8G14.6)                                                    EZPL1040
  200 FORMAT(20A4)                                                         EZPL1050
  300 FORMAT(/////1X,'AVERAGE ABSOLUTE DEVIATION',G14.6)                   EZPL1060
  400 FORMAT(26X,20A4//)                                                   EZPL1070
  500 FORMAT(1H1)                                                          EZPL1080
 1100 FORMAT(16I5)                                                         EZPL1090
      DATA IRHO,IDH,IVP/30,40,75/                                          EZPL1100
      READ 200,HEADER                                                      EZPL1110
      PRINT 500                                                            EZPL1120
      PRINT 400,HEADER                                                     EZPL1130
      PRINT 100                                                            EZPL1140
      PRINT 1600                                                           EZPL1150
 1600 FORMAT(5X,'DATAID',8X,'YEXP',8X,'YCALC',7X,'PERCENT',7X,'DELTA'     EZPL1160
     1  ,8X,'WEIGHT',6X,'CONTROL',9X,'X2',11X,'X3',11X,'X4'/57X,'X''S...'EZPL1170
     2  ,//)                                                              EZPL1180
      SUM1=0                                                               EZPL1190
      J0=0                                                                 EZPL1200
      SUM2=0                                                               EZPL1210
      SUM=0                                                                EZPL1220
```

```
      NDIM=N+NPARM                                                          EZPL1230
      DO 10 J=1,NPARM                                                       EZPL1240
      Z(N+J)=A1(J)                                                          EZPL1250
   10 CONTINUE                                                              EZPL1260
      DO 20 I=1,NPTS                                                        EZPL1270
      DO 50 J=1,N                                                           EZPL1280
      Z(J)=X(I,J)                                                           EZPL1290
   50 CONTINUE                                                              EZPL1300
      YC=FUNCN(Z,NDIM)                                                      EZPL1310
      PERC=100*(YC-Y(I))/Y(I)                                               EZPL1320
      DIFF=Y(I)-YC                                                          EZPL1330
      PRINT 2000,(DATAID(I,K),K=1,ND),Y(I),YC,PERC,DIFF,WEIGHT(I),          EZPL1340
     1 (X(I,K),K=1,N)                                                       EZPL1350
      J0=J0+1                                                               EZPL1360
      SUM=SUM+ABS(PERC)                                                     EZPL1370
      SUM1=SUM1+ABS(PERC)                                                   EZPL1380
      SUM2=SUM2+ABS(DIFF)                                                   EZPL1390
 2000 FORMAT(1X,3A4,1X,9G13.5,(/53X,6G13.5))                                EZPL1400
   20 CONTINUE                                                              EZPL1410
      SUM1=SUM1/J0                                                          EZPL1420
      SUM2=SUM2/J0                                                          EZPL1430
      PRINT 100                                                             EZPL1440
      CALL MESSG('AVE. ABS. PERCENT,NUMBER PTS.,AVE.ABS.DEVIATION ',48)     EZPL1450
      PRINT 100,SUM1,J0,SUM2                                                EZPL1460
      PRINT 100                                                             EZPL1470
      SUM=SUM/NPTS                                                          EZPL1480
      PRINT 300,SUM                                                         EZPL1490
      PRINT 100                                                             EZPL1500
      PRINT 100                                                             EZPL1510
      PRINT 500                                                             EZPL1520
      RETURN                                                                EZPL1530
      END                                                                   EZPL1540
```

```
//LKED.S4LIB DD DSN=S4.KGOIN.MOD,DISP=SHR                                 EZPL1550
//LKED.SYSIN DD *                                                         EZPL1560
   INCLUDE S4LIB(EZFIT)                                                   EZPL1570
   ENTRY MAIN                                                             EZPL1580
//GO.SYSIN DD *                                                           EZPL1590
```

```
    5                                   MINIMUN CURFIT OUTPUT
    3                                   SUBROUTINE DATA3     2
 0.001                                  MARQUART                                    3
25.
    0     0                               UNCONSTRAINED ,PRECISION     5
    5                                   NO ERROR MESSAGES
                                        DUMMY
    0     3
                                        DUMMY                                       9
    3     4
    1     2     3     4     5     6     7     8     9    10

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

```
   +1
10.7315
    1
   10
1.          1.01
2.          7.99
3.          27.01
4.          63.99
5.          75.01
6.          215.99
7.          343.01
8.           511.99
9.           729.01
10.         999.99
                    POLYNOMIAL REGRESSION    DEGREE 2
                    POLYNOMIAL REGRESSION    DEGREE 3
```

Example Output of EZFIT for a Polynomial Regression

PROGRAM STATUS SUMMARY

EZFIT IS OPERATING IN MODE TYPE 5

DATA READ BY ROUTINE DATA3
INITIAL VALUE OF ACCELERATION PARAMETER LAMBDA= 0.100000E-02
METHOD OF DERIVATIVE CALCULATION IS = 0
CONSTRAINT MODE IS = 0
ERROR MESSAGE CONTROL IS = 5
CONVERGENCE CRITERIA EPS= 0.100000E-02
WEIGHT METHOD IS = 1
UNIVERSAL GAS CONSTANT IS = 10.7315

TIME	NUMB	NOT FITTED PARMS	FITTED PARMS	NNTERM	FITTING RANGE	
25.0000	0	0	3	0	3	4

PARM FITTING ORDER

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

INITIAL VALUES

0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

NUMBER OF POINTS	NO OF INDEPENDENT VAR
10	1

NPTRHO	NPTH	NPTVP	NPTS
0	0	0	10

```
NUMBER OF PARAMETERS, NTERMS
             3                3

ITERATION     1

AVERAGE ABSOLUTE DEVIATION
   99.9998
INITIAL VALUE OF OBJECTIVE FCN
   1.42857

AVERAGE ABSOLUTE DERIVATIVE OF FCN
   1.00000         5.50000         38.5000

MAX SCALED PARM DELTA,PARM NO.
   0.21847                         3
TRIAL OBJECTIVE FCN
             0   0.125804

RELATIVE CHANGE IN PARAMETERS

  1: -1.00        2: -1.00        3: -1.00

LENGTH OF PARAMETER CHANGE
   14.7929

NEW PARMS

   6.23195        -11.7398         6.49380

OBJECTIVE FCN
  0.125804

PARM VARIANCE
  1:   11.4        2:   14.5        3:   3.62

ELASPED TIME
  0.217315


ITERATION     2

AVERAGE ABSOLUTE DEVIATION
   24.2912
```

```
INITIAL VALUE OF OBJECTIVE FCN
  0.125804

AVERAGE ABSOLUTE DERIVATIVE OF FCN
   1.00002          5.50006          38.5002

MAX SCALED PARM DELTA,PARM NO.
   1.79770                3
TRIAL OBJECTIVE FCN
               0   0.107375

RELATIVE CHANGE IN PARAMETERS

  1:-0.436        2:-0.346        3:-0.179

LENGTH OF PARAMETER CHANGE
   7.98680

NEW PARMS

   11.0531         -17.9469         7.91424

OBJECTIVE FCN
  0.107375

PARM VARIANCE
  1:   13.9        2:   17.8        3:   4.30

ELASPED TIME
  0.301577


ITERATION     3

AVERAGE ABSOLUTE DEVIATION
   21.3401
INITIAL VALUE OF OBJECTIVE FCN
  0.107375

AVERAGE ABSOLUTE DERIVATIVE OF FCN
  0.999995         5.49997          38.4998

MAX SCALED PARM DELTA,PARM NO.
  0.101995               3
TRIAL OBJECTIVE FCN
               0   0.107319
```

RELATIVE CHANGE IN PARAMETERS

1:-0.246E-01 2:-0.195E-01 3:-0.101E-01

LENGTH OF PARAMETER CHANGE
0.459960
RATIO OF CHANGE IN OBJECTIVE FUNCTION IS LESS THAN EPS 0.100000E-02

PART = 1 ITERATION = 3
WEIGHT CODE= 1

NUMBER	PARAMETER	STANDARD ERROR	VARIANCE	(A/SE)**2
1	11.0531	1.22257	13.9203	81.7361
2	-17.9469	1.38066	17.7529	168.969
3	7.91424	0.679306	4.29763	135.734

CHISQUARED 0.107375 DEGREES OF FREEDOM 7
F-STATISTIC FOR CORRELATION COEFFICIENT FR= 20.8128
F-STATISTIC ON CHANGE IN CHISQUARED FROM PREVIOUS PART= 1.98272
DEGREES OF FREEDOM ARE NU1= 3 NU2= 6

POLYNOMIAL REGRESSION DEGREE 2

DATAID		YEXP	YCALC	PERCENT	DELTA X'S...	WEIGHT	CONTROL
GEN	0001	1.0100	1.0204	1.0308	-0.10411E-01	0.98030	1.0000
GEN	0002	7.9900	6.8163	-14.690	1.1737	0.15664E-01	2.0000
GEN	0003	27.010	28.441	5.2965	-1.4306	0.13707E-02	3.0000
GEN	0004	63.990	65.893	2.9745	-1.9034	0.24422E-03	4.0000
GEN	0005	75.010	119.17	58.878	-44.165	0.17773E-03	5.0000
GEN	0006	215.99	188.28	-12.827	27.705	0.21435E-04	6.0000
GEN	0007	343.01	273.22	-20.346	69.787	0.84994E-05	7.0000
GEN	0008	511.99	373.99	-26.954	138.00	0.38148E-05	8.0000
GEN	0009	729.01	490.58	-32.705	238.43	0.18816E-05	9.0000
GEN	0010	999.99	623.01	-37.699	376.98	0.10000E-05	10.000

AVE. ABS. PERCENT	NUMBER PTS.	AVE. ABS. DEVIATION
21.3401	10	89.9582

AVERAGE ABSOLUTE DEVIATION 21.3401

```
NUMBER OF PARAMETERS, NTERMS
              4                4

ITERATION     1

AVERAGE ABSOLUTE DEVIATION
   21.3401
INITIAL VALUE OF OBJECTIVE FCN
  0.125271

AVERAGE ABSOLUTE DERIVATIVE OF FCN
  0.999995         5.49997          38.4998          302.500

MAX SCALED PARM DELTA,PARM NO.
   6.27766                4
TRIAL OBJECTIVE FCN
              0  0.873773E-01

RELATIVE CHANGE IN PARAMETERS

  1: 0.417       2: 0.513       3: 0.696       4: -1.00

LENGTH OF PARAMETER CHANGE
   7.63627

NEW PARMS

   7.79956        -11.8647         4.66699        0.434999

OBJECTIVE FCN
  0.873773E-01

PARM VARIANCE
  1:  14.5       2:  21.5       3:  9.05       4:  1.09

ELASPED TIME
  0.548258


ITERATION     2

AVERAGE ABSOLUTE DEVIATION
   16.4018
INITIAL VALUE OF OBJECTIVE FCN
  0.873773E-01

AVERAGE ABSOLUTE DERIVATIVE OF FCN
  0.999974         5.49986          38.4994          302.500
```

```
MAX SCALED PARM DELTA,PARM NO.
   18.8577                    4
TRIAL OBJECTIVE FCN
              0   0.448081E-01

RELATIVE CHANGE IN PARAMETERS

   1: -2.94        2: -2.85        3: -2.86        4:-0.618

LENGTH OF PARAMETER CHANGE
   22.9226

NEW PARMS

  -4.01558         6.40577        -2.51263         1.13866

OBJECTIVE FCN
  0.448081E-01

PARM VARIANCE
   1:  26.8        2:  41.1        3:  16.4        4:  1.73

ELASPED TIME
  0.647248


ITERATION    3

AVERAGE ABSOLUTE DEVIATION
   11.6921
INITIAL VALUE OF OBJECTIVE FCN
  0.448081E-01

AVERAGE ABSOLUTE DERIVATIVE OF FCN
   1.00004         5.49985         38.5002         302.494

MAX SCALED PARM DELTA,PARM NO.
   7.51088                    4
TRIAL OBJECTIVE FCN
              0   0.408196E-01

RELATIVE CHANGE IN PARAMETERS

   1:-0.540        2:-0.532        3:-0.531        4:-0.196

LENGTH OF PARAMETER CHANGE
   9.13138
```

```
NEW PARMS
  -8.73173         13.6827         -5.36026         1.41659

OBJECTIVE FCN
  0.408196E-01

PARM VARIANCE
  1:   31.3       2:   48.0       3:   19.1       4:   1.97

ELASPED TIME
  0.743612


ITERATION     4

AVERAGE ABSOLUTE DEVIATION
   11.3756
INITIAL VALUE OF OBJECTIVE FCN
  0.408196E-01

AVERAGE ABSOLUTE DERIVATIVE OF FCN
   1.00000         5.49999         38.5002         302.499

MAX SCALED PARM DELTA,PARM NO.
  0.302499                4
TRIAL OBJECTIVE FCN
              0   0.408136E-01

RELATIVE CHANGE IN PARAMETERS

  1:-0.213E-01   2:-0.210E-01   3:-0.209E-01   4:-0.783E-02

LENGTH OF PARAMETER CHANGE
  0.367744
RATIO OF CHANGE IN OBJECTIVE FUNCTION IS LESS THAN EPS  0.100000E-02
```

PART = 2 ITERATION = 4
WEIGHT CODE= 1

NUMBER	PARAMETER	STANDARD ERROR	VARIANCE	(A/SE)**2
1	-8.73173	1.12947	31.2520	59.7660
2	13.6827	1.39915	47.9582	95.6341
3	-5.36026	0.882329	19.0719	36.9071
4	1.41659	0.283790	1.97300	24.9170

CHISQUARED 0.406196E-01 DEGREES OF FREEDOM 6
F-STATISTIC FOR CORRELATION COEFFICIENT FR= 42.5062
F-STATISTIC ON CHANGE IN CHISQUARED FROM PREVIOUS PART= 10.3444
DEGREES OF FREEDOM ARE NU1= 4 NU2= 5

POLYNOMIAL REGRESSION DEGREE 3

DATAID		YEXP	YCALC	PERCENT	DELTA X'S...	WEIGHT	CONTROL
GEN	0001	1.0100	1.0073	-0.26590	0.26855E-02	0.98030	1.0000
GEN	0002	7.9900	8.5254	6.7008	-0.53540	0.15664E-01	2.0000
GEN	0003	27.010	22.322	-17.356	4.6879	0.13707E-02	3.0000
GEN	0004	63.990	50.897	-20.461	13.093	0.24422E-03	4.0000
GEN	0005	75.010	102.75	36.981	-27.740	0.17773E-03	5.0000
GEN	0006	215.99	186.38	-13.709	29.611	0.21435E-04	6.0000
GEN	0007	343.01	310.29	-9.5402	32.724	0.84994E-05	7.0000
GEN	0008	511.99	482.97	-5.6683	29.021	0.38148E-05	8.0000
GEN	0009	729.01	712.93	-2.2059	16.082	0.18816E-05	9.0000
GEN	0010	999.99	1008.7	0.86729	-8.6729	0.10000E-05	10.000

AVE. ABS. PERCENT. NUMBER PTS.. AVE. ABS. DEVIATION
11.3756 10 16.2163

AVERAGE ABSOLUTE DEVIATION 11.3756

```
  100 FORMAT (1X,8G14.6)                                                    EZMN0010
  200 FORMAT(1X,'F-STATISTIC FOR CORRELATION COEFFICIENT FR=',G14.6/        EZMN0020
     1' F-STATISTIC ON CHANGE IN CHISQUARED FROM PREVIOUS PART= ',G14.6/EZMN0030
     2' DEGREES OF FREEDOM ARE NU1=',I5,'  NU2= ',I5)                       EZMN0040
  300 FORMAT (1H1,'PART = ',I4,'    ITERATION = ',I4)                       EZMN0050
  400 FORMAT (6X,'YEXP',10X,'YFIT',10X,'PERCENT',8X,'X''S')                 EZMN0060
  500 FORMAT (1H1)                                                          EZMN0070
  600 FORMAT (1X,5A4,' WEIGHT CODE= ',I4)                                   EZMN0080
  700 FORMAT(1X,'  INPUT DATA     X''S  Y')                                EZMN0090
  800 FORMAT(1H0,'ITERATION',I5)                                            EZMN0100
  900 FORMAT(1X,'     ************  TIME EXCEDED *******')                  EZMN0110
 1200 FORMAT(16I5)                                                          EZMN0120
 1100 FORMAT(8F10.0)                                                        EZMN0130
 1300 FORMAT(1H1,5X,'YEXP',10X,'YFIT',10X,'PERCENT',8X,'X''S'//)            EZMN0140
 1400 FORMAT(20A4)                                                          EZMN0150
 1600 FORMAT(1X,3A4,8G14.6,(/13X,8G14.6))                                   EZMN0160
 2100 FORMAT(1X,8X,'NUMBER',4X,'PARAMETER',1X,'STANDARD ERROR',6X,          EZMN0170
     1 'VARIANCE',5X,'(A/SE)**2')                                           EZMN0180
 2200 FORMAT(1X,'CHISQUARED ',G14.6,'  DEGREES OF FREEDOM',I5)              EZMN0190
 2300 FORMAT (1X,'DENS%',G14.6,'  H%',G14.6,'  VP%',G14.6,                  EZMN0200
     1 'TOTAL%',G14.6)                                                      EZMN0210
 2400 FORMAT(1X,2A4,' TC=',G14.6,'PC=',G14.6,'RC=',G14.6,'MW=',G14.6,       EZMN0220
     1 'ALPHA=',G14.6,'BETA=',G14.6,/' OMEGA=',G14.6////)                   EZMN0230
 2500 FORMAT(1X,8G14.6,3A4)                                                 EZMN0240
 2600 FORMAT(1X,6G14.6,28X,3A4)                                             EZMN0250
 2700 FORMAT(//52X,'PROGRAM STATUS SUMMARY'///                              EZMN0260
     1 45X,'EZFIT IS OPERATING IN MODE TYPE',I5///)                         EZMN0270
 2800 FORMAT(6X,'TIME',16X,'NUMB',4X,'NOT FITTED PARMS',2X,'FITTED PARMSEZMN0280
     1',2X,'NNTERM',13X,'FITTING RANGE'/)                                   EZMN0290
 2900 FORMAT(/1X,'DATA READ BY ROUTINE DATA',I1,/' INITIAL VALUE OF ACCEEZMN0300
     1LERATION PARAMETER LAMBDA=',G14.6/' METHOD OF DERIVATIVE CALCULATIEZMN0310
     2ON IS =' I5     /' CONSTRAINT MODE IS ='  ,I5   /' ERROR MESSAGE CEZMN0320
     3ONTROL IS =',I5)                                                      EZMN0330
 3100 FORMAT(1X,'RATIO OF CHANGE IN OBJECTIVE FUNCTION IS LESS THAN EPS'EZMN0340
     1,G14.6)                                                               EZMN0350
 3200 FORMAT(11X,'NPTRHO',8X,'NPTH',10X,'NPTVP',9X,'NPTS')                  EZMN0360
 3300 FORMAT(1X,8(I3,':',G10.3),/(1X,8(I3,':',G10.3)))                      EZMN0370
 3400 FORMAT( 1X,'CONVERGENCE CRITERIA EPS= ',G14.6,                        EZMN0380
     1/' WLIGHT METHOD IS = ',I5/' UNIVERSAL GAS CONSTANT IS = ',G14.6/)EZMN0390
 3500 FORMAT(53X,'REGRESSION SERIES BEGINNING'////)                         EZMN0400
C                                                                           EZMN0410
C                      EZFIT COMMON BLOCKS                                  EZMN0420
C                                                                           EZMN0430
      COMMON /PRP/ICOMP(20),CPC(20),CRC(20),CMW(20),CW(20) ,CTC(20)         EZMN0440
     1 ,CA(20),CB(20),CNAME(20,2)                                           EZMN0450
      COMMON /PRM/RGAS,RENRGY,TCRIT,PCRIT,RHOC,W,ALPHA,BETA,XMW             EZMN0460
     1   ,A(40),B(7),NTERMS,NPARM,NUMB,RTOP,RMIDL,RMIDV                     EZMN0470
      COMMON /XTN/AXTN(60)                                                  EZMN0480
      COMMON /DAT/IPRES,ISTATE(20)                                          EZMN0490
C*************************EZFIT*************************************EZMN0500
```

```
      DIMENSION X(1000,3),Y(1000),SIGMAY(1000),YFIT(1000),                EZMN0510
     1 WEIGHT(1000),XX(3000),DATAID(1000,3),DD(3000)                      EZMN0520
C                     MODIFIED FOR EZ EXTENSION                          EZMN0530
       DIMENSION ITERM(100),A1(100),STORE(205),SIGMAA(100),STORED(100)    EZMN0540
      INTEGER DF  ,FPARM                                                  EZMN0550
      REAL NAME(5)                                                        EZMN0560
      EQUIVALENCE (XX(1),X(1,1)),(WEIGHT(1),SIGMAY(1))                    EZMN0570
      EQUIVALENCE (DD(1),DATAID(1,1))                                     EZMN0580
      CALL LBLEZ                                                          EZMN0590
      PRINT 500                                                           EZMN0600
      CALL CPUTIM                                                         EZMN0610
      DO 80 I=1,20                                                        EZMN0620
      ICOMP(I)=0                                                          EZMN0630
      ISTATE(I)=0                                                         EZMN0640
   80 CONTINUE                                                            EZMN0650
C                     INPUT CONTROL DATA                                  EZMN0660
      READ 1200,IOUT                                                      EZMN0670
      READ 1200,IDATA                                                     EZMN0680
      READ 1100,DFLMDA,EPS                                                EZMN0690
      IF(EPS.EQ.0)EPS=.001                                                EZMN0700
      READ 1100 ,TMAX                                                     EZMN0710
      READ 1200,ISTATE(3),ISTATE(5)                                       EZMN0720
      READ 1200,ISTATE(4)                                                 EZMN0730
      READ 1200,NUMB                                                      EZMN0740
      READ 1200 ,NFPARM,FPARM                                             EZMN0750
      READ 1200,NNTERM                                                    EZMN0760
      READ 1200,NU1FR,NU1TO                                               EZMN0770
      READ 1200, ITERM                                                    EZMN0780
      READ 1100,A1                                                        EZMN0790
      READ 1200 ,NCODE                                                    EZMN0800
      READ 1100,RGAS                                                      EZMN0810
      READ 1200,N                                                         EZMN0820
      READ 1200,NPTS                                                      EZMN0830
      PRINT 2700,IOUT                                                     EZMN0840
      PRINT 2900,IDATA,DFLMDA,ISTATE(5),ISTATE(3),ISTATE(4)               EZMN0850
      PRINT 3400,EPS,NCODE,RGAS                                           EZMN0860
      PRINT 2800                                                          EZMN0870
       PRINT 100,TMAX,NUMB,NFPARM,FPARM,NNTERM,NU1FR,NU1TO                EZMN0880
      PRINT 100                                                           EZMN0890
      CALL MESSG('PARM FITTING ORDER',18)                                 EZMN0900
      PRINT 100                                                           EZMN0910
      PRINT 100,ITERM                                                     EZMN0920
      PRINT 100                                                           EZMN0930
      CALL MESSG('INITIAL VALUES',14)                                     EZMN0940
      PRINT 100                                                           EZMN0950
      PRINT 100,A1                                                        EZMN0960
      PRINT 100                                                           EZMN0970
      CALL MESSG('NUMBER OF POINTS,NO OF INDEPENDENT VAR',40)             EZMN0980
      PRINT 100,NPTS,N                                                    EZMN0990
      PRINT 100                                                           EZMN1000
```

```
      ND=3                                                                  EZMN1010
C                     INPUT DATA                                            EZMN1020
      IF(IDATA.EQ.1) CALL DATA (X,N,Y,NPTS,WEIGHT,YBAR,YVAR,NCODE,          EZMN1030
     1  NPTRHO,NPTH,NPTVP,DATAID)                                           EZMN1040
      IF(IDATA.EQ.2) CALL DATA2(X,N,Y,NPTS,WEIGHT,YBAR,YVAR,NCODE,          EZMN1050
     1  NPTRHO,NPTH,NPTVP,DATAID)                                           EZMN1060
      IF(IDATA.EQ.3)CALL DATA3(X,N,Y,NPTS,WEIGHT,YBAR,YVAR,NCODE,           EZMN1070
     1 DATAID,ND)                                                          EZMN1080
      PRINT 100                                                             EZMN1090
      PRINT 3200                                                            EZMN1100
      PRINT 100,NPTRHO,NPTH,NPTVP,NPTS                                      EZMN1110
      ISTATE(2)=IOUT                                                        EZMN1120
      IF(IOUT.GE.3) GO TO 1130                                              EZMN1130
C                    DISPLAY DATA                                           EZMN1140
      PRINT 700                                                             EZMN1150
      DO 70 I=1,NPTS                                                        EZMN1160
      PRINT 1600,(DD(I+(K-1)*NPTS),K=1,3),(XX(I+(K-1)*NPTS),K=1,N),Y(I)     EZMN1170
   70 CONTINUE                                                              EZMN1180
 1130 CONTINUE                                                              EZMN1190
      PRINT 500                                                             EZMN1200
      PRINT 3500                                                            EZMN1210
      IPRES=0                                                               EZMN1220
      NPART=1                                                               EZMN1230
      CHI1=1                                                                EZMN1240
C                     START REGRESSION                                      EZMN1250
      DO 40 NU1=NU1FR,NU1TO                                                 EZMN1260
      NTERMS=NU1-NNTERM                                                     EZMN1270
      NPARM=NU1+NFPARM                                                      EZMN1280
      CALL MESSG('NUMBER OF PARAMETERS, NTERMS',28)                         EZMN1290
      PRINT 100,NPARM,NTERMS                                                EZMN1300
      DF=NPTS-NU1                                                           EZMN1310
      CHI=1.E+60                                                            EZMN1320
      DO 1160 LL=1,NPARM                                                    EZMN1330
      STORE(1+LL)=A1(LL)                                                    EZMN1340
 1160 CONTINUE                                                              EZMN1350
      IF(IOUT.LT.10) GO TO 1120                                             EZMN1360
C                      MODIFIED FOR EZ EXTENSION                            EZMN1370
      DO 3110 LL=1,40                                                       EZMN1380
 3110 A(LL)=A1(LL)                                                          EZMN1390
      DO 3120 LL=1,60                                                       EZMN1400
      AXTN(LL)=A1(LL+40)                                                    EZMN1410
 3120 CONTINUE                                                              EZMN1420
C                     PERFORM OUTPUT ONLY                                   EZMN1430
      CHISQR=-10                                                            EZMN1440
      GO TO 1110                                                            EZMN1450
 1120 CONTINUE                                                              EZMN1460
      FLAMDA=DFLMDA                                                         EZMN1470
      STORE(1)=CHI                                                          EZMN1480
      DO 260 L=1,NPARM                                                      EZMN1490
      STORE(1+L)=A1(L)                                                      EZMN1500
```

```
  260 CONTINUE                                                          EZMN1510
      DO 5 I=1,20                                                       EZMN1520
      PRINT 800,I                                                       EZMN1530
C                     PERFORM REGRESSION                              EZMN1540
      CALL CURFIT (X,N,Y,WEIGHT,NPTS,NU1,A1,SIGMAA,FLAMDA,              EZMN1550
     1 YFIT,CHISQR,NPARM,ITERM)                                         EZMN1560
      RMS=SQRT(CHISQR*DF/NPTS)                                          EZMN1570
      RMS=RMS*100                                                       EZMN1580
      SSQ=0                                                             EZMN1590
      DO 1170 L=1,NPARM                                                 EZMN1600
      DEL=STORE(L+1)-A1(L)                                              EZMN1610
      STORED(L)=0                                                       EZMN1620
      IF(A1(L).NE.0)STORED(L)=DEL/A1(L)                                 EZMN1630
      SSQ=SSQ+DEL*DEL                                                   EZMN1640
 1170 CONTINUE                                                          EZMN1650
      PRINT 100                                                         EZMN1660
      CALL MESSG('RELATIVE CHANGE IN PARAMETERS',29)                    EZMN1670
      PRINT 100                                                         EZMN1680
      PRINT 3300,(JJ,STORED(JJ),JJ=1,NPARM)                             EZMN1690
      PRINT 100                                                         EZMN1700
      SSQ=SQRT(SSQ)                                                     EZMN1710
      CALL MESSG('LENGTH OF PARAMETER CHANGE',26)                       EZMN1720
      PRINT 100,SSQ                                                     EZMN1730
      IF(I.NE.1) GO TO 1140                                             EZMN1740
      DO 1150 L=1,NU1                                                   EZMN1750
 1150 STORE(1+NPARM+L)=SIGMAA(L)                                        EZMN1760
 1140 CONTINUE                                                          EZMN1770
C                     CHECK RESULTS OF REGRESSION                     EZMN1780
      IF(CHI.LT.CHISQR) GO TO 220                                       EZMN1790
      IF(ABS(CHI-CHISQR).LE.EPS*CHISQR) GO TO 230                       EZMN1800
      IF(FLAMDA.GT.100.AND.CHI.GT.1.E+50) GO TO 240                     EZMN1810
      CHI=CHISQR                                                        EZMN1820
      PRINT 100                                                         EZMN1830
      CALL MESSG('NEW PARMS',9)                                         EZMN1840
      PRINT 100                                                         EZMN1850
      PRINT 100,(A1(L),L=1,NPARM)                                       EZMN1860
      PRINT 100                                                         EZMN1870
      CALL MESSG('OBJECTIVE FCN',13)                                    EZMN1880
      PRINT 100,CHI                                                     EZMN1890
      PRINT 100                                                         EZMN1900
      CALL MESSG('PARM VARIANCE',13)                                    EZMN1910
      PRINT 3300,(ITERM(L),SIGMAA(L),L=1,NU1)                           EZMN1920
      PRINT 100                                                         EZMN1930
      STORE(1)=CHI                                                      EZMN1940
      DO 20 L=1,NPARM                                                   EZMN1950
      STORE(1+L)=A1(L)                                                  EZMN1960
   20 CONTINUE                                                          EZMN1970
      DO 90 L=1,NU1                                                     EZMN1980
      STORE(1+NPARM+L)=SIGMAA(L)                                        EZMN1990
   90 CONTINUE                                                          EZMN2000
```

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      IF(I.EQ.1)CALL CPUTIM(STIME)                                      EZMN2010
      CALL CPUTIM(TIME,ST2)                                             EZMN2020
      CALL MESSG('ELASPED TIME',12)                                     EZMN2030
      PRINT 100,ST2                                                     EZMN2040
      PRINT 100                                                         EZMN2050
      PRINT 100                                                         EZMN2060
C                     CHECK TIME                                        EZMN2070
      IF(ISTATE(2).EQ.9.OR.ISTATE(2).EQ.8) GO TO 250                    EZMN2080
      IF(I.EQ.1.AND.(2*STIME).GT.TMAX) GO TO 210                        EZMN2090
      IF((TIME+STIME).LT.TMAX.AND.(TIME+ST2).LT.TMAX) GO TO 5           EZMN2100
  210 CONTINUE                                                          EZMN2110
      PRINT 900                                                         EZMN2120
      GO TO 8                                                           EZMN2130
    5 CONTINUE                                                          EZMN2140
      CALL MESSG('NO CONVERGENCE IN 20 ITERATIONS',31)                  EZMN2150
      GO TO 8                                                           EZMN2160
  220 CONTINUE                                                          EZMN2170
      CALL MESSG('OBJECTIVE FCN INCREASED',23)                          EZMN2180
      GO TO 8                                                           EZMN2190
  230 CONTINUE                                                          EZMN2200
      PRINT 3100,EPS                                                    EZMN2210
      GO TO 8                                                           EZMN2220
  240 CONTINUE                                                          EZMN2230
      CALL MESSG('NO IMPROVEMENT OVER INITIAL',27)                      EZMN2240
      GO TO 8                                                           EZMN2250
  250 CONTINUE                                                          EZMN2260
      CALL MESSG('NO REGRESSION MADE',18)                               EZMN2270
      GO TO 8                                                           EZMN2280
C           CONVERGED OUTPUT                                            EZMN2290
    8 CONTINUE                                                          EZMN2300
      CHISQR=STORE(1)                                                   EZMN2310
      DO 170 L=1,NPARM                                                  EZMN2320
      A1(L)=STORE(1+L)                                                  EZMN2330
  170 CONTINUE                                                          EZMN2340
 1110   CONTINUE                                                        EZMN2350
      PRINT 300,NPART,I                                                 EZMN2360
      DO 120 L=1,NU1                                                    EZMN2370
      SIGMAA(L)=STORE(1+NPARM+L)                                        EZMN2380
  120 CONTINUE                                                          EZMN2390
      NDIM=NPARM+N                                                      EZMN2400
      NPART=NPART+1                                                     EZMN2410
      PRINT 600,NAME,NCODE                                              EZMN2420
      PRINT 100                                                         EZMN2430
      PRINT 2100                                                        EZMN2440
      DO 60 J=1,NU1                                                     EZMN2450
      JJ=ITERM(J)                                                       EZMN2460
      SE=SQRT(SIGMAA(J)*CHISQR)                                         EZMN2470
      ASE=0                                                             EZMN2480
      IF(SE.NE.0)ASE=(A1(JJ)/SE)**2                                     EZMN2490
      PRINT 100,JJ,A1(JJ),SE,SIGMAA(J),ASE                              EZMN2500
```

```
   60 CONTINUE                                                          EZMN2510
      PRINT 100                                                         EZMN2520
C                     CALCULATE STATISTICS                            EZMN2530
      PRINT 2200,CHISQR,DF                                              EZMN2540
      NU2=NPTS-NU1-1                                                    EZMN2550
      CHIN=CHISQR*(NU2+1)                                               EZMN2560
      FR=(1-CHIN/YVAR)*NU2*YVAR/CHIN/NU1                                EZMN2570
      FCHI=(CHI1-CHIN)*NU2/CHIN                                         EZMN2580
      CHI1=CHIN                                                         EZMN2590
      PRINT 200,FR,FCHI,NU1,NU2                                         EZMN2600
      PRINT 100                                                         EZMN2610
      PRINT 100                                                         EZMN2620
      SAVE=ISTATE(4)                                                    EZMN2630
      ISTATE(4)=0.                                                      EZMN2640
C                   OUTPUT RESULTS FOR DATA POINTS                    EZMN2650
      CALL OUTPUT(X,N,Y,NPTS,NPARM,A1,WEIGHT,DATAID,ND)                 EZMN2660
      ISTATE(4)=SAVE                                                    EZMN2670
   40 CONTINUE                                                          EZMN2680
      STOP                                                              EZMN2690
      END                                                               EZMN2700
```

```
C    SUBROUTINE CONVR                                                    EZCN0010
C                                                                        EZCN0020
C    PURPOSE                                                             EZCN0030
C      CONVERTS A 4 DIGIT INTEGER INTO EBCDIC CODE                       EZCN0040
C                                                                        EZCN0050
C    USAGE                                                               EZCN0060
C      CALL CONVR(INUM,ICHAR,CHAR)                                       EZCN0070
C                                                                        EZCN0080
C    DESCRIPTION OF PARAMETERS                                           EZCN0090
C      INUM - INTEGER TO BE CONVERTED                                    EZCN0100
C      FCHAR - EBCDIC CODE IN AN INTEGER VARIABLE                        EZCN0110
C      CHAR - EBCDIC CODE IN A REAL VARIABLE                             EZCN0120
C                                                                        EZCN0130
      SUBROUTINE CONVR(INUM,ICHAR,CHAR)                                  EZCN0140
      EQUIVALENCE(IDUM,DUM)                                              EZCN0150
      ICHAR=0                                                            EZCN0160
      IFACT=1                                                            EZCN0170
      I=INUM                                                             EZCN0180
      DO 40 J=1,4                                                        EZCN0190
      I10=I/10                                                           EZCN0200
      ICHAR=(I-I10*10+240)*IFACT+ICHAR                                   EZCN0210
      I=I10                                                              EZCN0220
      IFACT=IFACT*256                                                    EZCN0230
   40 CONTINUE                                                           EZCN0240
      IDUM=ICHAR                                                         EZCN0250
      CHAR=DUM                                                           EZCN0260
      RETURN                                                             EZCN0270
      END                                                                EZCN0280
```

```
C    FUNCTION CP                                                         EZCP0010
C                                                                        EZCP0020
C    PURPOSE                                                             EZCP0030
C      CALCULATES HEAT CAPACITY OF PRESSURE BY NUMERICAL DERIV.          EZCP0040
C                                                                        EZCP0050
C    USUAGE                                                              EZCP0060
C      RESULT = CP(T,RHO)                                                EZCP0070
C                                                                        EZCP0080
C    DESCRIPTION OF PARAMETERS                                           EZCP0090
C        T-ABSOLUTE TEMPERATURE                                          EZCP0100
C      RHO-DENSITY                                                       EZCP0110
C                                                                        EZCP0120
C    SUBROUTINES NEEDED                                                  EZCP0130
C      ENTH(T,RHO)                                                       EZCP0140
```

```
C       CALCULATES ENTHALPY                                                    EZCP0150
C                                                                              EZCP0160
      FUNCTION CP(T,RHO)                                                       EZCP0170
      COMMON /PRM/RGAS,RENRGY,TCRIT,PCRIT,RHOC,W,ALPHA,BETA,XMW                EZCP0180
     1   ,A(40),B(7),NTERMS,NPARM,NUMB,RTOP,RMIDL,RMIDV                       EZCP0190
      EPMAX=.1                                                                 EZCP0200
      EPS=.0001                                                                EZCP0210
      SAVE=T                                                                   EZCP0220
      IF(ABS(SAVE).LT.EPS) GO TO 10                                            EZCP0230
      DEL=ABS(EPS*SAVE)                                                        EZCP0240
   14 CONTINUE                                                                 EZCP0250
      DO 12 IT=1,5                                                             EZCP0260
      T=SAVE+DEL                                                               EZCP0270
      F2=ENTH(T,RHO)                                                           EZCP0280
      T=SAVE-DEL                                                               EZCP0290
      F1=ENTH(T,RHO)                                                           EZCP0300
      DFDX=(F2-F1)/2./DEL                                                      EZCP0310
C                                                                              EZCP0320
C       TESTS PRECISION OF DERIVATIVE                                          EZCP0330
C                                                                              EZCP0340
      IF(ABS(DEL*2*DFDX).GE.((10**(-6+N))*ABS(F1)))GO TO 40                    EZCP0350
      IF(ABS(DFDX).LT.1.1E-65*ABS(F1)) DFDX=1.E-65*F1                          EZCP0360
      DEL=(10**(-6+N))*ABS(F1/DFDX)                                            EZCP0370
      IF(ABS(SAVE).LT.1.E-06) GO TO 20                                         EZCP0380
      IF(DEL.GT.ABS(SAVE*EPMAX)) DEL=ABS(SAVE*EPMAX)                           EZCP0390
      GO TO 12                                                                 EZCP0400
   20 IF (DEL.GT.EPMAX) DEL=EPMAX                                              EZCP0410
   12 CONTINUE                                                                 EZCP0420
      GO TO 40                                                                 EZCP0430
   10 DEL=EPS                                                                  EZCP0440
      GO TO 14                                                                 EZCP0450
   40 CP=DFDX                                                                  EZCP0460
      T=SAVE                                                                   EZCP0470
      RETURN                                                                   EZCP0480
      END                                                                      EZCP0490
```

```
C   SUBROUTINE CURFIT                                                          EZCR0010
C                                                                              EZCR0020
C   PURPOSE                                                                    EZCR0030
C     MAKE A LEAST-SQUARES FIT TO A NON-LINEAR FUNCTION                        EZCR0040
C       WITH A LINEARIZATION OF THE FITTING FUNCTION                           EZCR0050
C                                                                              EZCR0060
C   USAGE                                                                      EZCR0070
```

```
C      CALL CURFIT (X,N,Y,WEIGHT,NPTS,NTERMS,A,                          EZCR0080
C       SIGMAA,FLAMDA,YFIT,CHISQR,NPARM,ITERM)                           EZCR0090
C                                                                        EZCR0100
C    DESCRIPTION OF PARPMETERS                                           EZCR0110
C      X      - ARRAY OF DATA POINTS FOR INDEPENDENT VARIABLE            EZCR0120
C      Y      - ARRAY OF DATA POINTS FOR DEPENDENT VARIABLE              EZCR0130
C      WEIGHT - ARRAY OF WEIGHTS FOR DATA POINTS                         EZCR0140
C      N      - NUMBER OF INDEPENDENT VARIABLES                          EZCR0150
C      NPTS   - NUMBER OF PAIRS OF DATA POINTS                           EZCR0160
C      NTERMS - NUMBER OF PARAMETERS                                     EZCR0170
C      A      - ARRAY OF PARAMETERS                                      EZCR0180
C      SIGMAA - ARRAY OF STANDARD DEVIATIONS FOR PARAMETERS A            EZCR0190
C      FLAMDA - PROPORTION OF GRADIENT SEARCH INCLUDED                   EZCR0200
C      YFIT   - ARRAY OF CALCULATED VALUES OF Y                          EZCR0210
C      CHISQ1 - REDUCED CHI SQUARE FOR FIT                               EZCR0220
C      ITERMS - ARRAY OF INDICES TO BE REGRESSED                         EZCR0230
C                                                                        EZCR0240
C    SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                       EZCR0250
C      FUNCN (X,NDIM)                                                    EZCR0260
C         EVALUATES THE FITTING FUNCTION                                 EZCR0270
C      FCHISQ (Y,WEIGHT,NPTS,NFREE,YFIT)                                 EZCR0280
C         EVALUATES REDUCED CH SQUARE FOR FIT TO DATA                    EZCR0290
C      FDERIV (X,I,NDIM)                                                 EZCR0300
C         EVALUATES THE DERIVATIVES OF THE FITTING FUNCTION              EZCR0310
C         WITH RESPECT TO THE ITH VARIABLE                               EZCR0320
C      GJEL(ARRAY,NTERMS,NTERMS+1,DET,IER)                               EZCR0330
C      SOLVES A SYSTEM BY THE GAUSS JORDAN METHOD RETURNING THE          EZCR0340
C        DETERMINANT AND THE INVERSE IN PLACE                            EZCR0350
C                                                                        EZCR0360
C                                                                        EZCR0370
C    COMMENTS                                                            EZCR0380
C      DIMENSION STATEMENT VALID FOR NTERMS UP TO 10                     EZCR0390
C      SET FLAMDA =0.001 AT BEGINNING OF SEARCH                          EZCR0400
C                                                                        EZCR0410
      SUBROUTINE CURFIT (X,N,Y,WEIGHT,NPTS,NTERMS,A,                     EZCR0420
     1 SIGMAA,FLAMDA,YFIT,CHISQR,NPARM,ITERM)                            EZCR0430
      COMMON /DAT/IPRES,ISTATE(20)                                       EZCR0440
      DOUBLE PRECISION ALPHA,DSQRT,ARRAY                                 EZCR0450
      DOUBLE PRECISION DABS                                              EZCR0460
      DIMENSION X(NPTS,N),Y(NPTS),WEIGHT(NPTS),YFIT(NPTS)                EZCR0470
      DIMENSION SIGMAA(NPARM),A(NPARM),ITERM(NPARM)                      EZCR0480
      DIMENSION ALPHA(1830),BETA(60),DERIV(60),ARRAY(3660),B(60),Z(110)  EZCR0490
      DATA IC/5/                                                         EZCR0500
      DATA IBD/0/                                                        EZCR0510
  100 FORMAT (1X,8G14.6)                                                 EZCR0520
  700 FORMAT(1X,I3,':',8(I3,':',G10.3),/(5X,8(I3,':',G10.3))  )         EZCR0530
      IF(IBD.EQ.1) GO TO 5000                                            EZCR0540
      IBD=1                                                              EZCR0550
      CALL LBLEZ                                                         EZCR0560
 5000 CONTINUE                                                           EZCR0570
```

```
      FACT=.99                                                          EZCR0580
      SUM1=0.                                                           EZCR0590
      IF(NTERMS.LE.60) GO TO 6000                                       EZCR0600
      PRINT 600                                                         EZCR0610
  600 FORMAT(1X,10('*'),' MORE THAN 35 PARAMETERS FITTED.  ONLY 60' ,   EZCR0620
     4 6(4X,'*')////)                                                   EZCR0630
      NTERMS=60                                                         EZCR0640
 6000 CONTINUE                                                          EZCR0650
      NPN=N+NPARM                                                       EZCR0660
   11 NFREE =NPTS-NTERMS                                                EZCR0670
      IF (NFREE) 13,13,20                                               EZCR0680
   13 CONTINUE                                                          EZCR0690
      PRINT 2700,NFREE                                                  EZCR0700
 2700 FORMAT(//,'DEGRES OF FREEDOM ',I4,' IS LESS THAN 1. '//)          EZCR0710
      FLAMDA =1000.                                                     EZCR0720
      CHISQR=1.E+55                                                     EZCR0730
      GO TO 110                                                         EZCR0740
C                                                                       EZCR0750
C       EVALUATE ALPHA AND BETA MATRICES                                EZCR0760
C                                                                       EZCR0770
   20 CONTINUE                                                          EZCR0780
   31 DO 34 J=1,NTERMS                                                  EZCR0790
      BETA(J)=0                                                         EZCR0800
      DO 34 K=1,J                                                       EZCR0810
   34 ALPHA(K+J*(J-1)/2)=0                                              EZCR0820
C      NOTE - 1ST N OF Z ARE VARIABLES. (N+1-NTERMS) ARE PARAMETERS     EZCR0830
      DO 44 L=1,NPARM                                                   EZCR0840
   44 Z(L+N)=A(L)                                                       EZCR0850
      DO 230 J=1,NTERMS                                                 EZCR0860
      ARRAY(J)=0                                                        EZCR0870
  230 CONTINUE                                                          EZCR0880
      IF(ISTATE(2).LE.3)PRINT 3900                                      EZCR0890
 3900 FORMAT(4X,'Y',13X,'YFIT',10X,'PERCENT')                           EZCR0900
   41 DO 50 I=1,NPTS                                                    EZCR0910
      DO 45 L=1,N                                                       EZCR0920
   45 Z(L)=X(I,L)                                                       EZCR0930
      ISTATE(1)=I                                                       EZCR0940
   62 YFIT(I)=FUNCN(Z,NPN)                                              EZCR0950
      IF(Y(I).EQ.0) GO TO 290                                           EZCR0960
      PERC=100*(Y(I)-YFIT(I))/Y(I)                                      EZCR0970
      SUM1=SUM1+ABS(PERC)                                               EZCR0980
  290 CONTINUE                                                          EZCR0990
      IF(ISTATE(2).GT.3) GO TO 220                                      EZCR1000
      IF(IC.LT.5.AND.FLAMDA.EQ.0) GO TO 220                             EZCR1010
  210 PRINT 100, Y(I),YFIT(I)  ,PERC                                    EZCR1020
  220 CONTINUE                                                          EZCR1030
      DO 43 L=1,NTERMS                                                  EZCR1040
      JJ=ITERM(L)+N                                                     EZCR1050
      DERIV(L)=FDERIV(Z,JJ,NPN)                                         EZCR1060
      ARRAY(L)=ARRAY(L)+ABS(DERIV(L))                                   EZCR1070
```

```
      IF(ABS(DERIV(L)).LT.1.E-30) DERIV(L)=0.                          EZCR1080
   43 CONTINUE                                                         EZCR1090
      DO 46 J=1,NTERMS                                                 EZCR1100
      IF(FLAMDA.GE.0)                                                  EZCR1110
     1BETA(J)=BETA(J)+WEIGHT(I)*(Y(I)-YFIT(I))*DERIV(J)                EZCR1120
      IF(FLAMDA.LT.0)BETA(J)=BETA(J)+WEIGHT(I)*Y(I)*DERIV(J)           EZCR1130
      DO 46 K=1,J                                                      EZCR1140
      ALPHA(K+J*(J-1)/2)=ALPHA(K+J*(J-1)/2)+WEIGHT(I)*DERIV(J)*DERIV(K) EZCR1150
   46 CONTINUE                                                         EZCR1160
   50 CONTINUE                                                         EZCR1170
      SUM1=SUM1/NPTS                                                   EZCR1180
      PRINT 100                                                        EZCR1190
      CALL MESSG('AVERAGE ABSOLUTE DEVIATION',26)                      EZCR1200
      PRINT 100,SUM1                                                   EZCR1210
      IC=IC+1                                                          EZCR1220
      IF(IC.GT.5) IC=1                                                 EZCR1230
C                                                                      EZCR1240
C       EVALUTAE CHI SQUARE AT STARTING POINT                          EZCR1250
C                                                                      EZCR1260
   63 CHISQ1 = FCHISQ(Y,WEIGHT,NPTS,NFREE,YFIT)                        EZCR1270
      CALL MESSG('INITIAL VALUE OF OBJECTIVE FCN',30)                  EZCR1280
      PRINT 100,CHISQ1                                                 EZCR1290
      DO 240 J=1,NTERMS                                                EZCR1300
      ARRAY(J)=ARRAY(J)/NPTS                                           EZCR1310
  240 CONTINUE                                                         EZCR1320
      PRINT 100                                                        EZCR1330
      CALL MESSG('AVERAGE ABSOLUTE DERIVATIVE OF FCN',34)              EZCR1340
      PRINT 3300,(ITERM(J),ARRAY(J),J=1,NTERMS)                        EZCR1350
 3300 FORMAT(1X,8(I3,':',G10.3),/(1X,8(I3,':',G10.3)))                 EZCR1360
C                                                                      EZCR1370
C       INVERT MODIFIED CURVATURE MATRIX TO FIND NEW PARAMETERS        EZCR1380
C                                                                      EZCR1390
   71 CONTINUE                                                         EZCR1400
      DIAG=1                                                           EZCR1410
      IF(FLAMDA.GT.0)DIAG=DIAG+FLAMDA                                  EZCR1420
      DO 74 J=1,NTERMS                                                 EZCR1430
      IF(ALPHA(J*(J+1)/2).GT.0) GO TO 280                              EZCR1440
      JJ=ITERM(J)                                                      EZCR1450
      PRINT 300,J,JJ                                                   EZCR1460
  300 FORMAT(1X,I5,' DERIVATIVE IS NOT POS. FOR PARM ',I5,20('*'))     EZCR1470
      ALPHA(J*(J+1)/2)=1.E-40                                          EZCR1480
  280 CONTINUE                                                         EZCR1490
      ARRAY(NTERMS**2+J)=BETA(J)/DSQRT(ALPHA(J*(J+1)/2))               EZCR1500
      DO 73 K=1,J                                                      EZCR1510
      ARRAY(J+(K-1)*NTERMS)=ALPHA(K+J*(J-1)/2)/DSQRT(ALPHA(J*(J+1)/2)  EZCR1520
     1 *ALPHA(K*(K+1)/2))                                              EZCR1530
      ARRAY(K+(J-1)*NTERMS)=ARRAY(J+(K-1)*NTERMS)                      EZCR1540
   73 CONTINUE                                                         EZCR1550
   74 ARRAY(J+(J-1)*NTERMS)=DIAG                                       EZCR1560
      DELM=0.                                                          EZCR1570
```

```
      IF(NTERMS.GT.1) GO TO 80                                          EZCR1580
      ARRAY(1)=1/ARRAY(1)                                               EZCR1590
      ARRAY(2)=ARRAY(2)*ARRAY(1)                                        EZCR1600
      GO TO 81                                                          EZCR1610
   80 CALL GJEL(ARRAY,NTERMS,NTERMS+1,DET,IER)                          EZCR1620
      PRINT 100                                                         EZCR1630
      IF(ISTATE(2).EQ.8) GO TO 340                                      EZCR1640
      IF(ISTATE(2).EQ.9) GO TO 260                                      EZCR1650
   81 DO 84 J=1,NTERMS                                                  EZCR1660
      JJ=ITERM(J)                                                       EZCR1670
      IF(DABS(ARRAY(NTERMS**2+J)).LT.DELM) GO TO  250                   EZCR1680
      DELM=DABS(ARRAY(NTERMS**2+J))                                     EZCR1690
      JM=JJ                                                             EZCR1700
  250 CONTINUE                                                          EZCR1710
      B(J)=A(JJ)+ARRAY(NTERMS**2+J)/DSQRT(ALPHA(J*(J+1)/2))             EZCR1720
      IF(ISTATE(3).EQ.0.OR.B(J)*A(JJ).GT.0) GO TO 84                    EZCR1730
      CALL MESSG('OLD,NEW,PARM SIGN CHANGE',24)                         EZCR1740
      PRINT 100,B(J),A(JJ),JJ                                           EZCR1750
      B(J)=A(JJ)*(1-FACT)                                               EZCR1760
   84 CONTINUE                                                          EZCR1770
      CALL MESSG('MAX SCALED PARM DELTA,PARM NO.',30)                   EZCR1780
      PRINT 100,DELM,JM                                                 EZCR1790
C                                                                       EZCR1800
C       IF CHI SQUARE INCREASED, INCREASE FLAMDA AND TRY AGAIN          EZCR1810
C                                                                       EZCR1820
      DO 94 L=1,NTERMS                                                  EZCR1830
      JJ=ITERM(L)                                                       EZCR1840
   94 Z(JJ+N)=B(L)                                                      EZCR1850
   91 DO 92 I=1,NPTS                                                    EZCR1860
      DO 96 L=1,N                                                       EZCR1870
   96 Z(L)=X(I,L)                                                       EZCR1880
      ISTATE(1)=I                                                       EZCR1890
   92 YFIT(I)=FUNCN(Z,NPN)                                              EZCR1900
   93 CHISQR = FCHISQ(Y,WEIGHT,NPTS,NFREE,YFIT)                         EZCR1910
      CALL MESSG('TRIAL OBJECTIVE FCN',19)                              EZCR1920
      PRINT 100,IPRES,CHISQR                                            EZCR1930
      IF(FLAMDA.LE.0) GO TO 101                                         EZCR1940
      IF (CHISQ1-CHISQR) 95,101,101                                     EZCR1950
   95 FLAMDA =10*FLAMDA                                                 EZCR1960
      FACT=FACT/2.                                                      EZCR1970
      IF(FLAMDA.GT.1000) GO TO 135                                      EZCR1980
      IF(FLAMDA.GT.0.01) GO TO 71                                       EZCR1990
  115 DO 125 I=1,NTERMS                                                 EZCR2000
  125 SIGMAA(I)=ARRAY(I+(I-1)*NTERMS)/DSQRT(ALPHA(I*(I+1)/2))           EZCR2010
      GO TO 71                                                          EZCR2020
  340 CONTINUE                                                          EZCR2030
C    OUTPUT REGRESSION COEFFICIENTS                                     EZCR2040
      PRINT 100                                                         EZCR2050
      CALL MESSG('CORRELATION COEFFICIENTS',24)                         EZCR2060
       PRINT 100                                                        EZCR2070
```

```
      DO 320 I=1,NTERMS                                                    EZCR2080
      DO 330 J=1,I                                                         EZCR2090
      II=I+(I-1)*NTERMS                                                    EZCR2100
  330 B(J)=ARRAY(I+(J-1)*NTERMS)/DSQRT(ARRAY(II)*ARRAY(J+(J-1)*NTERMS))    EZCR2110
      PRINT 700,ITERM(I),(ITERM(JJ),B(JJ),JJ=1,I)                          EZCR2120
  320 CONTINUE                                                             EZCR2130
      PRINT 100                                                            EZCR2140
  260 CONTINUE                                                             EZCR2150
      DO 270 J=1,NTERMS                                                    EZCR2160
      SIGMAA(J)=ARRAY(J+(J-1)*NTERMS)/DSQRT(ALPHA(J*(J+1)/2))              EZCR2170
  270 CONTINUE                                                             EZCR2180
      CHISQR=CHISQ1                                                        EZCR2190
      RETURN                                                               EZCR2200
C                                                                          EZCR2210
C      EVALUATE PARAMETERS AND UNCERTAINTIES                               EZCR2220
C                                                                          EZCR2230
  101 DO 103 J=1,NTERMS                                                    EZCR2240
      JJ=ITERM(J)                                                          EZCR2250
      A(JJ)=B(J)                                                           EZCR2260
      IF(ARRAY(J+(J-1)*NTERMS).GT.0) GO TO 103                             EZCR2270
      PRINT 400,J,JJ                                                       EZCR2280
  400 FORMAT(1X,10('*'),' VARIANCE ',I3,' FOR PARAMETER',I3,               EZCR2290
     1 ' IS NEGATIVE.  CORRECTION TAKEN.',2X,10('*'))                      EZCR2300
      ARRAY(J+(J-1)*NTERMS)=1.E-30                                         EZCR2310
  103 SIGMAA(J)=ARRAY(J+(J-1)*NTERMS)/DSQRT(ALPHA(J*(J+1)/2))              EZCR2320
      FLAMDA =FLAMDA/10.                                                   EZCR2330
      IF(ISTATE(2).GT.4) GO TO 110                                         EZCR2340
C   OUTPUT REGRESSION COEFFICIENTS                                         EZCR2350
      PRINT 100                                                            EZCR2360
      CALL MESSG('CORRELATION COEFFICIENTS',24)                            EZCR2370
       PRINT 100                                                           EZCR2380
      DO 350 I=1,NTERMS                                                    EZCR2390
      II=I+(I-1)*NTERMS                                                    EZCR2400
      DO 360 J=1,I                                                         EZCR2410
  360 B(J)=ARRAY(I+(J-1)*NTERMS)/DSQRT(ARRAY(II)*ARRAY(J+(J-1)*NTERMS))    EZCR2420
      PRINT 700,ITERM(I),(ITERM(JJ),B(JJ),JJ=1,I)                          EZCR2430
  350 CONTINUE                                                             EZCR2440
      PRINT 100                                                            EZCR2450
      GO TO 110                                                            EZCR2460
  135 DO 140 L=1,NPARM                                                     EZCR2470
  140 Z(L+N)=A(L)                                                          EZCR2480
      DO 150 I=1,NPTS                                                      EZCR2490
      DO 160 L=1,N                                                         EZCR2500
  160 Z(L)=X(I,L)                                                          EZCR2510
      ISTATE(1)=I                                                          EZCR2520
  150 YFIT(I)=FUNCN(Z,NPN)                                                 EZCR2530
      CHISQR=CHISQ1                                                        EZCR2540
  110 RETURN                                                               EZCR2550
      END                                                                  EZCR2560
```

```
C    FUNCTION CV                                                        EZCV0040
C                                                                       EZCV0050
C    PURPOSE                                                            EZCV0060
C      CALCULATES HEAT CAPACITY OF SPECIFIC VOLUME BY NUMERICAL DERIV.  EZCV0070
C                                                                       EZCV0080
C    USUAGE                                                             EZCV0090
C      RESULT = CV(T,RHO)                                               EZCV0100
C                                                                       EZCV0110
C    DESCRIPTION OF PARAMETERS                                          EZCV0120
C        T-ABSOLUTE TEMPERATURE                                         EZCV0130
C      RHO-DENSITY                                                      EZCV0140
C                                                                       EZCV0150
C    SUBROUTINES NEEDED                                                 EZCV0160
C      U(T,RHO)                                                         EZCV0170
C        CALCULATES INTERNAL ENERGY                                     EZCV0180
C                                                                       EZCV0190
      FUNCTION CV(T,RHO)                                                EZCV0200
      COMMON /PRM/RGAS,RENRGY,TCRIT,PCRIT,RHOC,W,ALPHA,BETA,XMW         EZCV0210
     1   ,A(40),B(7),NTERMS,NPARM,NUMB,RTOP,RMIDL,RMIDV                 EZCV0220
      EPMAX=.1                                                          EZCV0230
      EPS=.0001                                                         EZCV0240
      SAVE=T                                                            EZCV0250
      IF(ABS(SAVE).LT.EPS) GO TO 10                                     EZCV0260
      DEL=ABS(EPS*SAVE)                                                 EZCV0270
   14 CONTINUE                                                          EZCV0280
      DO 12 IT=1,5                                                      EZCV0290
      T=SAVE+DEL                                                        EZCV0300
      F2=U(T,RHO)                                                       EZCV0310
      T=SAVE-DEL                                                        EZCV0320
      F1=U(T,RHO)                                                       EZCV0330
      DFDX=(F2-F1)/2./DEL                                               EZCV0340
C                                                                       EZCV0350
C       TESTS PRECISION OF DERIVATIVE                                   EZCV0360
C                                                                       EZCV0370
      IF(ABS(DEL*2*DFDX).GE.((10**(-6+N))*ABS(F1)))GO TO 40             EZCV0380
      IF(ABS(DFDX).LT.1.1E-65*ABS(F1)) DFDX=1.E-65*F1                   EZCV0390
      DEL=(10**(-6+N))*ABS(F1/DFDX)                                     EZCV0400
      IF(ABS(SAVE).LT.1.E-06) GO TO 20                                  EZCV0410
      IF(DEL.GT.ABS(SAVE*EPMAX)) DEL=ABS(SAVE*EPMAX)                    EZCV0420
      GO TO 12                                                          EZCV0430
   20 IF (DEL.GT.EPMAX) DEL=EPMAX                                       EZCV0440
   12 CONTINUE                                                          EZCV0450
      GO TO 40                                                          EZCV0460
   10 DEL=EPS                                                           EZCV0470
      GO TO 14                                                          EZCV0480
   40 CV=DFDX                                                           EZCV0490
      T=SAVE                                                            EZCV0500
```

```
      RETURN                                                                EZCV0510
      END                                                                   EZCV0520


C     SUBROUTINE DATA                                                       EZD10010
C                                                                           EZD10020
C     PURPOSE                                                               EZD10030
C       INPUTS DATA TO EZFIT IN PREBANKED FORMAT                            EZD10040
C                                                                           EZD10050
C       MODE    - DETERMINES METHOD OF WEIGHTING LEAST-SQUARES FIT          EZD10060
C                 +1 (INSTRUMENTAL) WEIGHT(I)=U/SIGMAY(I)**2                EZD10070
C             PERCENT ERROR CONSTANT                                        EZD10080
C                  0 (NO WEIGHTING) WEIGHT(I)= 1                            EZD10090
C                 -1 (STATISTICAL) WEIGHT =1/Y(I)                           EZD10100
      SUBROUTINE DATA (X,N,Y,NPTS,WEIGHT,YBAR,YVAR,NCODE,NPTRHO,            EZD10110
     1   NPTH,NPTVP,DATAID)                                                 EZD10120
 1100 FORMAT(8F10.0)                                                        EZD10130
 1200 FORMAT(16I5)                                                          EZD10140
 1300 FORMAT(3F10.0,I10)                                                    EZD10150
 1500 FORMAT(2A4,I2,7F10.0)                                                 EZD10160
      DIMENSION X(NPTS,N),Y(NPTS),WEIGHT(NPTS)                              EZD10170
     1  ,DATAID(NPTS,N)                                                     EZD10180
      COMMON /PRM/RGAS,RENRGY,TCRIT,PCRIT,RHOC,W,ALPHA,BETA,XMW             EZD10190
     1  ,A(40),B(7),NTERMS,NPARM,NUMB,RTOP,RMIDL,RMIDV                      EZD10200
      COMMON /PRP/ICOMP(20),CPC(20),CRC(20),CMW(20),CW(20) ,CTC(20)         EZD10210
     1 ,CA(20),CB(20),CNAME(20,2)                                           EZD10220
      INTEGER CODE                                                          EZD10230
      REAL NAME(40,2)                                                       EZD10240
      NPTRHO=0                                                              EZD10250
      NPTH=0                                                                EZD10260
      NPTVP=0                                                               EZD10270
      READ 1200,NCOMP                                                       EZD10280
      DO 30 L=1,NCOMP                                                       EZD10290
      READ 1500,(CNAME(L,J),J=1,2),IWHOLE,CTC(L),CPC(L),CRC(L),CMW(L),      EZD10300
     1CW(L),CA(L),CB(L)                                                     EZD10310
      ICOMP(L)=IWHOLE                                                       EZD10320
   30 CONTINUE                                                              EZD10330
      DO 40 I=1,NPTS                                                        EZD10340
      READ 1400,X(I,2),X(I,3),X(I,1),Y(I),(DATAID(I,J),J=1,3)               EZD10350
 1400 FORMAT(2X,4F10.4,26X,3A4)                                             EZD10360
      WEIGHT(I)=Y(I)                                                        EZD10370
      IWHOLE=ABS(X(I,1))+.005                                               EZD10380
C     IF(IWHOLE.GT.99) GO TO MIXTURE                                        EZD10390
      IFRACT=(ABS(X(I,1))-IWHOLE+.005)*100                                  EZD10400
```

```
      IF(IFRACT.EQ.0)NPTRHO=NPTRHO+1                                    EZD10410
      IF(IFRACT.EQ.10)NPTH=NPTH+1                                       EZD10420
      IF(IFRACT.EQ.20)NPTVP=NPTVP+1                                     EZD10430
   40 CONTINUE                                                          EZD10440
C       CACULATE AVERAGE AND VARIANCE                                   EZD10450
      SUM=0                                                             EZD10460
      SUMW=0                                                            EZD10470
      DO 60 I=1,NPTS                                                    EZD10480
C                                                                       EZD10490
C       EVALUATE WEIGHTS                                                EZD10500
C                                                                       EZD10510
      IF (NCODE) 1,2,3                                                  EZD10520
    1 IF (Y(I).EQ.0) GO TO 2                                            EZD10530
      WEIGHT(I)=1/ABS(Y(I))                                             EZD10540
      GO TO 10                                                          EZD10550
    2 WEIGHT(I)=1                                                       EZD10560
      GO TO 10                                                          EZD10570
    3 WEIGHT(I)=1/WEIGHT(I)**2                                          EZD10580
   10 CONTINUE                                                          EZD10590
      SUM=SUM+WEIGHT(I)*Y(I)                                            EZD10600
      SUMW=SUMW+WEIGHT(I)                                               EZD10610
   60 CONTINUE                                                          EZD10620
      SUM=SUM/SUMW                                                      EZD10630
      YBAR=SUM                                                          EZD10640
      SUMY=0                                                            EZD10650
      DO 50 I=1,NPTS                                                    EZD10660
      SUMY=SUMY+WEIGHT(I)*(Y(I)-SUM)**2                                 EZD10670
   50 CONTINUE                                                          EZD10680
      YVAR=SUMY*NPTS/SUMW/(NPTS-1)                                      EZD10690
      RETURN                                                            EZD10700
      END                                                               EZD10710
```

```
C    SUBROUTINE DATA2                                                   EZD20010
C                                                                       EZD20020
C    PURPOSE                                                            EZD20030
C      INPUTS DATA TO EZFIT FROM THE ORIGINAL STARLING-HAN FORMAT       EZD20040
C                                                                       EZD20050
      SUBROUTINE DATA2(X,N,Y,NPTS,WEIGHT,YBAR,YVAR,NCODE,NPTRHO,        EZD20060
     1   NPTH,NPTVP,DATAID)                                             EZD20070
  100 FORMAT(1X,8G14.6)                                                 EZD20080
 1100 FORMAT(8F10.0)                                                    EZD20090
 1200 FORMAT(16I5)                                                      EZD20100
 1300 FORMAT(3F10.0,I10)                                                EZD20110
```

```
1600 FORMAT(4I5,F10.0 )                                                    EZD20120
1800 FORMAT(1X,5G14.6,A4)                                                  EZD20130
     DIMENSION X(NPTS,N),Y(NPTS),WEIGHT(NPTS)                              EZD20140
    1,  DATAID(NPTS,N)                                                     EZD20150
     COMMON /PRM/RGAS,RENRGY,TCRIT,PCRIT,RHOC,W,ALPHA,BETA,XMW             EZD20160
    1   ,A(40),B(7),NTERMS,NPARM,NUMB,RTOP,RMIDL,RMIDV                    EZD20170
     COMMON /PRP/ICOMP(20),CPC(20),CRC(20),CMW(20),CW(20) ,CTC(20)         EZD20180
    1 ,CA(20),CB(20),CNAME(20,2)                                           EZD20190
     DATA D1,D2/' 006','S   '/                                             EZD20200
     INTEGER CODE                                                          EZD20210
     REAL NAME(40,2)                                                       EZD20220
     NPTL=0                                                                EZD20230
     NPTRHO=0                                                              EZD20240
     NPTH=0                                                                EZD20250
     NPTVP=0                                                               EZD20260
     CALL MESSG('DATA INPUT SUMMARY',18)                                   EZD20270
     READ 1200,NCOMP                                                       EZD20280
     CALL MESSG('NUMBER OF COMPONENTS',20)                                 EZD20290
     PRINT 100,NCOMP                                                       EZD20300
     CALL MESSG('DENSITY,ENTHALPY,   V.P.  , PRESET,GROUP WEIGHT',47)      EZD20310
     DO 30 L=1,NCOMP                                                       EZD20320
     READ 1500,(CNAME(L,J),J=1,2),IWHOLE,CTC(L),CPC(L),CRC(L),CMW(L),      EZD20330
    1CW(L),CA(L),CB(L)                                                     EZD20340
1500 FORMAT(2A4,I2,7F10.0)                                                 EZD20350
     ICOMP(L)=IWHOLE                                                       EZD20360
     TCRIT=CTC(L)                                                          EZD20370
     RHOC=CRC(L)                                                           EZD20380
     READ 1600,NPTRHL,NPTHL,NPTVPL,NPTA,SCALE                              EZD20390
     PRINT 1800,NPTRHL,NPTHL,NPTVPL,NPTA,SCALE,CNAME(L,1)                  EZD20400
     IF(SCALE.EQ.0.) SCALE=1.                                              EZD20410
     SCALE=SQRT(SCALE)                                                     EZD20420
     IF(NPTA.EQ.0) GO TO 160                                               EZD20430
     DO 140 JA=1,NPTA                                                      EZD20440
     I=NPTL+JA                                                             EZD20450
     READ 1400,X(I,2),X(I,3),X(I,1),Y(I),(DATAID(I,J),J=1,3)               EZD20460
1400 FORMAT(2X,4F10.4,26X,3A4)                                             EZD20470
     WEIGHT(I)=Y(I)/SCALE                                                  EZD20480
     IWHOLE=ABS(X(I,1))+.005                                               EZD20490
C    IF(IWHOLE.GT.99) GO TO MIXTURE                                        EZD20500
     IFRACT=(ABS(X(I,1))-IWHOLE+.005)*100                                  EZD20510
     IF(IFRACT.EQ.0)NPTRHO=NPTRHO+1                                        EZD20520
     IF(IFRACT.EQ.10)NPTH=NPTH+1                                           EZD20530
     IF(IFRACT.EQ.20)NPTVP=NPTVP+1                                         EZD20540
 140 CONTINUE                                                              EZD20550
     NPTL=NPTL+NPTA                                                        EZD20560
 160 CONTINUE                                                              EZD20570
     IF(NPTRHL.EQ.0) GO TO 130                                             EZD20580
     DO 70 J=1,NPTRHL                                                      EZD20590
     I=NPTL+J                                                              EZD20600
     DATAID(I,1)=D1                                                        EZD20610
```

```
      DATAID(I,2)=D2                                                    EZD20620
      READ 2100,T,P,RHO,CODE                                            EZD20630
      T=T+460                                                           EZD20640
      CODE=-1                                                           EZD20650
      IF(RHO.LT.RHOC)CODE=1                                             EZD20660
      IF (CODE)5,6,6                                                    EZD20670
    5 X(I,1)=-(IWHOLE+.3)                                               EZD20680
      GO TO 7                                                           EZD20690
    6 X(I,1)=IWHOLE+.3                                                  EZD20700
    7 X(I,3)=P                                                          EZD20710
      X(I,2)=T                                                          EZD20720
      Y(I)=RHO                                                          EZD20730
      WEIGHT(I)=Y(I)/SCALE                                              EZD20740
   70 CONTINUE                                                          EZD20750
      NPTRHO=NPTRHO+NPTRHL                                              EZD20760
      NPTL=NPTL+NPTRHL                                                  EZD20770
  130 IF(NPTHL.EQ.0) GO TO 110                                          EZD20780
      DO80 J=1,NPTHL                                                    EZD20790
      I=NPTL+J                                                          EZD20800
      DATAID(I,1)=D1                                                    EZD20810
      DATAID(I,2)=D2                                                    EZD20820
      READ 2100,T,P,DELH,CODE                                           EZD20830
 2100 FORMAT(3F10.0,20X,I5)                                             EZD20840
      T=T+460                                                           EZD20850
      IF(CODE)8,9,9                                                     EZD20860
    8 X(I,1)=-(IWHOLE+.4)                                               EZD20870
      GO TO 11                                                          EZD20880
    9 X(I,1)=+IWHOLE+.4                                                 EZD20890
   11 X(I,2)=T                                                          EZD20900
      X(I,3)=P                                                          EZD20910
      Y(I)=DELH                                                         EZD20920
      WEIGHT(I)=Y(I)/SCALE                                              EZD20930
   80 CONTINUE                                                          EZD20940
      NPTL=NPTL+NPTHL                                                   EZD20950
      NPTH=NPTH+NPTHL                                                   EZD20960
  110 IF(NPTVPL.EQ.0) GO TO 120                                         EZD20970
      DO 90 J=1,NPTVPL                                                  EZD20980
      I=NPTL+J                                                          EZD20990
      DATAID(I,1)=D1                                                    EZD21000
      DATAID(I,2)=D2                                                    EZD21010
      READ 2200,T,P                                                     EZD21020
 2200 FORMAT(F5.0,F10.0)                                                EZD21030
      T=T+460                                                           EZD21040
      X(I,1)=IWHOLE+.75                                                 EZD21050
      X(I,2)=T                                                          EZD21060
      X(I,3)=P                                                          EZD21070
      Y(I)=P                                                            EZD21080
      WEIGHT(I)=Y(I)/SCALE                                              EZD21090
   90 CONTINUE                                                          EZD21100
      NPTVP=NPTVP+NPTVPL                                                EZD21110
```

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      NPTL=NPTL+NPTVPL                                                  EZD21120
  120 CONTINUE                                                          EZD21130
   30 CONTINUE                                                          EZD21140
      NPTS=NPTL                                                         EZD21150
C      CACULATE AVERAGE AND VARIANCE                                    EZD21160
      SUM=0                                                             EZD21170
      SUMW=0                                                            EZD21180
      DO 60 I=1,NPTS                                                    EZD21190
      IF((DATAID(I,1).NE.D1).OR.(DATAID(I,2).NE.D2)) GO TO 170          EZD21200
      CALL CONVR(I,ICHAR,DATAID(I,3))                                   EZD21210
  170 CONTINUE                                                          EZD21220
C                                                                       EZD21230
C        EVALUATE WEIGHTS                                               EZD21240
C                                                                       EZD21250
      IF (NCODE) 1,2,3                                                  EZD21260
    1 IF (Y(I).EQ.0) GO TO 2                                            EZD21270
      WEIGHT(I)=1/ABS(Y(I))                                             EZD21280
      GO TO 10                                                          EZD21290
    2 WEIGHT(I)=1                                                       EZD21300
      GO TO 10                                                          EZD21310
    3 WEIGHT(I)=1/WEIGHT(I)**2                                          EZD21320
   10 CONTINUE                                                          EZD21330
      SUM=SUM+WEIGHT(I)*Y(I)                                            EZD21340
      SUMW=SUMW+WEIGHT(I)                                               EZD21350
   60 CONTINUE                                                          EZD21360
      SUM=SUM/SUMW                                                      EZD21370
      YBAR=SUM                                                          EZD21380
      SUMY=0                                                            EZD21390
      DO 50 I=1,NPTS                                                    EZD21400
      SUMY=SUMY+WEIGHT(I)*(Y(I)-SUM)**2                                 EZD21410
   50 CONTINUE                                                          EZD21420
      YVAR=SUMY*NPTS/SUMW/(NPTS-1)                                      EZD21430
      RETURN                                                            EZD21440
      END                                                               EZD21450
```

```
C    SUBROUTINE DATA3                                                   EZD30010
C    PURPOSE                                                            EZD30020
C      INPUTS DATA IN BANKED FORMAT AS BLOCKED WITH GROUP WEIGHT        EZD30030
C      A NEGATIVE GROUP WEIGHT CONVERTS TO EQUAL WEIGHTS                EZD30040
C                                                                       EZD30050
      SUBROUTINE DATA3(X,N,Y,NPTS,WEIGHT,YBAR,YVAR,NCODE,DATAID,ND)     EZD30060
C      MODE    - DETERMINES METHOD OF WEIGHTING LEAST-SQUARES FIT       EZD30070
C                +1 (INSTRUMENTAL) WEIGHT(I)=U/SIGMAY(I)**2             EZD30080
```

```
C          PERCENT ERROR CONSTANT                                                EZD30090
C                0 (NO WEIGHTING) WEIGHT(I)= 1                                   EZD30100
C               -1 (STATISTICAL) WEIGHT =1/Y(I)                                  EZD30110
      COMMON /PRM/RGAS,RENRGY,TCRIT,PCRIT,RHOC,W,ALPHA,BETA,XMW                  EZD30120
     1  ,A(40),B(7),NTERMS,NPARM,NUMB,RTOP,RMIDL,RMIDV                           EZD30130
      COMMON /PRP/ICOMP(20),CPC(20),CRC(20),CMW(20),CW(20) ,CTC(20)             EZD30140
     1 ,CA(20),CB(20),CNAME(20,2)                                               EZD30150
   20 FORMAT(4F10.0,26X,I2,3A4)                                                 EZD30160
 1100 FORMAT(8F10.0)                                                            EZD30170
 1200 FORMAT(16I5)                                                              EZD30180
 1300 FORMAT(3F10.0,I10)                                                        EZD30190
 1500 FORMAT(2A4,I2,7F10.0)                                                     EZD30200
 1600 FORMAT(6F10.0)                                                            EZD30210
 1700 FORMAT(2I5,F10.0,I5)                                                      EZD30220
      DIMENSION X(NPTS,N),Y(NPTS),WEIGHT(NPTS)                                  EZD30230
      DIMENSION DATAID(NPTS,ND)                                                 EZD30240
C     DATA INPUT                                                               EZD30250
      NPTL=0                                                                    EZD30260
      READ 1200,NBLKS                                                           EZD30270
      ICOMP(1)=0                                                                EZD30280
      L=1                                                                       EZD30290
      DO 300 JBLK=1,NBLKS                                                       EZD30300
      READ 1500,(CNAME(L,J),J=1,2),IWHOLE,CTC(L),CPC(L),CRC(L),CMW(L),          EZD30310
     1CW(L),CA(L),CB(L)                                                         EZD30320
      L1=L-1                                                                    EZD30330
      DO 160 JL=1,L1                                                            EZD30340
      IF(ICOMP(JL).EQ.IWHOLE) GO TO 170                                         EZD30350
  160 CONTINUE                                                                  EZD30360
      ICOMP(L)=IWHOLE                                                           EZD30370
      L=L+1                                                                     EZD30380
      IF(L.GT.20) GO TO 180                                                     EZD30390
      ICOMP(L)=0                                                                EZD30400
      GO TO 170                                                                 EZD30410
  180 CONTINUE                                                                  EZD30420
      PRINT 1400                                                                EZD30430
 1400 FORMAT(1X,20('*'),'MORE THAN 19 COMPOUNDS REQUESTED TO BE READ'//)        EZD30440
      STOP                                                                      EZD30450
  170 CONTINUE                                                                  EZD30460
      READ 1700,IFILE,NPTA,SCALE                                                EZD30470
      PRINT 1800,(CNAME(L,J),J=1,2),IWHOLE,IFILE,NPTA,SCALE                     EZD30480
 1800 FORMAT(1X,'COMPOUND ',2A4,'.',I3,' ON UNIT',I2,'.',I5,                    EZD30490
     1 ' DATA POINTS WITH WEIGHT ',G14.6  )                                     EZD30500
      IWT=0                                                                     EZD30510
      IF(SCALE.GE.0) GO TO 150                                                  EZD30520
      SCALE=ABS(SCALE)                                                          EZD30530
      IWT=1                                                                     EZD30540
  150 CONTINUE                                                                  EZD30550
      IF(SCALE.EQ.0)SCALE=1.                                                    EZD30560
      SCALE=SQRT(SCALE)                                                         EZD30570
      DO 40L=1,NPTA                                                             EZD30580
```

```
      I=NPTL+L                                                          EZD30590
      READ(IFILE,20,END=70)(X(I,J),J=1,3),Y(I),ICONT,(DATAID(I,K),K=1,3)EZD30600
      JL=3                                                              EZD30610
      IF(ICONT.EQ.0) GO TO 110                                          EZD30620
      DO 120 JJ=1,ICONT                                                 EZD30630
      JS=JL+1                                                           EZD30640
      JL=JS+5                                                           EZD30650
      IF(JL.GT.N)JL=N                                                   EZD30660
      READ(IFILE,1600)(X(I,JJJ),JJJ=JS,JL)                             EZD30670
  120 CONTINUE                                                          EZD30680
  110 CONTINUE                                                          EZD30690
      IF(JL.EQ.N) GO TO 130                                             EZD30700
      JL=JL+1                                                           EZD30710
      DO 140 JJJ=JL,N                                                   EZD30720
      X(I,JJJ)=0.                                                       EZD30730
  140 CONTINUE                                                          EZD30740
  130 CONTINUE                                                          EZD30750
 1110 CONTINUE                                                          EZD30760
C     PERCENT WEIGHTING. ASSUMES NCODE=1                                EZD30770
      WEIGHT(I)=1                                                       EZD30780
      IF(Y(I).NE.0) WEIGHT(I)=Y(I)                                      EZD30790
      WEIGHT(I)=WEIGHT(I)/SCALE                                         EZD30800
      IF(IWT.EQ.1)WEIGHT(I)=1/SCALE                                     EZD30810
   40 CONTINUE                                                          EZD30820
      NPTL=NPTL+NPTA                                                    EZD30830
  300 CONTINUE                                                          EZD30840
      NPTS=NPTL                                                         EZD30850
      GO TO 80                                                          EZD30860
   70 CONTINUE                                                          EZD30870
      I=I-1                                                             EZD30880
      PRINT 200,I                                                       EZD30890
  200 FORMAT(///1X,'****  TO FEW DATA. N=',G14.6)                       EZD30900
      STOP                                                              EZD30910
   80 CONTINUE                                                          EZD30920
C                                                                       EZD30930
C       EVALUATE WEIGHTS                                                EZD30940
C                                                                       EZD30950
      SUM=0                                                             EZD30960
      SUMW=0                                                            EZD30970
      DO 60 I=1,NPTS                                                    EZD30980
      IF (NCODE) 1,2,3                                                  EZD30990
    1 IF (Y(I).EQ.0) GO TO 2                                            EZD31000
      WEIGHT(I)=1/ABS(Y(I))                                             EZD31010
      GO TO 10                                                          EZD31020
    2 WEIGHT(I)=1                                                       EZD31030
      GO TO 10                                                          EZD31040
    3 WEIGHT(I)=1/WEIGHT(I)**2                                          EZD31050
   10 CONTINUE                                                          EZD31060
      SUM=SUM+WEIGHT(I)*Y(I)                                            EZD31070
      SUMW=SUMW+WEIGHT(I)                                               EZD31080
```

```
   60 CONTINUE                                                          EZD31090
      SUM=SUM/SUMW                                                      EZD31100
      YBAR=SUM                                                          EZD31110
      SUMY=0                                                            EZD31120
      DO 50 I=1,NPTS                                                    EZD31130
      SUMY=SUMY+WEIGHT(I)*(Y(I)-SUM)**2                                 EZD31140
   50 CONTINUE                                                          EZD31150
      YVAR=SUMY*NPTS/SUMW/(NPTS-1)                                      EZD31160
      YVAR=SUMY                                                         EZD31170
      RETURN                                                            EZD31180
      END                                                               EZD31190
```

```
C     FUNCTION DENSL(T,P)                                               EZDL0010
C                                                                       EZDL0020
C     PURPOSE                                                           EZDL0030
C       FINDS THE LIQUID DENSITY FOR TEMPERATURE AND PRESSURE           EZDL0040
C                                                                       EZDL0050
C     USUAGE                                                            EZDL0060
C       RESULT = DENSL(T,P)                                             EZDL0070
C                                                                       EZDL0080
C     DESCRIPTION OF PARAMETERS                                         EZDL0090
C       T - TEMPERATURE                                                 EZDL0100
C       P - PRESSURE                                                    EZDL0110
C                                                                       EZDL0120
C     SUBPROGRAMS NEEDED                                                EZDL0130
C       PRES(T,RHO)                                                     EZDL0140
C          CALCULATES PRESSURE AS FUNCTION OF TEMPERATURE AND DENSITY   EZDL0150
C                                                                       EZDL0160
        FUNCTION DENSL(T,P)                                             EZDL0170
        COMMON /PRM/RGAS,RENRGY,TCRIT,PCRIT,RHOC,W,ALPHA,BETA,XMW       EZDL0180
       1   ,A(40),B(7),NTERMS,NPARM,NUMB,RTOP,RMIDL,RMIDV               EZDL0190
        COMMON /DAT/IPRES,ISTATE(20)                                    EZDL0200
        DATA ITMAX,EPSP,EPSR/50,1.E-05,1.E-05/                          EZDL0210
        P0=P                                                            EZDL0220
        ITMAX=20                                                        EZDL0230
        DEL=RTOP/20.                                                    EZDL0240
        PMIN=1.E60                                                      EZDL0250
        CODE=0.                                                         EZDL0260
        RHO1=RTOP                                                       EZDL0270
        IT=1                                                            EZDL0280
        IF(T/TCRIT.LT.0.4) GO TO 30                                     EZDL0290
        IF(ISTATE(9).EQ.0) GO TO 210                                    EZDL0300
        RHO1=RHO2                                                       EZDL0310
```

```
  210 CONTINUE                                                                  EZDL0320
      RHO2=1.01*RHO1                                                            EZDL0330
      P1=PRES(T,RHO1)-P0                                                        EZDL0340
      P2=PRES(T,RHO2)-P0                                                        EZDL0350
   20 IF((ABS(P1-P2).LT.EPSP).OR.(ABS(RHO1-RHO2).LT.ABS(RHO2)*EPSR))            EZDL0360
     1   GO TO 40                                                             EZDL0370
      IF (IT.GT.ITMAX) GO TO 30                                                 EZDL0380
      RHO3=(RHO1*P2-RHO2*P1)/(P2-P1)                                            EZDL0390
      IF(RHO3.LT.RMIDL) GO TO 50                                                EZDL0400
      IF(RHO3.GT.RTOP) GO TO 190                                                EZDL0410
   60 CONTINUE                                                                  EZDL0420
      RHO1=RHO2                                                                 EZDL0430
      RHO2=RHO3                                                                 EZDL0440
      P1=P2                                                                     EZDL0450
      IT=IT+1                                                                   EZDL0460
      P2=PRES(T,RHO2)-P0                                                        EZDL0470
      GO TO 20                                                                  EZDL0480
   40 CONTINUE                                                                  EZDL0490
      RHO1=.99*RHO2                                                             EZDL0500
      P1=PRES(T,RHO1)-P0                                                        EZDL0510
      IF(RHO2.LT.RMIDL) GO TO 30                                                EZDL0520
      IF(P1.LT.P2) GO TO 130                                                    EZDL0530
      GO TO 30                                                                  EZDL0540
  190 CONTINUE                                                                  EZDL0550
      RHO3=RTOP*(50.+IT)/50.                                                    EZDL0560
      GO TO 220                                                                 EZDL0570
   50 CONTINUE                                                                  EZDL0580
      RHO3=RTOP*(50.+IT)/50.                                                    EZDL0590
  220 CONTINUE                                                                  EZDL0600
      IF(RHO1.LT.RHO2.AND.P1.GT.P2) GO TO 60                                    EZDL0610
      RHO2=RHO1                                                                 EZDL0620
      RHO1=RHO3                                                                 EZDL0630
      P2=P1                                                                     EZDL0640
      IT=IT+1                                                                   EZDL0650
      P1=PRES(T,RHO1)-P0                                                        EZDL0660
      GO TO 20                                                                  EZDL0670
   30 CONTINUE                                                                  EZDL0680
      ITMAX=40                                                                  EZDL0690
      RHO2=RTOP+DEL                                                             EZDL0700
      P2=PRES(T,RHO2)                                                           EZDL0710
C       CHECK FOR STARTING POINT                                                EZDL0720
      RHO1=RTOP                                                                 EZDL0730
      P1=PRES(T,RHO1)                                                           EZDL0740
      IF(P1.LT.P0)GO TO   150                                                   EZDL0750
   70 CONTINUE                                                                  EZDL0760
      P1=PRES(T,RHO1)                                                           EZDL0770
      IF(P1.LT.P0) GO TO 90                                                     EZDL0780
      IF(P1.LT.PMIN.AND.CODE.EQ.0.) GO TO 170                                   EZDL0790
      CODE=1.                                                                   EZDL0800
  180 CONTINUE                                                                  EZDL0810
```

```
      RHO2=RHO1                                                          EZDL0820
      P2=P1                                                              EZDL0830
      IF(RHO1.LT.RMIDL) GO TO 160                                        EZDL0840
      RHO1=RHO1-DEL                                                      EZDL0850
      GO TO 70                                                           EZDL0860
  170 CONTINUE                                                           EZDL0870
      PMIN=P1                                                            EZDL0880
      RHOMIN=RHO1                                                        EZDL0890
      GO TO 180                                                          EZDL0900
  160 CONTINUE                                                           EZDL0910
      IF(ISTATE(4).LT.5)                                                 EZDL0920
     1PRINT 200                                                          EZDL0930
  200 FORMAT(1X,'NO LIQUID ROOT.  MINIMUM USED')                         EZDL0940
      RHO2=RHOMIN                                                        EZDL0950
      GO TO 130                                                          EZDL0960
  150 CONTINUE                                                           EZDL0970
      IF(ISTATE(4).LT.5)                                                 EZDL0980
     1PRINT 300                                                          EZDL0990
  300 FORMAT(1X,'ROOT TOO LARGE')                                        EZDL1000
      RHO2=RHO1                                                          EZDL1010
      IF(ISTATE(9).EQ.0) GO TO 130                                       EZDL1020
C       CALLED FROM DERIVATIVE ROUTINE                                   EZDL1030
      P1=PRES(T,RHO2)                                                    EZDL1040
      IF(P1.LT.SP) GO TO 240                                             EZDL1050
      RHO2=RHO2-DEL                                                      EZDL1060
      GO TO 130                                                          EZDL1070
  240 CONTINUE                                                           EZDL1080
      RHO2=RHO2+DEL                                                      EZDL1090
      GO TO 130                                                          EZDL1100
   90 CONTINUE                                                           EZDL1110
C       SUCCESSIVE BISECTIONS                                            EZDL1120
      RHO3=(RHO1+RHO2)/2                                                 EZDL1130
      P3=PRES(T,RHO3)                                                    EZDL1140
      IF((ABS(P1-P2).LT.EPSP*P0).OR.ABS(RHO1-RHO2).LT.ABS(RHO2)*EPSR)    EZDL1150
     1 GO TO 130                                                         EZDL1160
      IT=IT+1                                                            EZDL1170
      IF(IT.GT.ITMAX) GO TO 80                                           EZDL1180
      IF(P3.GT.P0) GO TO 140                                             EZDL1190
      RHO1=RHO3                                                          EZDL1200
      P1=P3                                                              EZDL1210
      GO TO 90                                                           EZDL1220
  140 CONTINUE                                                           EZDL1230
      RHO2=RHO3                                                          EZDL1240
      P2=P3                                                              EZDL1250
      GO TO 90                                                           EZDL1260
   80 CONTINUE                                                           EZDL1270
      IF(ISTATE(4).LT.5)                                                 EZDL1280
     1PRINT 100,T,P,RHO1,P1,RHO2,P2                                      EZDL1290
  100 FORMAT (1X,'L DENSITY DIDNCT CONVERGE FOR T=',G11.4,'PRESSURE',    EZDL1300
     1 G11.4,'RHO1=',G11.4,'P1=',G11.4,'RHO2=',G11.4,'P2=',G11.4)        EZDL1310
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```
  130 CONTINUE                                                          EZDL1320
      DENSL=RHO2                                                        EZDL1330
      IF(ISTATE(9).EQ.1) GO TO 230                                      EZDL1340
C      NOT IN DERIVATIVE ROUTINE                                        EZDL1350
      SRHO=DENSL                                                        EZDL1360
      SP=PRES(T,SRHO)                                                   EZDL1370
  230 CONTINUE                                                          EZDL1380
      RETURN                                                            EZDL1390
      END                                                               EZDL1400
```

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```
C   FUNCTION DENSV(T,P)                                                 EZDV0010
C                                                                       EZDV0020
C   PURPOSE                                                             EZDV0030
C     FINDS THE VAPOR DENSITY FOR TEMPERATURE AND PRESSURE              EZDV0040
C                                                                       EZDV0050
C   USUAGE                                                              EZDV0060
C     RESULT = DENSV(T,P)                                               EZDV0070
C                                                                       EZDV0080
C   DESCRIPTION OF PARAMETERS                                           EZDV0090
C     T - TEMPERATURE                                                   EZDV0100
C     P - PRESSURE                                                      EZDV0110
C                                                                       EZDV0120
C   SUBPROGRAMS NEEDED                                                  EZDV0130
C     PRES(T,RHO)                                                       EZDV0140
C        CALCULATES PRESSURE AS FUNCTION OF TEMPERATURE AND DENSITY     EZDV0150
C                                                                       EZDV0160
      FUNCTION DENSV(T,P)                                               EZDV0170
      COMMON /PRM/RGAS,RENRGY,TCRIT,PCRIT,RHOC,W,ALPHA,BETA,XMW         EZDV0180
     1   ,A(40),B(7),NTERMS,NPARM,NUMB,RTOP,RMIDL,RMIDV                 EZDV0190
      COMMON /DAT/IPRES,ISTATE(20)                                      EZDV0200
      DATA ITMAX,EPSP,EPSR/50,1.E-05,1.E-05/                            EZDV0210
      ITMAX=20                                                          EZDV0220
      P0=P                                                              EZDV0230
      DEL=P0/RGAS/T/10.                                                 EZDV0240
      RHO1=.5*P0/RGAS/T                                                 EZDV0250
      IT=1                                                              EZDV0260
      IF(T/TCRIT.LT.0.4) GO TO 30                                       EZDV0270
      IF(ISTATE(9).EQ.0) GO TO 210                                      EZDV0280
      RHO1=RHO2                                                         EZDV0290
  210 CONTINUE                                                          EZDV0300
      RHO2=.8*RHO1                                                      EZDV0310
      P1=PRES(T,RHO1)-P0                                                EZDV0320
      P2=PRES(T,RHO2)-P0                                                EZDV0330
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   20 CONTINUE                                                          EZDV0340
      IF((ABS(P1-P2).LT.EPSP*P0).OR.ABS(RHO1-RHO2).LT.ABS(RHO2)*EPSR)   EZDV0350
     1   GO TO 40                                                       EZDV0360
      IF (IT.GT.ITMAX) GO TO 30                                         EZDV0370
C      PROJECTION                                                       EZDV0380
      RHO3=(RHO1*P2-RHO2*P1)/(P2-P1)                                    EZDV0390
      IF((RHO3.GT.RMIDV).OR.(RHO3.LT.0))RHO3=(1-IT/50.)*P0/RGAS/T       EZDV0400
      RHO1=RHO2                                                         EZDV0410
      RHO2=RHO3                                                         EZDV0420
      IT=IT+1                                                           EZDV0430
      P1=P2                                                             EZDV0440
      P2=PRES(T,RHO2)-P0                                                EZDV0450
      GO TO 20                                                          EZDV0460
   40 CONTINUE                                                          EZDV0470
      RHO1=.99*RHO2                                                     EZDV0480
      P1=PRES(T,RHO1)-P0                                                EZDV0490
      IF(RHO2.GT.RMIDV) GO TO 30                                        EZDV0500
      IF(P1.LT.P2 ) GO TO 130                                           EZDV0510
   30 CONTINUE                                                          EZDV0520
      ITMAX=40                                                          EZDV0530
      ITMAX=RMIDV/DEL+5                                                 EZDV0540
      IT=0                                                              EZDV0550
      P1=P1+P0                                                          EZDV0560
      P2=P2+P0                                                          EZDV0570
C      CHECK FOR STARTING POINT                                         EZDV0580
      RHO1=DEL                                                          EZDV0590
   70 CONTINUE                                                          EZDV0600
      P1=PRES(T,RHO1)                                                   EZDV0610
      IF(P1.LT.P0)GO TO 60                                              EZDV0620
      IF(ISTATE(4).LT.5)                                                EZDV0630
     1PRINT 300                                                         EZDV0640
  300 FORMAT(1X,'ROOT TOO SMALL')                                       EZDV0650
      RHO2=RHO1                                                         EZDV0660
      GO TO 130                                                         EZDV0670
   60 CONTINUE                                                          EZDV0680
      RHO2=RHO1+DEL                                                     EZDV0690
      CODE=0.                                                           EZDV0700
      PMAX=P1                                                           EZDV0710
      RHOMAX=RHO1                                                       EZDV0720
  110 CONTINUE                                                          EZDV0730
      P2=PRES(T,RHO2)                                                   EZDV0740
      IF(P2.GT.P0) GO TO 120                                            EZDV0750
      IF(P2.GT.PMAX.AND.CODE.EQ.0.) GO TO 160                           EZDV0760
      CODE=1.                                                           EZDV0770
  170 CONTINUE                                                          EZDV0780
      IT=IT+1                                                           EZDV0790
      RHO1=RHO2                                                         EZDV0800
      P1=P2                                                             EZDV0810
      RHO2=RHO2+DEL                                                     EZDV0820
      IF(IT.GT.ITMAX) GO TO 180                                         EZDV0830
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```
      IF(RHO1.LT.RMIDV) GO TO 110                                          EZDV0840
      IF(ISTATE(4).LT.5)                                                   EZDV0850
     1PRINT 200                                                            EZDV0860
  200 FORMAT(1X,'MAXIMUM USED')                                            EZDV0870
      RHO2=RHOMAX                                                          EZDV0880
      GO TO 130                                                            EZDV0890
  180 CONTINUE                                                             EZDV0900
      IF(ISTATE(4).LT.5)                                                   EZDV0910
     1 PRINT 500                                                           EZDV0920
  500 FORMAT(1X,'V ROOT NOT FOUND')                                        EZDV0930
      GO TO 130                                                            EZDV0940
  160 CONTINUE                                                             EZDV0950
      PMAX=P2                                                              EZDV0960
      RHOMAX=RHO2                                                          EZDV0970
      GO TO 170                                                            EZDV0980
  120 CONTINUE                                                             EZDV0990
      IT=0                                                                 EZDV1000
   90 CONTINUE                                                             EZDV1010
C       SUCCESSIVE BISECTIONS                                              EZDV1020
      RHO3=(RHO1+RHO2)/2                                                   EZDV1030
      P3=PRES(T,RHO3)                                                      EZDV1040
      IF((ABS(P1-P2).LT.EPSP*P0).OR.ABS(RHO1-RHO2).LT.ABS(RHO2)*EPSR)      EZDV1050
     1 GO TO 150                                                           EZDV1060
      IT=IT+1                                                              EZDV1070
      IF(IT.GT.ITMAX) GO TO 80                                             EZDV1080
      IF(P3.GT.P0) GO TO 140                                               EZDV1090
      RHO1=RHO3                                                            EZDV1100
      P1=P3                                                                EZDV1110
      GO TO 90                                                             EZDV1120
  150 CONTINUE                                                             EZDV1130
      RHO2=RHO3                                                            EZDV1140
      GO TO 130                                                            EZDV1150
  140 CONTINUE                                                             EZDV1160
      RHO2=RHO3                                                            EZDV1170
      P2=P3                                                                EZDV1180
      GO TO 90                                                             EZDV1190
   80 CONTINUE                                                             EZDV1200
      IF(ISTATE(4).LT.5)                                                   EZDV1210
     1PRINT 100,T,P,RHO1,P1,RHO2,P2                                        EZDV1220
  100 FORMAT (1X,'V DENSITY DIDNOT CONVERGE FOR T=',G11.4,'PRESSURE',      EZDV1230
     1 G11.4,'RHO1=',G11.4,'P1=',G11.4,'RHO2=',G11.4,'P2=',G11.4)          EZDV1240
  130 CONTINUE                                                             EZDV1250
      DENSV=RHO2                                                           EZDV1260
      RETURN                                                               EZDV1270
      END                                                                  EZDV1280
```

```
C    FUNCTION ENTH (T,RHO)                                                  EZDH0010
C                                                                           EZDH0020
C    PURPOSE                                                                EZDH0030
C      EVALUATES ENTHALPY AS A FUNCTION OF TEMPERATURE AND DENSITY          EZDH0040
C       MODIFIED FOR CURVE FITTING                                          EZDH0050
C                                                                           EZDH0060
C    USUAGE                                                                 EZDH0070
C      RESULT = ENTH(T,RHO)                                                 EZDH0080
C                                                                           EZDH0090
C    DESCRIPTION OF PARAMETERS                                              EZDH0100
C      T   - TEMPERATURE                                                    EZDH0110
C    RHO - DENSITY                                                          EZDH0120
C                                                                           EZDH0130
C    SUBROUTINES NEEDED                                                     EZDH0140
C      FI2(T,RHO)                                                           EZDH0150
C        CALCULATES THE INTEGRAL OF (DZDT)DLN(RHO)                          EZDH0160
C      PRES(T,RHO)                                                          EZDH0170
C        CALCULATES PRESSURE AT T AND RHO                                   EZDH0180
      FUNCTION ENTH(T,RHO)                                                  EZDH0190
      COMMON /PRM/RGAS,RENRGY,TCRIT,PCRIT,RHOC,W,ALPHA,BETA,XMW             EZDH0200
     1  ,A(40),B(7),NTERMS,NPARM,NUMB,RTOP,RMIDL,RMIDV                      EZDH0210
      TSTAR=ALPHA*T/TCRIT                                                   EZDH0220
      HDEV=-TSTAR*TSTAR*FI2(T,RHO)+TSTAR*(PRES(T,RHO)/RGAS/T/RHO-1.)        EZDH0230
      ENTH=HDEV*RENRGY*TCRIT/ALPHA                                          EZDH0240
      RETURN                                                                EZDH0250
      END                                                                   EZDH0260
```

```
C    FUNCTION ENTRPY(T,RHO)                                                 EZDS0010
C                                                                           EZDS0020
C    PURPOSE                                                                EZDS0030
C      CACULATES THE ENTROPY FOR TEMPERATURE AND DENSITY                    EZDS0040
C                                                                           EZDS0050
C    USUAGE                                                                 EZDS0060
C      RESULT = ENTRPY(T,RHO)                                               EZDS0070
C                                                                           EZDS0080
C    DESCRIPTION OF PARAMETERS                                              EZDS0090
C      T   - TERM                                                           EZDS0100
C      T   - TEMPERATURE                                                    EZDS0110
C      RHO - DENSITY                                                        EZDS0120
C                                                                           EZDS0130
C    SUBPROGRAMS NEEDED                                                     EZDS0140
C    SUBROUTINES NEEDED                                                     EZDS0150
C      FI2(T,RHO)                                                           EZDS0160
```

```
C       CALCULATES THE INTEGRAL OF (DZDT)DLN(RHO)                          EZDS0170
C     FII                                                                  EZDS0180
C       CALCULATES THE INTEGRAL OF (Z-1)D LN(RHO)                          EZDS0190
      FUNCTION ENTRPY(T,RHO)                                               EZDS0200
      COMMON /PRM/RGAS,RENRGY,TCRIT,PCRIT,RHOC,W,ALPHA,BETA,XMW            EZDS0210
     1  ,A(40),B(7),NTERMS,NPARM,NUMB,RTOP,RMIDL,RMIDV                     EZDS0220
      TSTAR=ALPHA*T/TCRIT                                                  EZDS0230
      ENTRPY=RENRGY*(-ALOG(RHO*RGAS*T)-FII(T,RHO)-TSTAR*FI2(T,RHO))        EZDS0240
      RETURN                                                               EZDS0250
      END                                                                  EZDS0260
```

```
C   FUNCTION FCHISQ                                                        EZFC0010
C                                                                          EZFC0020
C   PURPOSE                                                                EZFC0030
C        FCHISQ = SUM((Y-YFIT)**2/SIGMA**2)/NFREE                          EZFC0040
C     EVALUATE REDUCED CHI SQUARE FOR FIT TO DATA                          EZFC0050
C                                                                          EZFC0060
C   USUAGE                                                                 EZFC0070
C     RESULT = FCHISQ(Y,WEIGHT,NPTS,NFREE,YFIT)                            EZFC0080
C                                                                          EZFC0090
C   DESCRIPTION OF PARAMETERS                                              EZFC0100
C     Y       - ARRAY OF DATA POINTS                                       EZFC0110
C     WEIGHT  - ARRAY OF WEIGHTS FOR DATA POINTS                           EZFC0120
C     NPTS    - NUMBER OF DATA POINTS                                      EZFC0130
C     NFREE   - NUMBER OF DEGRES OF FREEDOM                                EZFC0140
C     YFIT    - ARRAY OF CALCULATED VALUES OF Y                            EZFC0150
C                                                                          EZFC0160
C   SUBROUTINES AND VUNCTION SUBPROGRAMS REQUIRED                          EZFC0170
C     NONE                                                                 EZFC0180
C                                                                          EZFC0190
      FUNCTION FCHISQ (Y,WEIGHT,NPTS,NFREE,YFIT)                           EZFC0200
      DOUBLE PRECISION CHISQ                                               EZFC0210
      DIMENSION Y(NPTS),WEIGHT(NPTS),YFIT(NPTS)                            EZFC0220
   11 CHISQ=0                                                              EZFC0230
   12 IF (NFREE) 13,13,20                                                  EZFC0240
   13 FCHISQ =0                                                            EZFC0250
      GO TO 40                                                             EZFC0260
C                                                                          EZFC0270
C       ACCUMULATE CHI SQUARE                                              EZFC0280
C                                                                          EZFC0290
   20 DO 30 I=1,NPTS                                                       EZFC0300
   30 CHISQ = CHISQ + WEIGHT(I)*(Y(I)-YFIT(I))**2                          EZFC0310
C                                                                          EZFC0320
```

```
C       DIVIDE BY NUMBER OF DEGREES OF FREEDOM                          EZFC0330
C                                                                       EZFC0340
   31 FREE =NFREE                                                       EZFC0350
   32 FCHISQ=CHISQ/FREE                                                 EZFC0360
   40, RETURN                                                           EZFC0370
      END                                                               EZFC0380
```

```
C    FUNCTION FDERIV                                                    EZFD0010
C                                                                       EZFD0020
C    PURPOSE                                                            EZFD0030
C        EVALUATE NUMERICALLY DERIVATIVE OF FUNCTN WITH RESPECT         EZFD0040
C        TO THE ITH VARIABLE                                            EZFD0050
C                                                                       EZFD0060
C    USUAGE                                                             EZFD0070
C      RESULT = FDERIV(X,I,NDIM)                                        EZFD0080
C                                                                       EZFD0090
C    DESCRIPTION OF PARAMETERS                                          EZFD0100
C      X     - ARRAY OF INDEPENDENT VARIABLE VALUES                     EZFD0110
C      I     - NUMBER OF VARIABLE FOR DERIVATIVE                        EZFD0120
C      NDIM  - NUMBER OF INDEPENDENT VARIABLES                          EZFD0130
C                                                                       EZFD0140
C    SUBROUTINES NEEDED                                                 EZFD0150
C      FUNCN(X,NDIM                                                     EZFD0160
C        EVALUATES THE FUNCTION AT POINT X                              EZFD0170
C                                                                       EZFD0180
      FUNCTION FDERIV (X,I,NDIM)                                        EZFD0190
      DIMENSION X(NDIM)                                                 EZFD0200
      COMMON /DAT/IPRES,ISTATE(20)                                      EZFD0210
      ISTATE(9)=1                                                       EZFD0220
      EPMAX=.1                                                          EZFD0230
      EPS=.01                                                           EZFD0240
      N=3                                                               EZFD0250
      SAVE=X(I)                                                         EZFD0260
      IF(ABS(SAVE).LT.EPS) GO TO 10                                     EZFD0270
      DEL=ABS(EPS*SAVE)                                                 EZFD0280
   14 CONTINUE                                                          EZFD0290
      DO 12 IT=1,3                                                      EZFD0300
      X(I)=SAVE+DEL                                                     EZFD0310
      F2=FUNCN(X,NDIM)                                                  EZFD0320
      X(I)=SAVE-DEL                                                     EZFD0330
      F1=FUNCN(X,NDIM)                                                  EZFD0340
      DFDX=(F2-F1)/2./DEL                                               EZFD0350
      IF(ISTATE(5).EQ.1) GO TO 40                                       EZFD0360
```

```
C                                                                       EZFD0370
C       TESTS PRECISION OF DERIVATIVE                                   EZFD0380
C                                                                       EZFD0390
      IF(ABS(F1-F2).LT.ABS(F1)*1.E-5) F2=F1                             EZFD0400
      IF(ABS(F1-F2)*(10**(6-N)).GT.ABS(F1)) GO TO 40                    EZFD0410
   20 CONTINUE                                                          EZFD0420
      EPS=EPS*10                                                        EZFD0430
      IF(ABS(SAVE).LT.1.E-6) GO TO 30                                   EZFD0440
      DEL=ABS(SAVE*EPS)                                                 EZFD0450
      GO TO 12                                                          EZFD0460
   30 CONTINUE                                                          EZFD0470
      DEL=EPS                                                           EZFD0480
   12 CONTINUE                                                          EZFD0490
      IF(ABS(F1-F2).LT.ABS(F1)*1.E-5) DFDX=0.                           EZFD0500
      GO TO 40                                                          EZFD0510
   10 DEL=EPS                                                           EZFD0520
      GO TO 14                                                          EZFD0530
   40 FDERIV=DFDX                                                       EZFD0540
  100 FORMAT(1X,8G14.6)                                                 EZFD0550
      X(I)=SAVE                                                         EZFD0560
      ISTATE(9)=0                                                       EZFD0570
      RETURN                                                            EZFD0580
      END                                                               EZFD0590
```

```
C   FUNCTION FLASHP                                                     EZFL0010
C                                                                       EZFL0020
C   PURPOSE                                                             EZFL0030
C     EVALUATES THE VAPOR PRESSURE FOR A GIVEN TEMPERATURE              EZFL0040
C      MODIFIED FOR CURVE FITTING                                       EZFL0050
C                                                                       EZFL0060
C   USUAGE                                                              EZFL0070
C     RESULT = FLASHP(T)                                                EZFL0080
C                                                                       EZFL0090
C   DESCRIPTION OF PARAMETERS                                           EZFL0100
C     T - TEMPERATURE                                                   EZFL0110
C                                                                       EZFL0120
C   SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                       EZFL0130
C     PRESS - CALCULATES PRESSURE GIVEN T,RHO                           EZFL0140
C     RHOL - CALCULATES LIQUID DENSITY                                  EZFL0150
C     RHOV - CALCULATES VAPOR DENSITY                                   EZFL0160
C     FUGCOF - CALCULATES THE FUGACITY COEFFICIENT                      EZFL017C
C                                                                       EZFL0180
      FUNCTION FLASHP(T,P0    )                                         EZFL0190
```

```
      COMMON /PRM/RGAS,RENRGY,TCRIT,PCRIT,RHOC,W,ALPHA,BETA,XMW          EZFL0200
     1  ,A(40),B(7),NTERMS,NPARM,NUMB,RTOP,RMIDL,RMIDV                   EZFL0210
      COMMON /DAT/IPRES,ISTATE(20)                                       EZFL0220
      REAL KVALUE                                                        EZFL0230
      EPS=0.001                                                          EZFL0240
      ITMAX=20                                                           EZFL0250
C     CURVE FITTING                                                      EZFL0260
      IF(ISTATE(9).EQ.1) GO TO 210                                       EZFL0270
      P=P0                                                               EZFL0280
  210 CONTINUE                                                           EZFL0290
      RHOL=DENSL(T,P)                                                    EZFL0300
      RHOV=DENSV(T,P)                                                    EZFL0310
      IT=1                                                               EZFL0320
   40 CONTINUE                                                           EZFL0330
      KVALUE=FUGCOF(T,RHOL)/FUGCOF(T,RHOV)                               EZFL0340
      P=P*KVALUE                                                         EZFL0350
      IF(P.LT.1.3*PCRIT) GO TO 30                                        EZFL0360
      P=1.3*PCRIT                                                        EZFL0370
      GO TO 20                                                           EZFL0380
   30 CONTINUE                                                           EZFL0390
      IF(ABS(1-KVALUE).LT.EPS) GO TO 25                                  EZFL0400
      IT=IT+1                                                            EZFL0410
      IF(IT.GE.ITMAX) GO TO 20                                           EZFL0420
      RHOV=DENSV(T,P)                                                    EZFL0430
      RHOL=DENSL(T,P)                                                    EZFL0440
      GO TO 40                                                           EZFL0450
   20 CONTINUE                                                           EZFL0460
      IF(ISTATE(4).LE.4) PRINT 200,T,P,KVALUE                            EZFL0470
  200 FORMAT (1X,'VAPOR PRESSURE DID NOT CONVERGE.  T=',G14.6,           EZFL0480
     1  'P=',G14.6,'KVALUE=',G14.6)                                       EZFL0490
   25 FLASHP=P                                                           EZFL0500
      RETURN                                                             EZFL0510
      END                                                                EZFL0520
```

```
C     FUNCTION FUGCOF(T,RHO)                                             EZFG0010
C                                                                        EZFG0020
C     PURPOSE                                                            EZFG0030
C       EVALUATES THE FUGACITY COEFFICIENT                               EZFG0040
C                                                                        EZFG0050
C     USUAGE                                                             EZFG0060
C       RESULT = FUGCOF(T,RHO)                                           EZFG0070
C                                                                        EZFG0080
C     DESCRIPTION OF PARAMETERS                                          EZFG0090
```

```
C      T - TEMPERATURE                                                    EZFG0100
C      RHO - DENSITY                                                      EZFG0110
C                                                                         EZFG0120
C    SUGROUTINES NEEDED                                                   EZFG0130
C      FI1                                                                EZFG0140
C        CALCULATES THE INTEGRAL OF (Z-1)D LN(RHO)                        EZFG0150
C      PRES(T,RHO)                                                        EZFG0160
C        CALCULATES PRESSURE AT T AND RHO                                 EZFG0170
       FUNCTION FUGCOF(T,RHO)                                             EZFG0180
       COMMON /PRM/RGAS,RENRGY,TCRIT,PCRIT,RHOC,W,ALPHA,BETA,XMW          EZFG0190
      1   ,A(40),B(7),NTERMS,NPARM,NUMB,RTOP,RMIDL,RMIDV                  EZFG0200
       FP=ALOG(RHO*RGAS*T)+FI1(T,RHO)+(PRES(T,RHO)/RHO/RGAS/T-1. )        EZFG0210
       IF(FP.GT.100)FP=100.                                               EZFG0220
       FUGCOF=EXP(FP)                                                     EZFG0230
       RETURN                                                             EZFG0240
       END                                                                EZFG0250
```

```
C    FUNCTION FUNCN(X,NDIM)                                               EZFN0010
C                                                                         EZFN0020
C    PURPOSE                                                              EZFN0030
C       EVALUATES THE FITTED FUNCTION AT THE POINT X                      EZFN0040
C                                                                         EZFN0050
C    USUAGE                                                               EZFN0060
C      RESULT = FUNCN(X,NDIM)                                             EZFN0070
C                                                                         EZFN0080
C    DESCRIPTION OF PARAMETERS                                            EZFN0090
C      X    - ARRAY OF VALUES OF INDEPENDENT VARIABLES                    EZFN0100
C      NDIM - NUMBER OF INDEPENDENT VARIABLES                             EZFN0110
C                                                                         EZFN0120
       FUNCTION FUNCN(X,NDIM)                                             EZFN0130
       DIMENSION X(NDIM)                                                  EZFN0140
       COMMON /PRM/RGAS,RENRGY,TCRIT,PCRIT,RHOC,W,ALPHA,BETA,XMW          EZFN0150
      1   ,A(40),B(7),NTERMS,NPARM,NUMB,RTOP,RMIDL,RMIDV                  EZFN0160
       COMMON /PRP/ICOMP(20),CPC(20),CRC(20),CMW(20),CW(20) ,CTC(20)      EZFN0170
      1 ,CA(20),CB(20),CNAME(20,2)                                        EZFN0180
       INTEGER SL                                                         EZFN0190
       DATA SL/-1/                                                        EZFN0200
       N=NDIM-NPARM                                                       EZFN0210
       DO 20 I=1,NPARM                                                    EZFN0220
   20  A(I)=X(N+I)                                                        EZFN0230
       XI=ABS(X(1))                                                       EZFN0240
       IWHOLE=XI+.005                                                     EZFN0250
       IFRACT=(XI-IWHOLE+.005)*100.                                       EZFN0260
```

```
      LIQVAP=SIGN(1.,X(1))                                              EZFN0270
C     IF(IWHOLE.GT.99) GO TO MIXTURE                                    EZFN0280
C          PURE                                                         EZFN0290
      DO 50 L=1,20                                                      EZFN0300
      IF(ICOMP(L).EQ.IWHOLE) GO TO 60                                   EZFN0310
   50 CONTINUE                                                          EZFN0320
      PRINT 200,IWHOLE                                                  EZFN0330
  200 FORMAT(1X,'COMPONENT',I5,'  NOT IN DATA SET')                     EZFN0340
      STOP                                                              EZFN0350
   60 CONTINUE                                                          EZFN0360
      IF(SL.EQ.L) GO TO 30                                              EZFN0370
      TCRIT=CTC(L)                                                      EZFN0380
      PCRIT=CPC(L)                                                      EZFN0390
      RHOC=CRC(L)                                                       EZFN0400
      RENRGY=1.9872/CMW(L)                                              EZFN0410
      W=CW(L)                                                           EZFN0420
      ALPHA=CA(L)                                                       EZFN0430
      BETA=CB(L)                                                        EZFN0440
      RTOP=4*RHOC                                                       EZFN0450
      RMIDL=RHOC                                                        EZFN0460
      RMIDV=RHOC                                                        EZFN0470
  100 FORMAT(1X,8G14.6)                                                 EZFN0480
      SL=L                                                              EZFN0490
   30 CONTINUE                                                          EZFN0500
C          CALCULATE PROPERTIES                                         EZFN0510
      IF(IFRACT.EQ.30.AND.LIQVAP.EQ.-1) GO TO 1                         EZFN0520
      IF(IFRACT.EQ.30.AND.LIQVAP.EQ.1) GO TO 2                          EZFN0530
      IF(IFRACT.EQ.40.AND.LIQVAP.EQ.-1) GO TO 3                         EZFN0540
      IF(IFRACT.EQ.40.AND.LIQVAP.EQ.1) GO TO 4                          EZFN0550
      IF(IFRACT.EQ.75) GO TO 5                                          EZFN0560
      IF(IFRACT.EQ.60) GO TO 6                                          EZFN0570
      IF(IFRACT.EQ.25) GO TO 7                                          EZFN0580
C                                                                       EZFN0590
C      LIQUID DENSITY                                                   EZFN0600
C                                                                       EZFN0610
    1 FUNCN=DENSL(X(2),X(3))                                            EZFN0620
      GO TO 40                                                          EZFN0630
C                                                                       EZFN0640
C      VAPOR DENSITY                                                    EZFN0650
C                                                                       EZFN0660
    2 FUNCN=DENSV(X(2),X(3))                                            EZFN0670
      GO TO 40                                                          EZFN0680
C                                                                       EZFN0690
C      LIQUID ENTHALPY                                                  EZFN0700
C                                                                       EZFN0710
    3 RHOL=DENSL(X(2),X(3))                                             EZFN0720
      FUNCN=ENTH(X(2),RHOL)                                             EZFN0730
      GO TO 40                                                          EZFN0740
C                                                                       EZFN0750
C      VAPOR ENTHALPY                                                   EZFN0760
```

```
C                                                                       EZFN0770
    4 RHOV=DENSV(X(2),X(3))                                             EZFN0780
      FUNCN=ENTH(X(2),RHOV)                                             EZFN0790
      GO TO 40                                                          EZFN0800
C                                                                       EZFN0810
C       VAPOR PRESSURE                                                  EZFN0820
    5 FUNCN=FLASHP(X(2),X(3))                                           EZFN0830
      GO TO 40                                                          EZFN0840
C                                                                       EZFN0850
C       PRESSURE                                                        EZFN0860
C                                                                       EZFN0870
    6 FUNCN=PRES(X(2),X(3))                                             EZFN0880
      GO TO 40                                                          EZFN0890
C                                                                       EZFN0900
C            SPCEIFIC VOLUME HEAT CAPACITY                              EZFN0910
C                                                                       EZFN0920
    7 FUNCN=CV(X(2),X(3))                                               EZFN0930
      GO TO 40                                                          EZFN0940
   40 RETURN                                                            EZFN0950
      END                                                               EZFN0960
```

```
C   SUBROUTINE GJEL(A,ND,MD,DETD,IER)                                   EZGJ0010
C                                                                       EZGJ0020
C   PURPOSE                                                             EZGJ0030
C      SIMULTANEOUS SOLUTION OF LINEAR EQUATIONS BY GAUSS-JORDAN        EZGJ0040
C   USUSGE                                                              EZGJ0050
C     CALL GEJEL(A,ND,MD,DETD,IER)                                      EZGJ0060
C                                                                       EZGJ0070
C   DESCRIPTION OF PARAMETERS                                           EZGJ0080
C    A IS THE ND BY MD AUGMENTED MATRIX                                 EZGJ0090
C    THE FIRST ND COLUMNS RETURNS THE INVERSE MATRIX                    EZGJ0100
C    THE LAST MD-ND COLUMNS CONTAIN THE SOLUTION VECTORS                EZGJ0110
C    DETD RETURNS THE DETERMINANT                                       EZGJ0120
C                                                                       EZGJ0130
C   SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                       EZGJ0140
C     NONE                                                              EZGJ0150
C                                                                       EZGJ0160
      SUBROUTINE GJEL(A,ND,MD,DETD,IER)                                 EZGJ0170
      DIMENSION A(ND,MD)                                                EZGJ0180
      DOUBLE PRECISION A,FACT,DABS                                      EZGJ0190
      INTEGER*2 PIVOTS(100),CPIVCT(100)                                 EZGJ0200
      DATA EPS/1.E-20/                                                  EZGJ0210
      IER=0                                                             EZGJ0220
```

```
      N=ND                                                                  EZGJ0230
      M=MD                                                                  EZGJ0240
      DET=1.                                                                EZGJ0250
      DO 4 I=1,N                                                            EZGJ0260
      IF(I.EQ.N) GO TO 30                                                   EZGJ0270
C      FIND LARGEST COLUMN PIVOT                                            EZGJ0280
      LPIVOT=I                                                              EZGJ0290
      IPIVOT=I                                                              EZGJ0300
      FACT=DABS(A(I,I))                                                     EZGJ0310
      DO 10 II=I,N                                                          EZGJ0320
      DO 10 JJ=I,N                                                          EZGJ0330
      IF(DABS(A(JJ,II)).LE.FACT) GO TO 10                                   EZGJ0340
      FACT=DABS(A(JJ,II))                                                   EZGJ0350
      LPIVOT=JJ                                                             EZGJ0360
      IPIVOT=II                                                             EZGJ0370
   10 CONTINUE                                                              EZGJ0380
C       TRADE COLUMNS                                                       EZGJ0390
      CPIVOT(I)=IPIVOT                                                      EZGJ0400
      DO 60 K=1,N                                                           EZGJ0410
      FACT=A(K,I)                                                           EZGJ0420
      A(K,I)=A(K,IPIVOT)                                                    EZGJ0430
      A(K,IPIVOT)=FACT                                                      EZGJ0440
   60 CONTINUE                                                              EZGJ0450
C       TRADE ROWS                                                          EZGJ0460
      PIVOTS(I)=LPIVOT                                                      EZGJ0470
      DO 20 K=1,M                                                           EZGJ0480
      FACT=A(I,K)                                                           EZGJ0490
      A(I,K)=A(LPIVOT,K)                                                    EZGJ0500
      A(LPIVOT,K)=FACT                                                      EZGJ0510
   20 CONTINUE                                                              EZGJ0520
   30 CONTINUE                                                              EZGJ0530
      CPIVOT(N)=N                                                           EZGJ0540
      PIVOTS(N)=N                                                           EZGJ0550
      IF(A(I,I))1,2,1                                                       EZGJ0560
    2 DET=0.                                                                EZGJ0570
      IER=N+1                                                               EZGJ0580
      RETURN                                                                EZGJ0590
    3 DET=0.                                                                EZGJ0600
      IER=I                                                                 EZGJ0610
      GO TO 8                                                               EZGJ0620
    1 IF(DABS(A(I,I)).LT.EPS) GO TO 3                                       EZGJ0630
C     FORM DETERMINANTS                                                     EZGJ0640
    8 DET=A(I,I)*DET                                                        EZGJ0650
      IF(ABS(DET).GE.1.E-60.OR.DET.EQ.0) GO TO 90                           EZGJ0660
      PRINT 200,DET                                                         EZGJ0670
      DET=0                                                                 EZGJ0680
   90 CONTINUE                                                              EZGJ0690
  200 FORMAT(1X,'MATRIX IS ILL CONDITIONED.  DETERMINANT IS ',G14.6)        EZGJ0700
      FACT=A(I,1)                                                           EZGJ0710
      A(I,1)=1.                                                             EZGJ0720
```

```
      DO 5 J=1,M                                                        EZGJ0730
C     NORMALIZE                                                         EZGJ0740
      A(I,J)=A(I,J)/FACT                                                EZGJ0750
    5 CONTINUE                                                          EZGJ0760
      DO 6 J=2,N                                                        EZGJ0770
      L=MOD(I+J-2,N)+1                                                  EZGJ0780
      IF(A(L,I).EQ.0.)GO TO 6                                           EZGJ0790
      FACT=A(L,I)                                                       EZGJ0800
      A(L,I)=0.                                                         EZGJ0810
      DO 7 K=1,M                                                        EZGJ0820
      LL=MOD(I+K-2,M)+1                                                 EZGJ0830
      IF(A(I,LL).EQ.0.)GO TO 7                                          EZGJ0840
C     REDUCE                                                            EZGJ0850
      A(L,LL)=A(L,LL)-A(I,LL)*FACT                                      EZGJ0860
    7 CONTINUE                                                          EZGJ0870
    6 CONTINUE                                                          EZGJ0880
    4 CONTINUE                                                          EZGJ0890
C       TRANSFER COLUMNS OF INVERSE                                     EZGJ0900
      DO 40 IR=1,N                                                      EZGJ0910
      I=N-IR+1                                                          EZGJ0920
      IF(PIVOTS(I).EQ.I) GO TO 40                                       EZGJ0930
      LPIVOT=PIVOTS(I)                                                  EZGJ0940
      DO 50 J=1,N                                                       EZGJ0950
      FACT=A(J,I)                                                       EZGJ0960
      A(J,I)=A(J,LPIVOT)                                                EZGJ0970
      A(J,LPIVOT)=FACT                                                  EZGJ0980
   50 CONTINUE                                                          EZGJ0990
   40 CONTINUE                                                          EZGJ1000
C       TRANSFER ROWS OF INVERSE                                        EZGJ1010
      DO 70 IR=1,N                                                      EZGJ1020
      I=N-IR+1                                                          EZGJ1030
      IF(CPIVOT(I).EQ.I) GO TO 70                                       EZGJ1040
      JPIVOT=CPIVOT(I)                                                  EZGJ1050
      DO 80 J=1,M                                                       EZGJ1060
      FACT=A(I,J)                                                       EZGJ1070
      A(I,J)=A(JPIVOT,J)                                                EZGJ1080
      A(JPIVOT,J)=FACT                                                  EZGJ1090
   80 CONTINUE                                                          EZGJ1100
   70 CONTINUE                                                          EZGJ1110
      DETD=DET                                                          EZGJ1120
      RETURN                                                            EZGJ1130
      END                                                               EZGJ1140
```

```
      SUBROUTINE LBLEZ                                                  EZLB0010
      DATA I/0/                                                         EZLB0020
      IF(I.EQ.0) PRINT 20                                               EZLB0030
   20 FORMAT(1H1,20(/),50X,'*',6(4X,'*')//50X,'*',12X,'EZFIT',12X,'*',  EZLB0040
     1//50X,'*',4X,'NONLINEAR REGRESSION',5X,'*',//50X,                 EZLB0050
     2'*',13X,'BY',14X,'*'//50X,'*',9X,'KEVIN GOIN',10X,'*'//           EZLB0060
     3 50X,'*',7X,'OCTOBER 20, 1976',6X,'*'//50X,'*',                   EZLB0070
     4 6(4X,'*')////)                                                   EZLB0080
      I=1                                                               EZLB0090
      RETURN                                                            EZLB0100
      END                                                               EZLB0110
```

```
C     SUBROUTINE MESSG(TEXT,NCHR)                                       EZMS0010
C                                                                       EZMS0020
C     PURPOSE                                                           EZMS0030
C       PRINTS A MESSAGE OF UP TO 80 CHARACTERS                         EZMS0040
C                                                                       EZMS0050
C     USAGE                                                             EZMS0060
C       CALL MESSG(TEXT,NCHR)                                           EZMS0070
C                                                                       EZMS0080
C     DESCRIPTION OF PARAMETERS                                         EZMS0090
C       TEXT - CHARACTER STRING TO BE PRINTED                           EZMS0100
C       NCHR - NUMBER OF CHARACTERS TO BE PRINTED                       EZMS0110
C                                                                       EZMS0120
      SUBROUTINE MESSG(TEXT,NCHR)                                       EZMS0130
      LOGICAL*1 TEXT                                                    EZMS0140
      DIMENSION TEXT(NCHR)                                              EZMS0150
      PRINT 2000,TEXT                                                   EZMS0160
 2000 FORMAT(1X,80A1)                                                   EZMS0170
      RETURN                                                            EZMS0180
      END                                                               EZMS0190
```

```
C                                                                       EZOU0010
C    SUBROUTINE OUTPUT(X,N,Y,NPTS,NAPRM,A1,WEIGHT,DATAID,ND)            EZOU0020
C                                                                       EZOU0030
C    PURPOSE                                                            EZOU0040
C      PRINTS TABULATED RESULTS OF A GIVEN SET OF PARAMETERS.           EZOU0050
C                                                                       EZOU0060
      SUBROUTINE OUTPUT(X,N,Y,NPTS,NPARM,A1,WEIGHT,DATAID,ND)           EZOU0070
      COMMON /PRM/RGAS,RENRGY,TCRIT,PCRIT,RHOC,W,ALPHA,BETA,XMW         EZOU0080
     1   ,A(40),B(7),NTERMS,NPAR1,NUMB,RTOP,RMIDL,RMIDV                 EZOU0090
      DIMENSION X(NPTS,N),Y(NPTS),A1(NPARM),WEIGHT(NPTS),DATAID(NPTS,ND)EZOU0100
      DIMENSION HEADER(20)                                              EZOU0110
      DIMENSION Z(110)                                                  EZOU0120
      DATA IPRINT/0/                                                    EZOU0130
  100 FORMAT(1X,8G14.6)                                                 EZOU0140
  200 FORMAT(20A4)                                                      EZOU0150
  300 FORMAT(/////1X,'AVERAGE ABSOLUTE DEVIATION',G14.6)                EZOU0160
  400 FORMAT(26X,20A4//)                                                EZOU0170
  500 FORMAT(1H1)                                                       EZOU0180
 1100 FORMAT(16I5)                                                      EZOU0190
      DATA IRHO,IDH,IVP/30,40,75/                                       EZOU0200
      READ 200,HEADER                                                   EZOU0210
      READ 1100,IXPRT,JXPRT                                             EZOU0220
      PRINT 400,HEADER                                                  EZOU0230
      LF=-1                                                             EZOU0240
      LW=-200                                                           EZOU0250
      SUM1=0                                                            EZOU0260
      J0=0                                                              EZOU0270
      SUM2=0                                                            EZOU0280
      SUM=0                                                             EZOU0290
      CHISQR=0                                                          EZOU0300
      RSUM=0.                                                           EZOU0310
      N1=0                                                              EZOU0320
      N2=0                                                              EZOU0330
      N3=0                                                              EZOU0340
      N4=0                                                              EZOU0350
      N5=0                                                              EZOU0360
      N6=0                                                              EZOU0370
      NDIM=N+NPARM                                                      EZOU0380
      DO 10 J=1,NPARM                                                   EZOU0390
      Z(N+J)=A1(J)                                                      EZOU0400
   10 CONTINUE                                                          EZOU0410
      DO 20 I=1,NPTS                                                    EZOU0420
      DO 50 J=1,N                                                       EZOU0430
      Z(J)=X(I,J)                                                       EZOU0440
   50 CONTINUE                                                          EZOU0450
      YC=FUNCN(Z,NDIM)                                                  EZOU0460
      PERC=100*(YC-Y(I))/Y(I)                                           EZOU0470
      DIFF=Y(I)-YC                                                      EZOU0480
      X1=ABS(Z(1))                                                      EZOU0490
      IWHOLE=X1+.003                                                    EZOU0500
```

```
      IFRACT=(X1-IWHOLE+.003)*100                                          EZOU0510
      IF(IWHOLE.EQ.LW.AND.IFRACT.EQ.LF) GO TO 140                          EZOU0520
C     PREPARE SUMMARIES AND GROUP HEADING                                  EZOU0530
      IF(IPRINT.EQ.1) GO TO 240                                            EZOU0540
      IPRINT=1                                                             EZOU0550
      GO TO 250                                                            EZOU0560
  240 CONTINUE                                                             EZOU0570
C      SUMMARY                                                             EZOU0580
      IF(J0.NE.0)SUM1=SUM1/J0                                              EZOU0590
      IF(J0.NE.0)SUM2=SUM2/J0                                              EZOU0600
      PRINT 100                                                            EZOU0610
      CALL MESSG('AVE. ABS. PERCENT.NUMBER PTS..AVE.ABS.DEVIATION ',48)    EZOU0620
      PRINT 100,SUM1,J0,SUM2                                               EZOU0630
      PRINT 100                                                            EZOU0640
      CALL MESSG('CONTRIBUTION TO CHISQUARED',26)                          EZOU0650
      PRINT 100,CHISQR                                                     EZOU0660
      PRINT 100                                                            EZOU0670
      CHISQR=0                                                             EZOU0680
  250 CONTINUE                                                             EZOU0690
C    HEADING                                                               EZOU0700
      PRINT 500                                                            EZOU0710
      PRINT 400,HEADER                                                     EZOU0720
      IF(IWHOLE.NE.LW) PRINT 1900,IWHOLE                                   EZOU0730
      IF(IFRACT.NE.LF.OR.IWHOLE.NE.LW) PRINT 1800,IFRACT                   EZOU0740
 1800 FORMAT(57X,'DATA TYPE',I5///)                                        EZOU0750
 1900 FORMAT(55X,'COMPOUND CODE',I5///)                                    EZOU0760
      PRINT 1600                                                           EZOU0770
 1600 FORMAT(5X,'DATAID',8X,'YEXP',8X,'YCALC',7X,'PERCENT',7X,'DELTA'      EZOU0780
     1  ,8X,'WEIGHT',6X,'CONTROL',9X,'X2',11X,'X3',11X,'X4'/57X,'X''S...'EZOU0790
     2  ,//)                                                              EZOU0800
      SUM1=0                                                               EZOU0810
      SUM2=0.                                                              EZOU0820
      J0=0                                                                 EZOU0830
      LF=IFRACT                                                            EZOU0840
      LW=IWHOLE                                                            EZOU0850
  140 CONTINUE                                                             EZOU0860
      J0=J0+1                                                              EZOU0870
      SUM=SUM+ABS(PERC)                                                    EZOU0880
      SUM1=SUM1+ABS(PERC)                                                  EZOU0890
      SUM2=SUM2+ABS(DIFF)                                                  EZOU0900
      CHISQR=CHISQR+WEIGHT(I)*DIFF*DIFF                                    EZOU0910
      IF(IFRACT.EQ.60) GO TO 220                                           EZOU0920
      IF(JXPRT.EQ.0)                                                       EZOU0930
     1PRINT 2000,(DATAID(I,K),K=1,ND),Y(I),YC,PERC,DIFF,WEIGHT(I),         EZOU0940
     1 (X(I,K),K=1,N)                                                     EZOU0950
 2000 FORMAT(1X,3A4,1X,9G13.5,(/53X,6G13.5))                               EZOU0960
      IF(IXPRT.EQ.0) GO TO 20                                              EZOU0970
      IF(IFRACT.EQ.IDH) GO TO 220                                          EZOU0980
      IF(IFRACT.EQ.IRHC) GO TO 210                                         EZOU0990
      IF(IFRACT.EQ.IVP) GO TO 230                                          EZOU1000
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      GO TO 20                                                          EZOU1010
  220 CONTINUE                                                          EZOU1020
C       MODIFIED FOR DELTA P OUTPUT                                     EZOU1030
      P=Y(I)+RGAS*Z(2)*Z(3)                                             EZOU1040
      IF(Z(1).LE.0) RHO=DENSL(Z(2),P)                                   EZOU1050
      IF(Z(1).GT.0) RHO=DENSV(Z(2),P)                                   EZOU1060
      PECR=(Z(3)-RHO)*100/Z(3)                                          EZOU1070
      RSUM=RSUM+ABS(PECR)                                               EZOU1080
      APECR=ABS(PECR)                                                   EZOU1090
      IF(APECR.LT..01) N1=N1+1                                          EZOU1100
      IF(APECR.LT..1.AND.APECR.GE..01)N2=N2+1                           EZOU1110
      IF(APECR.LT.1..AND.APECR.GE..1) N3=N3+1                           EZOU1120
      IF(APECR.LT.10..AND.APECR.GE.1.)N4=N4+1                           EZOU1130
      IF(APECR.LT.100..AND.APECR.GE.10.)N5=N5+1                         EZOU1140
      IF(APECR.GE.100)N6=N6+1                                           EZOU1150
      IF(JXPRT.EQ.0)                                                    EZOU1160
     1PRINT 2100,(DATAID(I,K),K=1,ND),Y(I),YC,PERC,DIFF,WEIGHT(I),      EZOU1170
     1 (X(I,K),K=1,N),RHO,PECR                                          EZOU1180
 2100 FORMAT(1X,3A4,1X,8G13.5,F8.5,F7.2)                                EZOU1190
      GO TO 20                                                          EZOU1200
  230 CONTINUE                                                          EZOU1210
      RHOL=DENSL(Z(2),Z(3))                                             EZOU1220
      RHOV=DENSV(Z(2),Z(3))                                             EZOU1230
      PRINT 2200,RHOV,RHOL                                              EZOU1240
 2200 FORMAT(68X,'SATURATION VAPOR AND LIQUID DENSITIES',2G13.5)        EZOU1250
      GO TO 20                                                          EZOU1260
  210 CONTINUE                                                          EZOU1270
      PRESC= PRES(Z(2),Y(I))                                            EZOU1280
      PERC2=(Z(3)-PRESC)*100/Z(3)                                       EZOU1290
 1700 FORMAT(69X,'PEXP,PCALC,PERCENT',5X,3G13.5)                        EZOU1300
      PRINT 1700,Z(3),PRESC,PERC2                                       EZOU1310
   20 CONTINUE                                                          EZOU1320
      SUM1=SUM1/J0                                                      EZOU1330
      SUM2=SUM2/J0                                                      EZOU1340
      PRINT 100                                                         EZOU1350
      CALL MESSG('AVE. ABS. PERCENT.NUMBER PTS.,AVE.ABS.DEVIATION ',48) EZOU1360
      PRINT 100,SUM1,J0,SUM2                                            EZOU1370
      PRINT 100                                                         EZOU1380
      CALL MESSG('CONTRIBUTION TO CHISQUARED',26)                       EZOU1390
      PRINT 100,CHISQR                                                  EZOU1400
      PRINT 100                                                         EZOU1410
      CHISQR=0                                                          EZOU1420
      PRINT 100                                                         EZOU1430
      IF (RSUM.EQ.0) GO TO 260                                          EZOU1440
      RSUM=RSUM/NPTS                                                    EZOU1450
      CALL MESSG('DENSITY AAPD',12)                                     EZOU1460
      PRINT 100,RSUM                                                    EZOU1470
      PRINT 100                                                         EZOU1480
      PRINT 2300,N1,N2,N3,N4,N5,N6                                      EZOU1490
 2300 FORMAT(/1X,'DENSITY ERROR DISTRIBUTION',/,7X,'<.01',4X,'.01-.1',5XEZOU1500
```

```
     1  ,'.1-1.',4X,'1.-10.',2X,'10.-100.',5X,'>100.',/1X,6I10//)          EZDU1510
  260 CONTINUE                                                            EZDU1520
      SUM=SUM/NPTS                                                        EZDU1530
      PRINT 300,SUM                                                       EZDU1540
      PRINT 100                                                           EZDU1550
      PRINT 100                                                           EZDU1560
      PRINT 100                                                           EZDU1570
      IPRINT=0.                                                           EZDU1580
      RETURN                                                              EZDU1590
      END                                                                 EZDU1600
```

```
C     FUNCTION U(T,RHO))                                                  EZDU0010
C                                                                         EZDU0020
C     PURPOSE                                                             EZDU0030
C       CALCULATES THE INTERNAL ENERGY                                    EZDU0040
C                                                                         EZDU0050
C     USUAGE                                                              EZDU0060
C       RESULT=U(T,RHO)                                                   EZDU0070
C     DESCRIPTION OF PARAMETERS                                           EZDU0080
C          T-ABSOLUTE TEMPERATURE                                         EZDU0090
C       RHO-DENSITY                                                       EZDU0100
C                                                                         EZDU0110
C     SUBROUTINES NEEDED                                                  EZDU0120
C       FI2(T,RHO)                                                        EZDU0130
C         CALCULATES THE INTEGRAL OF (DZDT)DLN(RHO)                       EZDU0140
C                                                                         EZDU0150
      FUNCTION U(T,RHO)                                                   EZDU0160
      COMMON /PRM/RGAS,RENRGY,TCRIT,PCRIT,RHOC,W,ALPHA,BETA,XMW           EZDU0170
     1   ,A(40),B(7),NTERMS,NPARM,NUMB,RTOP,RMIDL,RMIDV                   EZDU0180
      TSTAR=ALPHA*T/TCRIT                                                 EZDU0190
      U=RENRGY*TCRIT*(-TSTAR*TSTAR*FI2(T,RHO))/ALPHA                      EZDU0200
      RETURN                                                              EZDU0210
      END                                                                 EZDU0220
```

```
C                                                                       EZPR0010
C                                                                       EZPR0020
C     FUNCTION PRES                                                     EZPR0030
C                                                                       EZPR0040
C     PURPOSE                                                           EZPR0050
C       CALCULATES THE PRESSURE FOR THE TCHEBYCHEF POLYNOMIAL EQUATION  EZPR0060
C            PURE COMPONENT FORM                                        EZPR0070
C                                                                       EZPR0080
C     USUAGE                                                            EZPR0090
C       RESULT = PRES(T,RHO)                                            EZPR0100
C                                                                       EZPR0110
C     DESCRIPTION OF PARAMETERS                                         EZPR0120
C         T-ABSOLUTE TEMPERATURE                                        EZPR0130
C       RHO - DENSITY                                                   EZPR0140
C                                                                       EZPR0150
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                     EZPR0160
C       NONE                                                            EZPR0170
C                                                                       EZPR0180
       FUNCTION PRES(T,RHO)                                             EZPR0190
       COMMON /PRM/RGAS,RENRGY,TCRIT,PCRIT,RHOC,W,ALPHA,BETA,XMW        EZPR0200
      1  ,A(40),B(7),NTERMS,NPARM,NUMB,RTOP,RMIDL,RMIDV                 EZPR0210
       COMMON /XTN/AXTN(60)                                             EZPR0220
       REAL*8 Z,X,X6,X4,C1,C2,C3,C4,C5,C6,C7,C8,C9                      EZPR0230
       Y1(U)=U                                                          EZPR0240
       Y2(U)=2*U*U-1                                                    EZPR0250
       Y3(U)=(4*U*U-3)*U                                                EZPR0260
       Y4(U)=(8*U*U-8)*U*U+1                                            EZPR0270
       Y5(U)=((16*U*U-20)*U*U+5)*U                                      EZPR0280
       Y6(U)=((32*U*U-48)*U*U+18)*U*U-1                                 EZPR0290
       Y7(U)=(((64*U*U-112)*U*U+56)*U*U-7)*U                            EZPR0300
       Y8(U)=(((128*U*U-256)*U*U+160)*U*U-32)*U*U+1                     EZPR0310
       TSTAR=ALPHA*T/TCRIT                                              EZPR0320
       RHOS=BETA*RHO/RHOC                                               EZPR0330
       X=1/TSTAR                                                        EZPR0340
       Y=RHOS/4.                                                        EZPR0350
       C1=(((((A(6)*X+A(5))*X+A(4))*X+A(3))*X+A(2))*X+A(1))             EZPR0360
       C2=(((((A(12)*X+A(11))*X+A(10))*X+A(9))*X+A(8))*X+A(7))          EZPR0370
       C3=(((((A(18)*X+A(17))*X+A(16))*X+A(15))*X+A(14))*X+A(13) )      EZPR0380
       C4=(((((A(24)*X+A(23))*X+A(22))*X+A(21))*X+A(20))*X+A(19) )      EZPR0390
       C5=((A(28)*X+A(27))*X+A(26))*X+A(25)                             EZPR0400
       C6=((A(32)*X+A(31))*X+A(30))*X+A(29)                             EZPR0410
       C7=((A(36)*X+A(35))*X+A(34))*X+A(33)                             EZPR0420
       C8=((A(40)*X+A(39))*X+A(38))*X+A(37)                             EZPR0430
       X6=X**6                                                          EZPR0440
       X4=X**4                                                          EZPR0450
       C1=C1+(AXTN(6)*X+AXTN(5))*X6                                     EZPR0460
       C2=C2+(AXTN(8)*X+AXTN(7))*X6                                     EZPR0470
       C3=C3+(AXTN(10)*X+AXTN(9))*X6                                    EZPR0480
       C4=C4+(AXTN(12)*X+AXTN(11))*X6                                   EZPR0490
       C5=C5+(((AXTN(16)*X+AXTN(15))*X+AXTN(14))*X+AXTN(13))*X4         EZPR0500
```

```
      C6=C6+(((AXTN(20)*X+AXTN(19))*X+AXTN(18))*X+AXTN(17))*X4          EZPR0510
      C7=C7+(((AXTN(24)*X+AXTN(23))*X+AXTN(22))*X+AXTN(21))*X4          EZPR0520
      C8=C8+(((AXTN(28)*X+AXTN(27))*X+AXTN(26))*X+AXTN(25))*X4          EZPR0530
      C9=((((((AXTN(32)*X+AXTN(31))*X+AXTN(30))*X+AXTN(29))*X           EZPR0540
     1   +AXTN(4))*X+AXTN(3))*X+AXTN(2))*X+AXTN(1)                      EZPR0550
      Z=C1+C2*Y1(Y)+C3*Y2(Y)+C4*Y3(Y)+C5*Y4(Y)+C6*Y5(Y)+C7*Y6(Y)         EZPR0560
      Z=(Z+C8*Y7(Y)+C9*Y8(Y))*Y+1                                       EZPR0570
      PRES=Z*T*RHO*RGAS                                                 EZPR0580
      RETURN                                                            EZPR0590
      END                                                               EZPR0600
```

```
C     FUNCTION FI1                                                      EZI10010
C                                                                       EZI10020
C     PURPOSE                                                           EZI10030
C       CALCULATES THE INTEGRAL OF (Z-1)DLN(RHO) FOR DERIVED PROPERTIES EZI10040
C            PURE COMPONENT FORM                                        EZI10050
C                                                                       EZI10060
C     USUAGE                                                            EZI10070
C       RESULT=FI1(T,RHO)                                               EZI10080
C     DESCRIPTION OF PARAMETERS                                         EZI10090
C        T-ABSOLUTE TEMPERATURE                                         EZI10100
C       RHO-DENSITY                                                     EZI10110
C                                                                       EZI10120
C     SUBROUTINES NEEDED                                                EZI10130
C       NONE                                                            EZI10140
C                                                                       EZI10150
      FUNCTION FI1(T,RHO)                                               EZI10160
      COMMON /XTN/AXTN(60)                                              EZI10170
      COMMON /PRM/RGAS,RENRGY,TCRIT,PCRIT,RHOC,W,ALPHA,BETA,XMW         EZI10180
     1   ,A(40),B(7),NTERMS,NPARM,NUMB,RTOP,RMIDL,RMIDV                 EZI10190
      YI0(U)=U                                                          EZI10200
      YI1(U)=U*U/2                                                      EZI10210
      YI2(U)=(.666667*U*U-1)*U                                          EZI10220
      YI3(U)=(U*U-1.5)*U*U                                              EZI10230
      YI4(U)=((1.6*U*U-2.66667)*U*U+1)*U                                EZI10240
      YI5(U)=((2.66667*U*U-5.)*U*U+2.5)*U*U                             EZI10250
      YI6(U)=(((4.57143*U*U-9.6)*U*U+6.)*U*U-1.)*U                      EZI10260
      YI7(U)=(((8.*U*U-18.6667)*U*U+14.)*U*U-3.5)*U*U                   EZI10270
      YI8(U)=((((14.2222*U*U-36.5714)*U*U+32.)*U*U-10.6667)*U*U+1)*U    EZI10280
      TSTAR=ALPHA*T/TCRIT                                               EZI10290
      RHOS=BETA*RHO/RHOC                                                EZI10300
      X=1/TSTAR                                                         EZI10310
      Y=RHOS/4.                                                         EZI10320
```

```
      C1=(((((A(6)*X+A(5))*X+A(4))*X+A(3))*X+A(2))*X+A(1))                    EZI10330
      C2=(((((A(12)*X+A(11))*X+A(10))*X+A(9))*X+A(8))*X+A(7))                 EZI10340
      C3=(((((A(18)*X+A(17))*X+A(16))*X+A(15))*X+A(14))*X+A(13) )             EZI10350
      C4=(((((A(24)*X+A(23))*X+A(22))*X+A(21))*X+A(20))*X+A(19) )             EZI10360
      C5=((A(28)*X+A(27))*X+A(26))*X+A(25)                                    EZI10370
      C6=((A(32)*X+A(31))*X+A(30))*X+A(29)                                    EZI10380
      C7=((A(36)*X+A(35))*X+A(34))*X+A(33)                                    EZI10390
      C8=((A(40)*X+A(39))*X+A(38))*X+A(37)                                    EZI10400
      X6=X**6                                                                 EZI10410
      X4=X**4                                                                 EZI10420
      C1=C1+(AXTN(6)*X+AXTN(5))*X6                                            EZI10430
      C2=C2+(AXTN(8)*X+AXTN(7))*X6                                            EZI10440
      C3=C3+(AXTN(10)*X+AXTN(9))*X6                                           EZI10450
      C4=C4+(AXTN(12)*X+AXTN(11))*X6                                          EZI10460
      C5=C5+(((AXTN(16)*X+AXTN(15))*X+AXTN(14))*X+AXTN(13))*X4                EZI10470
      C6=C6+(((AXTN(20)*X+AXTN(19))*X+AXTN(18))*X+AXTN(17))*X4                EZI10480
      C7=C7+(((AXTN(24)*X+AXTN(23))*X+AXTN(22))*X+AXTN(21))*X4                EZI10490
      C8=C8+(((AXTN(28)*X+AXTN(27))*X+AXTN(26))*X+AXTN(25))*X4                EZI10500
      C9=(((((AXTN(32)*X+AXTN(31))*X+AXTN(30))*X+AXTN(29))*X                  EZI10510
     1   +AXTN(4))*X+AXTN(3))*X+AXTN(2))*X+AXTN(1)                            EZI10520
      FI1=C1*YI0(Y)+C2*YI1(Y)+C3*YI2(Y)+C4*YI3(Y)+C5*YI4(Y)+C6*YI5(Y)         EZI10530
      FI1=FI1+C7*YI6(Y)+C8*YI7(Y)+C9*YI8(Y)                                   EZI10540
      RETURN                                                                  EZI10550
      END                                                                     EZI10560
```

```
C    FUNCTION FI2                                                           EZI20010
C                                                                           EZI20020
C    PURPOSE                                                                EZI20030
C      CALCULATES THE INTEGRAL OF DZDT*DLN(RHO) FOR DERIVED PROPERTIES      EZI20040
C           PURE COMPONENT FORM                                             EZI20050
C                                                                           EZI20060
C    USUAGE                                                                 EZI20070
C      RESULT=FI2(T,RHO)                                                    EZI20080
C    DESCRIPTION OF PARAMETERS                                              EZI20090
C        T-ABSOLUTE TEMPERATURE                                             EZI20100
C      RHO-DENSITY                                                          EZI20110
C                                                                           EZI20120
C   SUBROUTINES NEEDED                                                      EZI20130
C      NONE                                                                 EZI20140
C                                                                           EZI20150
      FUNCTION FI2(T,RHO)                                                   EZI20160
      COMMON /XTN/AXTN(60)                                                  EZI20170
      COMMON /PRM/RGAS,RENRGY,TCRIT,PCRIT,RHOC,W,ALPHA,BETA,XMW             EZI20180
```

```
1   ,A(40),B(7),NTERMS,NPARM,NUMB,RTOP,RMIDL,RMIDV                          EZI20190
 YI0(U)=U                                                                  EZI20200
 YI1(U)=U*U/2                                                              EZI20210
 YI2(U)=(.666667*U*U-1)*U                                                  EZI20220
 YI3(U)=(U*U-1.5)*U*U                                                      EZI20230
 YI4(U)=((1.6*U*U-2.66667)*U*U+1)*U                                        EZI20240
 YI5(U)=((2.66667*U*U-5.)*U*U+2.5)*U*U                                     EZI20250
 YI6(U)=(((4.57143*U*U-9.6)*U*U+6.)*U*U-1.)*U                              EZI20260
 YI7(U)=(((8.*U*U-18.6667)*U*U+14.)*U*U-3.5)*U*U                           EZI20270
 YI8(U)=((((14.2222*U*U-36.5714)*U*U+32.)*U*U-10.6667)*U*U+1)*U            EZI20280
 TSTAR=ALPHA*T/TCRIT                                                       EZI20290
 RHOS=BETA*RHO/RHOC                                                        EZI20300
 X=1/TSTAR                                                                 EZI20310
 Y=RHOS/4.                                                                 EZI20320
 DC1=-((((   ((AXTN(6)*X*7+AXTN(5)*6)*X+A(6)*5)*X+A(5)*4)*X+              EZI20330
1   A(4)*3)*X+A(3)*2)*X+A(2))*X*X                                          EZI20340
 DC2=-(((   (((AXTN(8)*X*7+AXTN(7)*6)*X+A(12)*5)*X+A(11)*4)*X+            EZI20350
1   A(10)*3)*X+A(9)*2)*X+A(8))*X*X                                         EZI20360
 DC3=-(((((AXTN(10)*X*7+AXTN(9)*6)*X+A(18)*5)*X+A(17)*4 )*X+              EZI20370
1   A(16)*3)*X+A(15)*2)*X+A(14))*X*X                                       EZI20380
 DC4=-(((((AXTN(12)*X*7+AXTN(11)*6)*X+A(24)*5)*X+A(23)*4)*X+              EZI20390
1   A(22)*3)*X+A(21)*2)*X+A(20))*X*X                                       EZI20400
 DC5=-(((((AXTN(16)*X*7+AXTN(15)*6)*X+AXTN(14)*5)*X+AXTN(13)*4)*X          EZI20410
1+A(28)*3)*X+A(27)*2)*X+A(26))*X*X                                         EZI20420
 DC6=-(((((AXTN(20)*X*7+AXTN(19)*6)*X+AXTN(18)*5)*X+AXTN(17)*4)*X          EZI20430
1  +A(32)*3)*X+A(31)*2)*X+A(30))*X*X                                       EZI20440
 DC7=-(((((AXTN(24)*X*7+AXTN(23)*6)*X+AXTN(22)*5)*X+AXTN(21)*4)*X          EZI20450
1  +A(36)*3)*X+A(35)*2)*X+A(34))*X*X                                       EZI20460
    DC8=-(((((AXTN(28)*X*7+AXTN(27)*6)*X+AXTN(26)*5)*X+AXTN(25)*4)         EZI20470
1*X+A(40)*3)*X+A(39)*2)*X+A(38))*X*X                                       EZI20480
 DC9=-(((((AXTN(32)*X*7+AXTN(31)*6)*X+AXTN(30)*5)*X+AXTN(29)*4)           EZI20490
1*X+AXTN(4)*3)*X+AXTN(3)*2)*X+AXTN(2))*X*X                                 EZI20500
 FI2=DC1*YI0(Y)+DC2*YI1(Y)+DC3*YI2(Y)+DC4*YI3(Y)+DC5*YI4(Y)                EZI20510
1  +DC6*YI5(Y)+DC7*YI6(Y)+DC8*YI7(Y)+DC9*YI8(Y)                            EZI20520
 RETURN                                                                    EZI20530
 END                                                                       EZI20540
```

APPENDIX C

BANKED

Bank for Experimental Data

Abstract

BANKED is a flexible data structure based on computer cards that will handle experimental data for a maximum of 999 chemical species, 99 data types and mixtures of 999 components. It features identification of each data point along with the bibliographical source. Because of its basic structure the cards can be arranged from disorder by simple sorting. It also supplies a set of physical properties for the species in BANKED.

Basic Structure

The BANKED Data base consists of three types of cards: The experimental data, the bibliographic information and physical properties information. The experimental data cards contain the independent variables, the dependent variable, control information identifying data type, bibliographic reference and data point reference number. The bibliographic cards have the reference code that is on the data card and the journal reference from which the data was obtained. The

physical properties card contains an acronym the for species, the data bank's species code, and various physical properties for the species, such as critical properties and molecular weight.

Experimental Data Cards

Several items of information are required for a data card. The method here identifies the data point as to the source, which actual point it is, the type of data, the independent variables and the dependent variable. The cards are laid out in six ten column fields, a two digit sequence number, a four character bibliographic reference and a seven digit data point reference number. The sequence number identifies the number of data cards needed for that type of point and also their order.

The first card for a data point has the control variable, two independent variables, usually temperature and pressure, the independent variable, the sequence number, bibliography code and data point identification number. (The format is 4F10.0, 26X, I2, 1X, A4,I7) The sequence number is one less than the number of cards needed for the data point. For explanation of the bibliography code see below. The following cards consist of six additional independent variables, a sequence number, bibliography code and data point identification number. (The format is 6F10.0,6X,12,1X,A4,I7.) The sequence numbers for each card for a specific point decrease so that the last card for the point has a sequence number of

0. Some examples of various data types are given in Figure 1.

The control variable contains information to specify the exact type of data that the point is. It's basic form is

$$X_1 = \text{SHXXX.DD}$$

(See Table III for a summary of its meaning.) The control variable is punched on the card so that SHXXX and DD can be read as separate integers (I6,1X,I2). The value of H specifies whether the datum is for a mixture or pure fluid. When it has the value 0, the point is a pure fluid and when it is 1 it is for a mixture. Therefore, for pure fluids the absolute value of X_1 is less than 1000. The sign, S, specifies whether the point is for a gas(+), i.e. $\rho < \rho_c$ or a liquid(-), $\rho > \rho_c$. The term DD is the code for the type of data this point is. Some of these types are given in Table II. There is room for 99 data types. The remaining term, XXX, has different meanings according to whether the point is for a mixture or pure fluid.

For pure fluids XXX is the code for the chemical species. These codes are given in Table I. There is a capability of handling 999 species with this system. For mixtures XXX specifies the number of components. With this and the data point type, the exact number of independent variables is fixed. Following the first card, the first XXX variables are the coded overall composition for mixtures.

TABLE I

Codes for Chemical Species

XXX	Specie
026	Ammonia
016	Argon
017	Carbon dioxide
018	Carbon monoxide

Freons

036	R-11 C Cl_3 F
037	R-12 C Cl_2 F_2
038	R-13 C Cl F_3
039	R-14 C F_4
040	R-21 C H Cl_2 F
041	R-22 C H Cl F_2
042	R-23 C H F_3
043	R-113 C Cl_2 F C Cl F_2
044	R-114 C Cl F_2 C Cl F_2
045	R-115 C_2 Cl F_5
046	R-C318 C_4 F_8
047	R-500 C Cl_2 F_2/C H_3 C H F_2
048	R-502 C H Cl F_2/C Cl F_2 C F_2
049	R-142b
050	R-152a

XXX	Specie
019	Helium
031	Hydrogen
028	Hydrogen Chloride
035	Hydrogen Sulfide
021	Nitric Oxide
024	Nitrogen
020	Nitrous Oxide
027	Water

Hydrocarbons

032	Acetylene
033	Benzene
004	Butane
030	Cyclohexane
029	Cyclopentane
010	Decane
012	Dodecane
002	Ethane
022	Ethylene
007	Heptane
006	Hexane
014	Isobutane
015	Isopentane
001	Methane
009	Nonane
008	Octane
005	Pentane
003	Propane
023	Propylene
034	Toluene
013	Tridecane
012	Undecane

TABLE II

Codes for Data Types

DD	Type	Variable Order
05	T_B, Bubble point temperature	Control, pressure, blank, T_B; compositions
06	P_B, Bubble point pressure	Control, temperature, blank, P_B; compositions
10	Adiabatic flash pressure	Control, temperature, V/L ratio, P; compositions
12	Δu, Internal energy departure	Control, temperature, density, ΔU; (mixture: compositions)
14	ΔS, entropy departure	Control, temperature, density, ΔS; (mixture: compositions)
15	Adiabatic flash temperature	Control, pressure, V/L ratio, T; compositions
20	C_p, specific heat at constant P	Control, temperature, density, C_p; (mixture: compositions)
21	C_p	Control, temperature, pressure, C_p; (mixture: compositions)
25	C_v, specific heat at constant v	Control, temperature, density, C_v; (mixture: compositions)
26	C_v	Control, temperature, pressure, C_v; (mixture: compositions)
30	ρ, density	Control, temperature, pressure, ρ; (mixture: compositions)
35	a, diffusivity	Control, temperature, pressure, a; (mixture: compositions)
36	a, diffusivity	Control, temperature, density, a; (mixture: compositions)
40	ΔH, enthalpy departure	Control, temperature, pressure, ΔH; (mixture: compositions)

TABLE II (continued)

DD	Type	Variable Order
41	ΔH, enthalpy departure	Control, temperature, density, ΔH; (mixture: compositions)
45	Flash V/L ratio	Control, temperature, pressure, V/L; compositions, K-values
50	H_J, Joule Thompson coefficient	Control, temperature, pressure, H_J; (mixture: compositions)
60	P, pressure	Control, temperature, density, P; (mixture: compositions)
65	W, speed of sound	Control, temperature, density, W; (mixture: compositions)
70	K, thermal conductivity	Control, temperature, density, K; (mixture: compositions)
75	$P\sigma$, vapor pressure	Control, temperature, pressure, $P\sigma$
80	B_2, 2nd Virial coefficient	Control, temperature, blank, B_2
85	B_3, 3rd Virial coefficient	Control, temperature, blank, B_3
90	ν, viscosity	Control, temperature, density, ν ; (mixture: compositions)
95	T_D, dew point temperature	Control, pressure, blank, T_D; (mixture: compositions)
96	P_D, dew point pressure	Control, temperature, blank, P_D; (mixture: compositions

TABLE III

Format of Control Variable, X_1

$$X_1 = SHXXX.DD$$

$S = \begin{cases} + \text{ Gas, } \rho<\rho_c \\ - \text{ Liquid, } \rho>\rho_c \end{cases}$

$H = \begin{cases} 0 \text{ Pure Fluid} \\ 1 \text{ Mixture} \end{cases}$

Pure Fluid	Mixture
XXX = Code for Chemical Species	XXX = Number of Components
DD = Code for Data Type	DD = Code for Data Type

```
(a)  -1.30    216.000    3638.45 1.68180                                    0 0016    1011

(b) 1002.60    582.011 0.0624100     377.000                                01 0033    1915
     1.98700    3.01300                                                     00 0033    1915

(c) 1004.55    504.000    1071.000    10.95                                02 0043    1392
     1.95000    3.03750    7.01245  10.00005     3.5         1.13          01 0043    1392
      .001                                                                  00 0043    1392
```

Figure 1. Example Data Cards: (a) Methane density; (b) Pressure for methane and propane mixture; (c) K-value for light component in mixture of methane, propane, heptane, and decane.

The whole portion of the variable is the species code and the fraction is the mole fraction of that specie. These are punched so that they could be read as separate numbers (F4.0,F6.5). The data type then specifies how many other variables are needed.

Bibliographic Card

The bibliographic cards are used to reference the source of the experimental data. The card consists of a four character code and a seventy-six character reference field. The code consists of a three digit sequence number and the initial of the author. The typical card is:

001M, MICHELS, WIJKER, WIJKER, "ISOTHERMS OF ARGON..."PHYSICA, XV, NO. 7, P62 (1949).

The reference field is in a standard journal reference style.

Physical Properties Card

The physical properties cards are used to supply information on each chemical specie. For each substance there is a set of four cards. On the first card the first field is a twelve character acronym identifying the species. The second field is a three digit code used on the data cards to identify the species. These codes are listed in Table I. The next four fields, which are fifteen columns wide, contain the critical properties and molecular weight. The last five columns in each card are used to sequence the cards. The first three digits are the species code and the last two are

the card number. The following cards consist of five fifteen column data fields and a five digit sequence number. The arrangement of the data on the cards is as follows:

Card 1 Acronym, species code, critical temperature, critical pressure, critical density molecular weight, species code, 01

Card 2 Acentric factor, L-Jε, L-Jσ, boiling point, melting point, specie code, 02

Card 3 Ideal gas parameter 1,2,3,4,5, species code, 03

Card 4 Ideal gas parameter 6,7, blank, blank, blank, species code, 04

The ideal gas parameters are for the equation for ideal gas enthalpy

$$H^* = B_1 + B_2T + B_3T^2 + B_4T^3 + B_5T^4 + B_6T^5$$

where the enthalpy is in BTU/lb and temperature, T, in degrees R. For the heat capacity

$$C_p^* = B_2 + 2B_3T - 3B_4T^2 + 4B_5T^3 + 5B_6T^4$$

and for entropy

$$S^* = B_2 \ln T/T_B + 2B_3(T-T_B) + \frac{3}{2} B_4(T^2-T_B^2) + \frac{4}{3} B_5(T^3-T_B^3)$$

$$+ \frac{5}{4} B_6(T^4-T_B^4) + B_7$$

Where T_B is the base temperature for the entropy equations(1°R). The data bases are 0 Btu/lb at 0°R for enthalpy and 0 Btu/lb at 0°R and 1 atm pressure for entropy. The coefficients for

the hydrocarbons were extracted from the work of Passut and Danner[1]. The properties are given in psia, Btu/lb, lb mole/ft^3, and °R. The primary reference for them is Sherwood and Reid[2].

The physical properties information also has a short summary version which takes only one card. It has a short eight digit acronym, two digit compound code, and then in F10.0 formats, critical temperature critical pressure, critical density, molecular weight, acentric factor, α a temperature scaling factor and β a density scaling factor.

References

(1) Passut, C. and Danner, R., "Correlation of Ideal Gas Enthalpy, Heat Capacity and Entropy", IEC, Process Design and Development, Vol. II, pp. 543-546 (1972).

(2) Sherwood and Reid, Properties of Gases and Liquids, 2nd Ed., McGraw-Hill, New York (1966).

APPENDIX D

TABULATED RESULTS FOR 43 PARAMETER EQUATION OF STATE

TABLE 1. THE PREDICTION OF EXPERIMENTAL DENSITY DATA OF THE WORKING DATA SET. PRESSURES BELOW 10,000 PSIA.

DATA ID		T RANKINE	P PSIA	RHO EXP LBMOL/FT3	RHO CALC LBMOL/FT3	ERROR PERCENT
001H	153	707.67	2900.760	3.303990	3.296171	-0.24
001H	161	707.67	4351.137	3.319804	3.303509	-0.49
001H	169	707.67	5801.520	3.335448	3.310596	-0.75
001H	177	707.67	7251.895	3.350917	3.317452	-1.00
001H	145	707.67	1450.380	3.287703	3.288570	0.03
001H	162	779.67	4351.137	3.202991	3.192388	-0.33
001H	170	779.67	5801.520	3.221436	3.202519	-0.59
001H	178	779.67	7251.895	3.239182	3.212213	-0.83
001H	146	779.67	1450.380	3.164415	3.170595	0.20
001H	154	779.67	2900.760	3.184170	3.181765	-0.08
001H	179	851.67	7251.895	3.110493	3.090551	-0.64
001H	147	851.67	1450.380	3.018449	3.029179	0.36
001H	155	851.67	2900.760	3.043347	3.046144	0.09
001H	163	851.67	4351.137	3.066489	3.061918	-0.15
001H	171	851.67	5801.520	3.088283	3.076671	-0.40
001H	164	923.67	4351.137	2.907853	2.900694	-0.33
001H	172	923.67	5801.520	2.936414	2.928997	-0.25
001H	180	923.67	7251.895	2.963260	2.949272	-0.47
001H	148	923.67	1450.380	2.843719	2.855227	0.40
001H	156	923.67	2900.760	2.877216	2.882515	0.18
001H	165	995.67	4351.137	2.717596	2.717540	-0.00
001H	173	995.67	5801.520	2.756696	2.752568	-0.15
001H	181	995.67	7251.895	2.792431	2.783003	-0.34
001H	149	995.67	1450.380	2.622060	2.627680	0.21
001H	157	995.67	2900.760	2.673396	2.676924	0.13
001H	174	1067.67	5801.520	2.537271	2.534334	-0.12
001H	182	1067.67	7251.895	2.588981	2.583420	-0.21
001H	158	1067.67	2900.760	2.403463	2.394662	-0.37
001H	166	1067.67	4351.137	2.476576	2.474079	-0.10
001H	183	1139.67	7251.895	2.335173	2.335078	0.02
001H	175	1139.67	5801.520	2.249156	2.248029	-0.06
001H	167	1139.67	4351.137	2.131257	2.119596	-0.55
001H	184	1211.67	7251.895	1.998961	2.007324	0.42
001H	33	1247.67	8702.273	1.955015	1.963391	0.43
001H	159	1139.67	2900.760	1.900331	1.850967	-2.60
001H	176	1211.67	5801.520	1.803535	1.811907	0.46
001H	25	1247.67	6526.703	1.660219	1.662582	0.14
001H	34	1319.67	8702.273	1.548993	1.564987	1.03
001H	35	1391.67	8702.273	1.170501	1.166372	-0.35
001H	17	1247.67	5076.324	1.124578	1.122955	-0.14
001H	36	1463.67	8702.273	0.922884	0.913092	-1.06
001H	37	1535.67	8702.273	0.772599	0.766183	-0.83
001H	27	1391.67	6526.703	0.744249	0.740161	-0.55
001H	38	1607.67	8702.273	0.674616	0.671890	-0.40
001H	28	1463.67	6526.703	0.608136	0.605166	-0.49
001H	39	1679.67	8702.273	0.605165	0.604039	-0.09
001H	40	1751.67	8702.273	0.552965	0.553996	0.19
001H	105	1787.67	8702.273	0.531525	0.532657	0.25
001H	29	1535.67	6526.703	0.527483	0.526007	-0.28
001H	108	2003.67	8702.273	0.440071	0.440889	0.19
001H	20	1463.67	5076.324	0.428649	0.429022	0.09
001H	19	1391.67	5076.324	0.498806	0.498596	-0.04
001H	31	1679.67	6526.703	0.430565	0.431788	0.28
001H	30	1607.67	6526.703	0.471735	0.471939	0.05
001H	109	2075.67	8702.273	0.421461	0.418705	-0.65
001H	107	1931.67	8702.273	0.465405	0.466610	0.24
001H	106	1859.67	8702.273	0.495174	0.496633	0.29
001H	99	1931.67	6526.703	0.341930	0.342964	0.30

TABLE 1. CONTINUED. PRESSURES BELOW 10,000 PSIA.

DATA ID		T RANKINE	P PSIA	RHO EXP LBMOL/FT3	RHO CALC LBMOL/FT3	ERROR PERCENT
001H	10	1319.67	3625.950	0.361120	0.360677	-0.12
001H	98	1859.67	6526.703	0.361572	0.363031	0.40
001H	11	1391.67	3625.950	0.311301	0.312295	0.32
001H	24	1751.67	5076.324	0.300902	0.302433	0.51
001H	23	1679.67	5076.324	0.322114	0.323675	0.48
001H	22	1607.67	5076.324	0.348668	0.349790	0.32
001H	21	1535.67	5076.324	0.382550	0.383275	0.19
001H	160	1211.67	2900.760	0.347898	0.346298	-0.46
001H	32	1751.67	6526.703	0.398460	0.400168	0.43
001H	101	2075.67	6526.703	0.309854	0.310337	0.16
001H	100	2003.67	6526.703	0.324920	0.325895	0.21
001H	97	1787.67	6526.703	0.384928	0.386647	0.45
001H	112	2291.67	8702.273	0.365882	0.366375	0.13
001H	111	2219.67	8702.273	0.381037	0.381909	0.23
001H	110	2147.67	8702.273	0.398460	0.399221	0.19
001H	16	1751.67	3625.950	0.208425	0.209459	0.50
001H	15	1679.67	3625.950	0.221327	0.222369	0.47
001H	14	1607.67	3625.950	0.236656	0.237684	0.43
001H	13	1535.67	3625.950	0.255371	0.256380	0.39
001H	12	1463.67	3625.950	0.279131	0.280147	0.36
001H	81	1787.67	3625.950	0.202819	0.203707	0.44
001H	96	2291.67	5076.324	0.211347	0.211831	0.23
001H	95	2219.67	5076.324	0.219784	0.220028	0.11
001H	94	2147.67	5076.324	0.228773	0.229029	0.11
001H	93	2075.67	5076.324	0.238643	0.238968	0.14
001H	92	2003.67	5076.324	0.249565	0.250050	0.19
001H	91	1931.67	5076.324	0.261771	0.262522	0.29
001H	90	1859.67	5076.324	0.275604	0.276731	0.41
001H	89	1787.67	5076.324	0.291739	0.293167	0.49
001H	104	2291.67	6526.703	0.272872	0.273580	0.26
001H	103	2219.67	6526.703	0.284139	0.284599	0.16
001H	102	2147.67	6526.703	0.296377	0.296773	0.13
001H	82	1859.67	3625.950	0.192678	0.193330	0.34
001H	152	1211.67	1450.380	0.131321	0.131917	0.45
001H	150	1067.67	1450.380	0.180073	0.178315	-0.98
001H	83	1931.67	3625.950	0.183794	0.184188	0.21
001H	84	2003.67	3625.950	0.175783	0.176042	0.15
001H	85	2075.67	3625.950	0.168523	0.168713	0.11
001H	86	2147.67	3625.950	0.161914	0.162068	0.09
001H	88	2291.67	3625.950	0.150203	0.150436	0.15
001H	87	2219.67	3625.950	0.155804	0.156003	0.13
001H	4	1463.67	2175.570	0.154142	0.154701	0.36
001H	5	1535.67	2175.570	0.143909	0.144546	0.44
001H	151	1139.67	1450.380	0.148722	0.149271	0.37
001H	6	1607.67	2175.570	0.135265	0.135654	0.29
001H	8	1751.67	2175.570	0.121308	0.121675	0.30
001H	7	1679.67	2175.570	0.127789	0.128191	0.31
001H	74	1859.67	2175.570	0.113044	0.113261	0.19
001H	73	1787.67	2175.570	0.118369	0.118707	0.29
001H	76	2003.67	2175.570	0.103838	0.103936	0.09
001H	75	1931.67	2175.570	0.108248	0.108367	0.11
001H	80	2291.67	2175.570	0.089525	0.089624	0.11
001H	79	2219.67	2175.570	0.092708	0.092781	0.08
001H	78	2147.67	2175.570	0.096125	0.096193	0.07
001H	77	2075.67	2175.570	0.099833	0.099898	0.06
001U	3	509.67	452.052	3.469329	3.454296	-0.43
001U	5	559.67	2718.304	3.469329	3.460434	-0.26
001U	4	584.67	4807.340	3.469329	3.448634	-0.60

TABLE 1. CONTINUED. PRESSURES BELOW 10,000 PSIA.

DATA ID		T RANKINE	P PSIA	RHO EXP LBMOL/FT3	RHO CALC LBMOL/FT3	ERROR PERCENT
0010	7	529.67	1003.522	3.469329	3.464945	-0.13
0010	6	539.67	1464.684	3.469329	3.465229	-0.12
0010	12	734.67	3344.042	3.265253	3.258132	-0.22
0010	13	719.67	1344.379	3.265253	3.269740	0.14
0010	11	759.67	6795.867	3.265253	3.240275	-0.76
0010	17	834.67	3255.107	3.083851	3.083945	0.00
0010	16	859.67	6587.645	3.083851	3.069387	-0.47
0010	18	819.67	1291.138	3.083851	3.093740	0.32
0010	22	959.67	2701.389	2.775464	2.781717	0.23
0010	21	1009.67	8111.273	2.775464	2.765104	-0.37
0010	23	939.67	576.326	2.775464	2.789671	0.51
0010	26	1109.67	9176.320	2.523149	2.516731	-0.25
0010	27	1059.67	4755.152	2.523149	2.521695	-0.05
0010	25	1034.67	2575.500	2.523149	2.522989	-0.01
0010	31	1159.67	6746.285	2.220370	2.221826	0.07
0010	32	1134.67	5059.477	2.220370	2.216275	-0.18
0010	36	1259.67	9696.043	1.982475	1.994162	0.59
0010	37	1209.67	6948.297	1.982475	1.986902	0.20
0010	38	1159.67	4277.137	1.982475	1.964454	-0.91
0010	41	1259.67	7432.641	1.734666	1.740597	0.34
0010	42	1209.67	5308.883	1.734666	1.724694	-0.57
0010	43	1159.67	3303.629	1.734666	1.694545	-2.31
0010	45	1359.67	9759.395	1.500250	1.508348	0.54
0010	46	1259.67	6297.555	1.500250	1.498277	-0.13
0010	50	1359.67	8342.117	1.261574	1.258078	-0.28
0010	51	1259.67	5631.852	1.261574	1.255915	-0.45
0010	59	1459.67	7780.344	0.792990	0.786680	-0.80
0010	63	1959.67	9602.172	0.504630	0.506310	0.33
0010	64	1459.67	5688.734	0.504630	0.503982	-0.13
0010	70	1209.67	2372.065	0.252315	0.252582	0.02
0010	68	1959.67	5006.074	0.252315	0.253751	0.56
0010	69	1459.67	3322.942	0.252315	0.253462	0.45
0010	67	2459.67	6564.293	0.252315	0.252884	0.23
0010	66	2859.67	7812.117	0.252315	0.253411	0.43
0010	79	1009.67	871.402	0.100926	0.100915	-0.01
0010	78	1059.67	948.238	0.100926	0.101324	0.39
0010	77	1109.67	1020.631	0.100926	0.101460	0.53
0010	76	1159.67	1089.934	0.100926	0.101481	0.55
0010	75	1209.67	1157.043	0.100926	0.101461	0.53
0010	71	2859.67	3104.061	0.100926	0.101233	0.30
0010	72	2459.67	2644.306	0.100926	0.101134	0.21
0010	73	1959.67	2069.674	0.100926	0.101264	0.34
0010	74	1459.67	1474.609	0.100926	0.101370	0.44
0010	80	2859.67	852.205	0.027755	0.027787	0.12
0010	81	2459.67	730.966	0.027755	0.027776	0.08
0010	82	1959.67	579.492	0.027755	0.027784	0.10
0010	83	1459.67	426.617	0.027755	0.027805	0.17
0010	84	1159.67	332.747	0.027755	0.027830	0.27
0010	85	959.67	267.416	0.027755	0.027876	0.44
0010	86	859.67	232.317	0.027755	0.027870	0.42
0010	87	2859.67	170.363	0.005551	0.005552	0.02
0010	88	2459.67	146.450	0.005551	0.005552	0.01
0010	89	1959.67	116.564	0.005551	0.005552	0.02
0010	90	1459.67	86.624	0.005551	0.005553	0.04
0010	91	1159.67	68.574	0.005551	0.005554	0.06
0010	92	959.67	56.442	0.005551	0.005556	0.12
0010	93	859.67	50.300	0.005551	0.005561	0.18
0010	94	759.67	44.034	0.005551	0.005566	0.27

TABLE 1. CONTINUED. PRESSURES BELOW 10,000 PSIA.

DATA ID		T RANKINE	P PSIA	RHO EXP LBMOL/FT3	RHO CALC LBMOL/FT3	ERROR PERCENT
0010	95	2859.67	34.069	0.001110	0.001110	-0.00
0010	96	2459.67	29.301	0.001110	0.001110	-0.00
0010	98	1459.67	17.377	0.001110	0.001110	0.00
0010	97	1959.67	23.340	0.001110	0.001110	0.00
0010	99	1159.67	13.796	0.001110	0.001110	0.01
0010	100	959.67	11.404	0.001110	0.001110	0.02
0010	101	859.67	10.206	0.001110	0.001111	0.04
0010	102	759.67	9.003	0.001110	0.001111	0.06
0010	103	659.67	7.790	0.001110	0.001111	0.10
0010	104	2859.67	3.407	0.000111	0.000111	0.02
0010	105	2459.67	2.930	0.000111	0.000111	0.00
0010	106	1959.67	2.335	0.000111	0.000111	0.03
0010	107	1459.67	1.739	0.000111	0.000111	0.02
0010	108	1159.67	1.381	0.000111	0.000111	-0.01
0010	109	959.67	1.143	0.000111	0.000111	0.01
0010	110	859.67	1.024	0.000111	0.000111	0.04
0010	111	759.67	0.905	0.000111	0.000111	0.07
0010	112	659.67	0.785	0.000111	0.000111	-0.00
0010	113	559.67	0.666	0.000111	0.000111	0.09
002K	1	545.67	62.063	3.453388	3.459388	0.17
002K	2	545.67	324.939	3.456499	3.460155	0.11
002K	3	545.67	682.358	3.460219	3.461201	0.03
002K	4	545.67	1120.520	3.464846	3.462475	-0.07
002K	5	545.67	1558.696	3.469402	3.463734	-0.18
002K	6	545.67	1996.843	3.473966	3.464982	-0.26
002K	7	545.67	2435.004	3.478447	3.466228	-0.35
002K	8	545.67	2873.137	3.482901	3.467458	-0.44
002K	9	545.67	3311.282	3.487295	3.468681	-0.53
002K	10	545.67	3749.429	3.491697	3.469891	-0.62
002K	11	545.67	4187.570	3.496019	3.471095	-0.71
002K	12	545.67	4625.730	3.500315	3.472287	-0.80
0010	60	1022.67	1160.667	2.506104	2.502576	-0.14
0010	59	1013.67	1079.793	2.539873	2.538849	-0.04
0010	58	1004.67	1003.300	2.572274	2.572c09	0.05
0010	57	995.67	931.017	2.603557	2.606995	0.13
0010	56	986.67	862.788	2.633807	2.639102	0.20
0010	55	977.67	798.456	2.663132	2.670035	0.26
0010	54	968.67	737.836	2.691446	2.699870	0.31
0010	53	959.67	680.814	2.719089	2.728702	0.35
0010	52	950.67	627.207	2.745783	2.756563	0.39
0010	51	941.67	576.399	2.771898	2.783536	0.42
0010	50	932.67	529.734	2.797160	2.809669	0.45
0010	49	923.67	485.585	2.821737	2.835005	0.47
0010	48	914.67	444.323	2.845817	2.859595	0.46
0010	47	905.67	405.806	2.869362	2.883474	0.49
0010	46	896.67	369.906	2.892094	2.906686	0.50
0010	45	887.67	336.510	2.914454	2.929254	0.51
0010	44	878.67	305.489	2.936165	2.951213	0.51
0010	43	869.67	276.729	2.957709	2.972598	0.50
0010	42	860.67	250.118	2.978527	2.993428	0.50
0010	41	851.67	225.540	2.998875	3.013732	0.50
0010	40	842.67	202.896	3.018711	3.033529	0.49
0010	39	833.67	182.059	3.038280	3.052541	0.48
0010	38	824.67	162.943	3.057297	3.071692	0.47
0010	37	815.67	145.434	3.076009	3.090093	0.46
0010	36	806.67	129.441	3.094395	3.108064	0.44
0010	35	797.67	114.873	3.112166	3.125620	0.43
0010	34	788.67	101.636	3.129861	3.142776	0.41

TABLE 1. CONTINUED. PRESSURES BELOW 10,000 PSIA.

DATA ID		T RANKINE	P PSIA	RHO EXP LBMOL/FT3	RHO CALC LBMOL/FT3	ERROR PERCENT
0010	33	779.67	89.640	3.146898	3.159547	0.40
0010	32	770.67	78.800	3.163837	3.175935	0.38
0010	31	761.67	69.033	3.180082	3.191959	0.37
0010	30	752.67	60.253	3.196201	3.207626	0.36
0010	29	743.67	52.410	3.211890	3.222945	0.34
0010	28	734.67	45.405	3.227130	3.237917	0.33
0010	27	725.67	39.177	3.242215	3.252555	0.32
0010	26	716.67	33.661	3.256828	3.266857	0.31
0010	25	707.67	28.795	3.270960	3.280824	0.30
0010	24	698.67	24.520	3.284900	3.294464	0.29
0010	23	689.67	20.779	3.298333	3.307782	0.29
0010	22	680.67	17.520	3.311243	3.320735	0.29
0010	21	671.67	14.696	3.323621	3.333358	0.29
0010	20	662.67	12.259	3.336086	3.345622	0.29
0010	19	653.67	10.168	3.348004	3.357531	0.28
0010	18	644.67	8.384	3.359355	3.369055	0.29
0010	17	635.67	6.869	3.370454	3.380167	0.29
0010	16	626.67	5.591	3.380969	3.390886	0.29
0010	15	617.67	4.519	3.390884	3.401136	0.30
0010	14	608.67	3.627	3.400526	3.410892	0.30
0010	13	599.67	2.889	3.409888	3.420105	0.30
0010	12	590.67	2.283	3.418630	3.428720	0.30
0010	11	581.67	1.789	3.426734	3.436655	0.29
0010	10	572.67	1.390	3.434099	3.443820	0.28
0010	9	563.67	1.070	3.441050	3.450083	0.26
0010	8	554.67	0.815	3.447342	3.455265	0.23
0010	7	545.67	0.615	3.452935	3.459206	0.18
0010	6	536.67	0.459	3.457791	3.461527	0.11
0010	5	527.67	0.339	3.461830	3.461791	-0.00
0010	4	518.67	0.247	3.464907	3.459270	-0.16
0010	3	509.67	0.178	3.466985	3.452724	-0.41
0010	2	500.67	0.126	3.467920	3.439583	-0.82
0010	1	491.67	0.089	3.467471	3.412505	-1.69

THE AVERAGE ABSOLUTE ERROR IN PERCENT IS 0.31
FOR 265 DATA POINTS.

TABLE 2. THE PREDICTION OF EXPERIMENTAL DENSITY DATA OF THE WORKING DATA SET. PRESSURES ABOVE 10,000 PSIA.

DATA ID		T RANKINE	P PSIA	RHO EXP LBMOL/FT3	RHO CALC LBMOL/FT3	ERROR PERCENT
001H	209	707.67	20305.316	3.474451	3.371170	-2.97
001H	201	707.67	17404.547	3.449228	3.360277	-2.58
001H	193	707.67	13053.406	3.409220	3.342912	-1.94
001H	210	779.67	20305.316	3.378994	3.285140	-2.78
001H	185	707.67	10152.656	3.380639	3.330545	-1.48
001H	194	779.67	13053.406	3.305564	3.247353	-1.76
001H	202	779.67	17404.547	3.350917	3.270712	-2.39
001H	186	779.67	10152.656	3.273430	3.230444	-1.31
001H	203	851.67	17404.547	3.240397	3.170572	-2.15
001H	187	851.67	10152.656	3.150901	3.116120	-1.10
001H	195	851.67	13053.406	3.188561	3.139300	-1.54
001H	204	923.67	17404.547	3.117762	3.059091	-1.88
001H	212	923.67	20305.316	3.155201	3.083850	-2.26
001H	213	995.67	20305.316	3.026880	2.967161	-1.97
001H	188	923.67	10152.656	3.012680	2.985515	-0.90
001H	196	923.67	13053.406	3.057297	3.017357	-1.31
001H	197	995.67	13053.406	2.911029	2.879411	-1.09
001H	205	995.67	17404.547	2.933396	2.935046	-1.62
001H	189	995.67	10152.656	2.855659	2.835302	-0.71
001H	206	1067.67	17404.547	2.835813	2.797414	-1.35
001H	214	1067.67	20305.316	2.887279	2.838863	-1.68
001H	198	1067.67	13053.406	2.746869	2.723166	-0.86
001H	215	1139.67	20305.316	2.736467	2.698881	-1.37
001H	190	1067.67	10152.656	2.674840	2.661508	-0.50
001H	207	1139.67	17404.547	2.673603	2.645826	-1.05
001H	199	1139.67	13053.406	2.560690	2.546257	-0.56
001H	216	1211.67	20305.316	2.565234	2.547704	-0.68
001H	65	1247.67	20305.316	2.480828	2.468224	-0.51
001H	191	1139.67	10152.656	2.464258	2.458313	-0.24
001H	208	1211.67	17404.547	2.491521	2.479607	-0.48
001H	66	1319.67	20305.316	2.310591	2.302430	-0.35
001H	57	1247.67	17404.547	2.396820	2.391379	-0.23
001H	200	1211.67	13053.406	2.348136	2.346023	-0.09
001H	49	1247.67	14503.789	2.293781	2.295533	0.07
001H	58	1319.67	17404.547	2.206232	2.205198	-0.05
001H	192	1211.67	10152.656	2.217518	2.217257	-0.01
001H	41	1247.67	11603.027	2.158181	2.165918	0.36
001H	67	1391.67	20305.316	2.135590	2.129516	-0.28
001H	50	1319.67	14503.789	2.068096	2.078241	0.49
001H	59	1391.67	17404.547	2.005698	2.008413	0.15
001H	68	1463.67	20305.316	1.957222	1.953329	-0.20
001H	60	1463.67	17404.547	1.801661	1.807523	0.31
001H	42	1319.67	11603.027	1.874701	1.894294	1.05
001H	51	1391.67	14503.789	1.830182	1.844132	0.76
001H	69	1535.67	20305.316	1.779475	1.779940	0.03
001H	70	1607.67	20305.316	1.614617	1.616924	0.14
001H	61	1535.67	17404.547	1.607135	1.613228	0.38
001H	52	1463.67	14503.789	1.598246	1.607036	0.55
001H	43	1391.67	11603.027	1.580044	1.594682	0.93
001H	71	1679.67	20305.316	1.472070	1.470792	-0.09
001H	62	1607.67	17404.547	1.434917	1.438913	0.28
001H	53	1535.67	14503.789	1.390615	1.391790	0.08
001H	44	1463.67	11603.027	1.315704	1.314510	-0.09
001H	72	1751.67	20305.316	1.347395	1.344566	-0.21
001H	63	1679.67	17404.547	1.292174	1.291684	-0.04
001H	54	1607.67	14503.789	1.217766	1.216303	-0.12
001H	137	1787.67	20305.316	1.292174	1.288652	-0.26
001H	129	1787.67	17404.547	1.123484	1.119905	-0.32

TABLE 2. CONTINUED. PRESSURES ABOVE 10,000 PSIA.

DATA ID		T RANKINE	P PSIA	RHO EXP LBMOL/FT3	RHO CALC LBMOL/FT3	ERROR PERCENT
001H	139	1931.67	20305.316	1.109822	1.108205	-0.15
001H	138	1859.67	20305.316	1.193871	1.190622	-0.28
001H	64	1751.67	17404.547	1.174465	1.171308	-0.27
001H	45	1535.67	11603.027	1.108758	1.101235	-0.68
001H	130	1859.67	17404.547	1.034664	1.031532	-0.30
001H	55	1679.67	14503.789	1.083472	1.080622	-0.26
001H	140	2003.67	20305.316	1.038382	1.038094	-0.03
001H	131	1931.67	17404.547	0.960454	0.958645	-0.19
001H	46	1607.67	11603.027	0.958066	0.951978	-0.64
001H	56	1751.67	14503.789	0.979441	0.976052	-0.35
001H	121	1787.67	14503.789	0.935581	0.932627	-0.32
001H	141	2075.67	20305.316	0.976956	0.978018	0.11
001H	142	2147.67	20305.316	0.923130	0.928987	0.61
001H	132	2003.67	17404.547	0.897800	0.897605	-0.02
001H	133	2075.67	17404.547	0.844460	0.845700	0.15
001H	123	1931.67	14503.789	0.800231	0.799226	-0.13
001H	122	1859.67	14503.789	0.861023	0.859129	-0.22
001H	47	1679.67	11603.027	0.849008	0.845622	-0.40
001H	144	2291.67	20305.316	0.834705	0.840221	0.66
001H	143	2219.67	20305.316	0.876029	0.880455	0.51
001H	134	2147.67	17404.547	0.798205	0.800938	0.34
001H	136	2291.67	17404.547	0.722843	0.727542	0.62
001H	124	2003.67	14503.789	0.749233	0.749313	0.01
001H	125	2075.67	14503.789	0.705779	0.706928	0.16
001H	48	1751.67	11603.027	0.767640	0.766365	-0.17
001H	113	1787.67	11603.027	0.734477	0.733762	-0.10
001H	135	2219.67	17404.547	0.758076	0.761851	0.50
001H	126	2147.67	14503.789	0.668247	0.670352	0.32
001H	128	2291.67	14503.789	0.606647	0.610056	0.56
001H	115	1931.67	11603.027	0.633345	0.633665	0.05
001H	114	1859.67	11603.027	0.678575	0.678675	0.01
001H	127	2219.67	14503.789	0.635551	0.638361	0.44
001H	116	2147.67	11603.027	0.534391	0.535804	0.26
001H	117	2075.67	11603.027	0.562745	0.563765	0.18
001H	116	2003.67	11603.027	0.595399	0.595968	0.10
001H	119	2219.67	11603.027	0.509355	0.511207	0.36
001H	120	2291.67	11603.027	0.487107	0.489326	0.46
001U	1	669.67	14694.000	3.469329	3.393675	-2.17
001U	2	659.67	13368.641	3.469329	3.400455	-1.99
001U	3	634.67	10222.074	3.469329	3.417151	-1.50
001U	9	809.67	14063.938	3.265253	3.210285	-1.68
001U	10	784.67	10370.430	3.265253	3.224321	-1.25
001U	14	919.67	14805.695	3.083851	3.041807	-1.36
001U	15	909.67	13417.594	3.083851	3.045779	-1.25
001U	19	1079.67	15720.836	2.775464	2.745149	-1.09
001U	20	1059.67	13851.844	2.775464	2.750630	-0.89
001U	24	1169.67	14470.148	2.523149	2.506520	-0.66
001U	25	1159.67	13593.023	2.523149	2.508456	-0.56
001U	29	1259.67	13575.109	2.220370	2.221801	0.06
001U	34	1359.67	15202.945	1.982475	1.989923	0.38
001U	35	1309.67	12459.277	1.982475	1.994264	0.59
001U	39	1429.67	14864.297	1.734866	1.744894	0.58
001U	40	1359.67	11806.418	1.734666	1.748603	0.80
001U	44	1459.67	13253.949	1.500250	1.508500	0.55
001U	48	1559.67	13776.328	1.261574	1.262823	0.10
001U	49	1459.67	11073.102	1.261574	1.262007	0.03
001U	58	1959.67	14775.563	0.792990	0.795593	0.33
001U	62	2459.67	13178.977	0.504630	0.505573	0.19

TABLE 2. CONTINUED. PRESSURES ABOVE 10,000 PSIA.

DATA ID		T RANKINE	P PSIA	RHO EXP LBMOL/FT3	RHO CALC LBMOL/FT3	ERROR PERCENT
0010	30	1209.67	10162.066	2.220370	2.225070	0.21

THE AVERAGE ABSOLUTE ERROR IN PERCENT IS 0.68
FOR 117 DATA POINTS.

TABLE 3. THE PREDICTION OF EXPERIMENTAL DENSITY DATA OF HOLSER AND KENNEDY, AM. J. OF SCI.,V. 256, 744(1958).

DATA ID		T RANKINE	P PSIA	RHO EXP LBMOL/FT3	RHO CALC LBMOL/FT3	ERROR PERCENT
001H	1	1247.67	2175.570	0.205706	0.206447	0.36
001H	2	1319.67	2175.570	0.182825	0.183794	0.53
001H	3	1391.67	2175.570	0.166580	0.167426	0.51
001H	4	1463.67	2175.570	0.154142	0.154701	0.36
001H	5	1535.67	2175.570	0.143909	0.144346	0.30
001H	6	1607.67	2175.570	0.135265	0.135654	0.29
001H	7	1679.67	2175.570	0.127789	0.128191	0.31
001H	8	1751.67	2175.570	0.121308	0.121675	0.30
001H	9	1247.67	3625.950	0.457606	0.453154	-0.97
001H	10	1319.67	3625.950	0.361120	0.360677	-0.12
001H	11	1391.67	3625.950	0.311301	0.312293	0.32
001H	12	1463.67	3625.950	0.279131	0.280147	0.36
001H	13	1535.67	3625.950	0.255371	0.256380	0.39
001H	14	1607.67	3625.950	0.236656	0.237684	0.43
001H	15	1679.67	3625.950	0.221327	0.222369	0.47
001H	16	1751.67	3625.950	0.208425	0.209459	0.50
001H	17	1247.67	5076.324	1.124578	1.122955	-0.14
001H	18	1319.67	5076.324	0.640007	0.630754	-1.45
001H	19	1391.67	5076.324	0.498806	0.498596	-0.04
001H	20	1463.67	5076.324	0.428649	0.429022	0.09
001H	21	1535.67	5076.324	0.382550	0.383275	0.19
001H	22	1607.67	5076.324	0.348662	0.349790	0.32
001H	23	1679.67	5076.324	0.322114	0.323675	0.48
001H	24	1751.67	5076.324	0.300902	0.302433	0.51
001H	25	1247.67	6526.703	1.660219	1.662582	0.14
001H	26	1319.67	6526.703	1.058022	1.044664	-1.26
001H	27	1391.67	6526.703	0.744249	0.740161	-0.55
001H	28	1463.67	6526.703	0.608136	0.605166	-0.49
001H	29	1535.67	6526.703	0.527483	0.526007	-0.28
001H	30	1607.67	6526.703	0.471735	0.471989	0.05
001H	31	1679.67	6526.703	0.430565	0.431788	0.28
001H	32	1751.67	6526.703	0.398460	0.400168	0.43
001H	33	1247.67	8702.273	1.955015	1.963391	0.43
001H	34	1319.67	8702.273	1.548993	1.564987	1.03
001H	35	1391.67	8702.273	1.170501	1.166373	-0.35
001H	36	1463.67	8702.273	0.922884	0.913092	-1.06
001H	37	1535.67	8702.273	0.772599	0.766183	-0.83
001H	38	1607.67	8702.273	0.674616	0.671590	-0.45
001H	39	1679.67	8702.273	0.605165	0.604639	-0.09
001H	40	1751.67	8702.273	0.552965	0.553996	0.19
001H	41	1247.67	11603.027	2.158181	2.165918	0.36
001H	42	1319.67	11603.027	1.874701	1.894294	1.05
001H	43	1391.67	11603.027	1.580044	1.594682	0.93
001H	44	1463.67	11603.027	1.315704	1.314510	-0.09
001H	45	1535.67	11603.027	1.108758	1.101233	-0.68
001H	46	1607.67	11603.027	0.958066	0.951978	-0.64
001H	47	1679.67	11603.027	0.849008	0.845622	-0.40
001H	48	1751.67	11603.027	0.767640	0.766363	-0.17
001H	49	1247.67	14503.789	2.293781	2.295333	0.07
001H	50	1319.67	14503.789	2.068096	2.078241	0.49
001H	51	1391.67	14503.789	1.830182	1.844132	0.76
001H	52	1463.67	14503.789	1.598248	1.607036	0.55
001H	53	1535.67	14503.789	1.390615	1.391790	0.08
001H	54	1607.67	14503.789	1.217766	1.216303	-0.12
001H	55	1679.67	14503.789	1.083472	1.080622	-0.26
001H	56	1751.67	14503.789	0.979441	0.976052	-0.35
001H	57	1247.67	17404.547	2.396820	2.391379	-0.23
001H	58	1319.67	17404.547	2.206232	2.205198	-0.05
001H	59	1391.67	17404.547	2.008898	2.008413	0.13

TABLE 3. CONTINUED. HOLSER AND KENNEDY.

DATA ID		T RANKINE	P PSIA	RHO EXP LBMOL/FT3	RHO CALC LBMOL/FT3	ERROR PERCENT
001H	60	1463.67	17404.547	1.801661	1.807323	0.31
001H	61	1535.67	17404.547	1.607135	1.613228	0.38
001H	62	1607.67	17404.547	1.434917	1.438913	0.28
001H	63	1679.67	17404.547	1.292174	1.291684	-0.04
001H	64	1751.67	17404.547	1.174465	1.171308	-0.27
001H	65	1247.67	20305.316	2.480828	2.468224	-0.51
001H	66	1319.67	20305.316	2.310591	2.302430	-0.35
001H	67	1391.67	20305.316	2.138590	2.129516	-0.28
001H	68	1463.67	20305.316	1.957222	1.953329	-0.20
001H	69	1535.67	20305.316	1.779475	1.779940	0.03
001H	70	1607.67	20305.316	1.614617	1.616924	0.14
001H	71	1679.67	20305.316	1.472070	1.470792	-0.09
001H	72	1751.67	20305.316	1.347395	1.344566	-0.21
001H	73	1787.67	2175.570	0.118369	0.118707	0.29
001H	74	1859.67	2175.570	0.113044	0.113261	0.19
001H	75	1931.67	2175.570	0.108246	0.108367	0.11
001H	76	2003.67	2175.570	0.103838	0.103936	0.09
001H	77	2075.67	2175.570	0.099833	0.099896	0.06
001H	78	2147.67	2175.570	0.096125	0.096193	0.07
001H	79	2219.67	2175.570	0.092708	0.092781	0.08
001H	80	2291.67	2175.570	0.089525	0.089624	0.11
001H	81	1787.67	3625.950	0.202819	0.203707	0.44
001H	82	1859.67	3625.950	0.192678	0.193330	0.34
001H	83	1931.67	3625.950	0.183794	0.184188	0.21
001H	84	2003.67	3625.950	0.175783	0.176042	0.15
001H	85	2075.67	3625.950	0.168523	0.168713	0.11
001H	86	2147.67	3625.950	0.161914	0.162068	0.09
001H	87	2219.67	3625.950	0.155804	0.156003	0.13
001H	88	2291.67	3625.950	0.150203	0.150436	0.15
001H	89	1787.67	5076.324	0.291739	0.293167	0.49
001H	90	1859.67	5076.324	0.275604	0.276731	0.41
001H	91	1931.67	5076.324	0.261771	0.262522	0.29
001H	92	2003.67	5076.324	0.249565	0.250050	0.19
001H	93	2075.67	5076.324	0.238643	0.238968	0.14
001H	94	2147.67	5076.324	0.228773	0.229025	0.11
001H	95	2219.67	5076.324	0.219784	0.220028	0.11
001H	96	2291.67	5076.324	0.211347	0.211631	0.23
001H	97	1787.67	6526.703	0.384928	0.386647	0.45
001H	98	1859.67	6526.703	0.361572	0.363031	0.40
001H	99	1931.67	6526.703	0.341930	0.342964	0.30
001H	100	2003.67	6526.703	0.324920	0.325595	0.21
001H	101	2075.67	6526.703	0.309854	0.310337	0.16
001H	102	2147.67	6526.703	0.296377	0.296773	0.13
001H	103	2219.67	6526.703	0.284139	0.284599	0.16
001H	104	2291.67	6526.703	0.272872	0.273580	0.26
001H	105	1787.67	8702.273	0.531525	0.532857	0.25
001H	106	1859.67	8702.273	0.495174	0.496633	0.29
001H	107	1931.67	8702.273	0.465405	0.466510	0.24
001H	108	2003.67	8702.273	0.440071	0.440889	0.19
001H	109	2075.67	8702.273	0.421461	0.418705	-0.65
001H	110	2147.67	8702.273	0.398460	0.399221	0.19
001H	111	2219.67	8702.273	0.381037	0.381909	0.23
001H	112	2291.67	8702.273	0.365882	0.366375	0.13
001H	113	1787.67	11603.027	0.734477	0.733762	-0.10
001H	114	1859.67	11603.027	0.678575	0.678675	0.01
001H	115	1931.67	11603.027	0.633345	0.633665	0.05
001H	116	2003.67	11603.027	0.595399	0.595968	0.10
001H	117	2075.67	11603.027	0.562745	0.563763	0.18
001H	118	2147.67	11603.027	0.534391	0.535804	0.26

TABLE 3. CONTINUED. HOLSER AND KENNEDY.

DATA ID		T RANKINE	P PSIA	RHO EXP LBMOL/FT3	RHO CALC LBMOL/FT3	ERROR PERCENT
001H	119	2219.67	11603.027	0.509355	0.511207	0.36
001H	120	2291.67	11603.027	0.487107	0.489328	0.46
001H	121	1787.67	14503.789	0.935581	0.932627	-0.32
001H	122	1859.67	14503.789	0.861023	0.859129	-0.22
001H	123	1931.67	14503.789	0.800231	0.799226	-0.13
001H	124	2003.67	14503.789	0.749233	0.749313	0.01
001H	125	2075.67	14503.789	0.705779	0.706928	0.16
001H	126	2147.67	14503.789	0.668247	0.670352	0.32
001H	127	2219.67	14503.789	0.635551	0.638361	0.44
001H	128	2291.67	14503.789	0.606647	0.610056	0.56
001H	129	1787.67	17404.547	1.123484	1.119905	-0.32
001H	130	1859.67	17404.547	1.034664	1.031532	-0.30
001H	131	1931.67	17404.547	0.960454	0.958645	-0.19
001H	132	2003.67	17404.547	0.897800	0.897605	-0.02
001H	133	2075.67	17404.547	0.844460	0.845700	0.15
001H	134	2147.67	17404.547	0.798205	0.800938	0.34
001H	135	2219.67	17404.547	0.758076	0.761851	0.50
001H	136	2291.67	17404.547	0.722843	0.727342	0.62
001H	137	1787.67	20305.316	1.292174	1.288852	-0.26
001H	138	1859.67	20305.316	1.193871	1.190822	-0.26
001H	139	1931.67	20305.316	1.109822	1.108203	-0.15
001H	140	2003.67	20305.316	1.038382	1.038094	-0.03
001H	141	2075.67	20305.316	0.976958	0.978018	0.11
001H	142	2147.67	20305.316	0.923130	0.925987	0.31
001H	143	2219.67	20305.316	0.876029	0.880455	0.51
001H	144	2291.67	20305.316	0.834705	0.840221	0.66
001H	145	707.67	1450.380	3.287703	3.288570	0.03
001H	146	779.67	1450.380	3.164415	3.170595	0.20
001H	147	851.67	1450.380	3.018449	3.029176	0.36
001H	148	923.67	1450.380	2.843719	2.855227	0.40
001H	149	995.67	1450.380	2.622060	2.627680	0.21
001H	150	1067.67	1450.380	0.180073	0.178315	-0.98
001H	151	1139.67	1450.380	0.148722	0.149271	0.37
001H	152	1211.67	1450.380	0.131321	0.131917	0.45
001H	153	707.67	2900.760	3.303990	3.296171	-0.24
001H	154	779.67	2900.760	3.184170	3.181765	-0.08
001H	155	851.67	2900.760	3.043347	3.046144	0.09
001H	156	923.67	2900.760	2.877216	2.882515	0.18
001H	157	995.67	2900.760	2.673396	2.676924	0.13
001H	158	1067.67	2900.760	2.403463	2.394662	-0.37
001H	159	1139.67	2900.760	1.900381	1.850967	-2.60
001H	160	1211.67	2900.760	0.347898	0.346298	-0.46
001H	161	707.67	4351.137	3.319804	3.303509	-0.49
001H	162	779.67	4351.137	3.202991	3.192388	-0.33
001H	163	851.67	4351.137	3.066489	3.061918	-0.15
001H	164	923.67	4351.137	2.907853	2.906894	-0.03
001H	165	995.67	4351.137	2.717596	2.717540	-0.00
001H	166	1067.67	4351.137	2.476576	2.474079	-0.10
001H	167	1139.67	4351.137	2.131257	2.119596	-0.55
001H	168	1211.67	4351.137	1.232479	1.265021	2.64
001H	169	707.67	5801.520	3.335448	3.310596	-0.75
001H	170	779.67	5801.520	3.221436	3.202519	-0.59
001H	171	851.67	5801.520	3.088883	3.076671	-0.40
001H	172	923.67	5801.520	2.936414	2.928997	-0.25
001H	173	995.67	5801.520	2.756696	2.752368	-0.16
001H	174	1067.67	5801.520	2.537271	2.534334	-0.12
001H	175	1139.67	5801.520	2.249156	2.248029	-0.05
001H	176	1211.67	5801.520	1.803535	1.811907	0.46
001H	177	707.67	7251.895	3.350917	3.317452	-1.00

TABLE 3. CONTINUED. HOLSER AND KENNEDY.

DATA ID		T RANKINE	P PSIA	RHO EXP LBMOL/FT3	RHO CALC LBMOL/FT3	ERROR PERCENT
001H	178	779.67	7251.895	3.239188	3.212213	-0.83
001H	179	851.67	7251.895	3.110493	3.090551	-0.64
001H	180	923.67	7251.895	2.963260	2.949272	-0.47
001H	181	995.67	7251.895	2.792431	2.783003	-0.34
001H	182	1067.67	7251.895	2.588581	2.583420	-0.21
001H	183	1139.67	7251.895	2.335173	2.335678	0.02
001H	184	1211.67	7251.895	1.998961	2.007324	0.42
001H	185	707.67	10152.656	3.380639	3.330545	-1.48
001H	186	779.67	10152.656	3.273430	3.230444	-1.31
001H	187	851.67	10152.656	3.150901	3.116120	-1.10
001H	188	923.67	10152.656	3.012680	2.985515	-0.90
001H	189	995.67	10152.656	2.855659	2.835368	-0.71
001H	190	1067.67	10152.656	2.674840	2.661508	-0.50
001H	191	1139.67	10152.656	2.464258	2.458313	-0.24
001H	192	1211.67	10152.656	2.217518	2.217257	-0.01
001H	193	707.67	13053.406	3.409220	3.342912	-1.94
001H	194	779.67	13053.406	3.305564	3.247363	-1.76
001H	195	851.67	13053.406	3.188561	3.139300	-1.54
001H	196	923.67	13053.406	3.057297	3.017357	-1.31
001H	197	995.67	13053.406	2.911025	2.879411	-1.09
001H	198	1067.67	13053.406	2.746869	2.723166	-0.86
001H	199	1139.67	13053.406	2.560690	2.546257	-0.56
001H	200	1211.67	13053.406	2.348136	2.346023	-0.09
001H	201	707.67	17404.547	3.449228	3.360277	-2.58
001H	202	779.67	17404.547	3.350917	3.270712	-2.39
001H	203	851.67	17404.547	3.240397	3.170572	-2.15
001H	204	923.67	17404.547	3.117762	3.059091	-1.88
001H	205	995.67	17404.547	2.983396	2.935046	-1.62
001H	206	1067.67	17404.547	2.835813	2.797414	-1.35
001H	207	1139.67	17404.547	2.673603	2.645626	-1.05
001H	208	1211.67	17404.547	2.491521	2.479607	-0.48
001H	209	707.67	20305.316	3.474451	3.371170	-2.97
001H	210	779.67	20305.316	3.378994	3.285140	-2.79
001H	211	851.67	20305.316	3.272502	3.189548	-2.53
001H	212	923.67	20305.316	3.155201	3.083850	-2.26
001H	213	995.67	20305.316	3.026880	2.967161	-1.97
001H	214	1067.67	20305.316	2.887279	2.838863	-1.68
001H	215	1139.67	20305.316	2.736467	2.698681	-1.37
001H	216	1211.67	20305.316	2.565234	2.547704	-0.68

THE AVERAGE ABSOLUTE ERROR IN PERCENT IS 0.90
FOR 216 DATA POINTS.

TABLE 4. THE PREDICTION OF EXPERIMENTAL DENSITY DATA OF KEENAN, KEYES, ET AL., "STEAM TABLES" JOHN WILEY, 1969

DATA ID		T RANKINE	P PSIA	RHO EXP LBMOL/FT3	RHO CALC LBMOL/FT3	ERROR PERCENT
0010	1	669.67	14694.000	3.469329	3.393879	-2.17
0010	2	659.67	13368.641	3.469329	3.400455	-1.99
0010	3	634.67	10222.074	3.469329	3.417151	-1.50
0010	4	584.67	4607.340	3.469329	3.448634	-0.60
0010	5	559.67	2718.304	3.469329	3.460434	-0.26
0010	6	539.67	1464.684	3.469329	3.465229	-0.12
0010	7	529.67	1003.522	3.469329	3.464945	-0.13
0010	8	509.67	452.052	3.469329	3.454296	-0.43
0010	9	809.67	14063.938	3.265253	3.210286	-1.68
0010	10	784.67	10370.430	3.265253	3.224321	-1.25
0010	11	759.67	6793.867	3.265253	3.240275	-0.76
0010	12	734.67	3344.042	3.265253	3.258132	-0.22
0010	13	719.67	1344.379	3.265253	3.269740	0.14
0010	14	919.67	14805.695	3.083851	3.041807	-1.36
0010	15	909.67	13417.554	3.083851	3.045779	-1.23
0010	16	859.67	6587.645	3.083851	3.069357	-0.47
0010	17	854.67	3255.107	3.083851	3.083945	0.00
0010	18	819.67	1291.138	3.083851	3.093740	0.32
0010	19	1079.67	15720.836	2.775464	2.745149	-1.09
0010	20	1059.67	13551.844	2.775464	2.750630	-0.89
0010	21	1009.67	8111.273	2.775464	2.765104	-0.37
0010	22	959.67	2701.889	2.775464	2.781717	0.23
0010	23	939.67	576.326	2.775464	2.789671	0.51
0010	24	1169.67	14470.148	2.523149	2.506520	-0.66
0010	25	1159.67	13593.023	2.523149	2.509456	-0.56
0010	26	1109.67	9176.320	2.523149	2.516731	-0.35
0010	27	1059.67	4755.152	2.523149	2.521883	-0.05
0010	28	1034.67	2575.500	2.523149	2.522989	-0.01
0010	29	1259.67	13575.109	2.220370	2.221601	0.06
0010	30	1209.67	10162.066	2.220370	2.225070	0.21
0010	31	1159.67	6746.285	2.220370	2.221826	0.07
0010	32	1134.67	5059.477	2.220370	2.216275	-0.18
0010	34	1359.67	15202.945	1.982475	1.989923	0.38
0010	35	1309.67	12459.277	1.982475	1.994204	0.59
0010	36	1259.67	9696.043	1.982475	1.994162	0.59
0010	37	1209.67	6948.297	1.982475	1.986502	0.20
0010	38	1159.67	4277.137	1.982475	1.964454	-0.91
0010	39	1429.67	14864.297	1.734666	1.744694	0.58
0010	40	1359.67	11806.418	1.734666	1.743603	0.50
0010	41	1259.67	7432.641	1.734666	1.740597	0.34
0010	42	1209.67	5308.883	1.734666	1.724094	-0.57
0010	43	1159.67	3303.629	1.734666	1.694545	-2.31
0010	44	1459.67	13253.945	1.500250	1.508500	0.55
0010	45	1359.67	9759.395	1.500250	1.508343	0.54
0010	46	1259.67	6297.355	1.500250	1.498277	-0.13
0010	47	1209.67	4637.852	1.500250	1.494387	-0.39
0010	48	1559.67	13776.328	1.261574	1.268823	0.15
0010	49	1459.67	11073.102	1.261574	1.262007	0.03
0010	50	1359.67	8342.117	1.261574	1.258078	-0.28
0010	51	1259.67	5631.852	1.261574	1.255913	-0.45
0010	52	1209.67	4320.469	1.261574	1.286336	1.96
0010	57	1209.67	4188.379	1.110185	1.147456	3.36
0010	58	1959.67	14775.563	0.792990	0.793592	0.08
0010	59	1459.67	7780.344	0.792990	0.786680	-0.80
0010	60	1259.67	4720.324	0.792990	0.781001	-1.51
0010	61	1209.67	3919.446	0.792990	0.783591	-1.19
0010	62	2459.67	13170.977	0.504630	0.505575	0.19
0010	63	1959.67	9602.172	0.504630	0.506310	0.33

TABLE 4. CONTINUED. KEENAN,KEYES, ET AL.

DATA ID		T RANKINE	P PSIA	RHO EXP LBMOL/FT3	RHO CALC LBMOL/FT3	ERROR PERCENT
0010	64	1459.67	5688.734	0.504630	0.503982	-0.13
0010	65	1209.67	3434.606	0.504630	0.495319	-1.85
0010	66	2859.67	7812.117	0.252315	0.253411	0.43
0010	67	2459.67	6564.293	0.252315	0.252804	0.23
0010	68	1959.67	5006.074	0.252315	0.253731	0.56
0010	69	1459.67	3322.942	0.252315	0.253462	0.45
0010	70	1209.67	2372.065	0.252315	0.252382	0.03
0010	71	2859.67	3104.061	0.100926	0.101233	0.30
0010	72	2459.67	2644.306	0.100926	0.101134	0.21
0010	73	1959.67	2069.674	0.100926	0.101264	0.34
0010	74	1459.67	1474.609	0.100926	0.101375	0.44
0010	75	1209.67	1157.043	0.100926	0.101461	0.53
0010	76	1159.67	1089.934	0.100926	0.101481	0.55
0010	77	1109.67	1020.631	0.100926	0.101460	0.53
0010	78	1059.67	948.238	0.100926	0.101324	0.39
0010	79	1009.67	871.402	0.100926	0.100915	-0.01
0010	80	2859.67	852.205	0.027755	0.027787	0.12
0010	81	2459.67	730.966	0.027755	0.027776	0.08
0010	82	1959.67	579.492	0.027755	0.027784	0.10
0010	83	1459.67	426.617	0.027755	0.027803	0.17
0010	84	1159.67	332.747	0.027755	0.027830	0.27
0010	85	959.67	267.416	0.027755	0.027876	0.44
0010	86	859.67	232.317	0.027755	0.027870	0.42
0010	87	2859.67	170.363	0.005551	0.005559	0.12
0010	88	2459.67	146.460	0.005551	0.005552	0.01
0010	89	1959.67	116.564	0.005551	0.005552	0.02
0010	90	1459.67	86.624	0.005551	0.005553	0.04
0010	91	1159.67	68.574	0.005551	0.005554	0.06
0010	92	959.67	56.442	0.005551	0.005558	0.12
0010	93	859.67	50.300	0.005551	0.005561	0.18
0010	94	759.67	44.034	0.005551	0.005565	0.27
0010	95	2859.67	34.069	0.001110	0.001110	-0.00
0010	96	2459.67	29.301	0.001110	0.001110	-0.00
0010	97	1959.67	23.340	0.001110	0.001110	0.00
0010	98	1459.67	17.377	0.001110	0.001110	0.00
0010	99	1159.67	13.796	0.001110	0.001110	0.01
0010	100	959.67	11.404	0.001110	0.001110	0.02
0010	101	859.67	10.206	0.001110	0.001111	0.04
0010	102	759.67	9.003	0.001110	0.001111	0.06
0010	103	659.67	7.790	0.001110	0.001111	0.10
0010	104	2859.67	3.407	0.000111	0.000111	0.02
0010	105	2459.67	2.930	0.000111	0.000111	0.00
0010	106	1959.67	2.335	0.000111	0.000111	0.03
0010	107	1459.67	1.739	0.000111	0.000111	0.02
0010	108	1159.67	1.381	0.000111	0.000111	-0.01
0010	109	959.67	1.143	0.000111	0.000111	0.01
0010	110	859.67	1.024	0.000111	0.000111	0.04
0010	111	759.67	0.905	0.000111	0.000111	0.07
0010	112	659.67	0.785	0.000111	0.000111	-0.00
0010	113	559.67	0.666	0.000111	0.000111	0.09

THE AVERAGE ABSOLUTE ERROR IN PERCENT IS 0.45
FOR 108 DATA POINTS.

TABLE 5. THE PREDICTION OF EXPERIMENTAL DENSITY DATA OF KENNEDY, AM. J. OF SCI., V. 255, 724(1957).

DATA ID		T RANKINE	P PSIA	RHO EXP LBMOL/FT3	RHO CALC LBMOL/FT3	ERROR PERCENT
001K	1	851.67	145.038	0.016852	0.016895	0.25
001K	2	869.67	145.038	0.016406	0.016451	0.27
001K	3	887.67	145.038	0.015990	0.016036	0.29
001K	4	887.67	290.076	0.033919	0.034063	0.43
001K	5	905.67	145.038	0.015601	0.015648	0.30
001K	6	905.67	290.076	0.032899	0.033040	0.43
001K	7	923.67	145.038	0.015573	0.015283	-1.86
001K	8	923.67	290.076	0.031974	0.032103	0.41
001K	9	923.67	435.114	0.050868	0.050957	0.17
001K	10	941.67	145.038	0.014891	0.014939	0.32
001K	11	941.67	290.076	0.031122	0.031240	0.38
001K	12	941.67	435.114	0.049139	0.049293	0.31
001K	13	959.67	145.038	0.014517	0.014613	0.66
001K	14	959.67	290.076	0.030330	0.030440	0.36
001K	15	959.67	435.114	0.047607	0.047789	0.38
001K	16	959.67	580.152	0.066954	0.067117	0.24
001K	17	977.67	145.038	0.014220	0.014304	0.59
001K	18	977.67	290.076	0.029592	0.029695	0.35
001K	19	977.67	435.114	0.046224	0.046418	0.42
001K	20	977.67	580.152	0.064597	0.064825	0.35
001K	21	977.67	725.190	0.085424	0.085448	0.03
001K	22	995.67	145.038	0.013901	0.014010	0.79
001K	23	995.67	290.076	0.028904	0.028997	0.32
001K	24	995.67	435.114	0.044960	0.045159	0.44
001K	25	995.67	580.152	0.062490	0.062769	0.45
001K	26	995.67	725.190	0.082049	0.082222	0.21
001K	27	995.67	870.228	0.104527	0.104128	-0.38
001K	28	1013.67	145.038	0.013714	0.013730	0.12
001K	29	1013.67	290.076	0.028256	0.028341	0.30
001K	30	1013.67	435.114	0.043801	0.043995	0.44
001K	31	1013.67	580.152	0.060612	0.060906	0.49
001K	32	1013.67	725.190	0.079092	0.079375	0.36
001K	33	1013.67	870.228	0.099833	0.099837	0.00
001K	34	1013.67	1015.266	0.123688	0.122969	-0.58
001K	35	1031.67	145.038	0.013448	0.013462	0.11
001K	36	1031.67	290.076	0.027646	0.027723	0.28
001K	37	1031.67	435.114	0.042738	0.042913	0.41
001K	38	1031.67	580.152	0.058923	0.059205	0.48
001K	39	1031.67	725.190	0.076493	0.076829	0.44
001K	40	1031.67	870.228	0.095886	0.096106	0.23
001K	41	1031.67	1015.266	0.117686	0.117505	-0.15
001K	42	1031.67	1160.304	0.143018	0.141761	-0.88
001K	43	1049.67	145.038	0.013192	0.013207	0.11
001K	44	1049.67	290.076	0.027068	0.027138	0.26
001K	45	1049.67	435.114	0.041745	0.041902	0.38
001K	46	1049.67	580.152	0.057382	0.057639	0.45
001K	47	1049.67	725.190	0.074170	0.074527	0.48
001K	48	1049.67	870.228	0.092485	0.092809	0.35
001K	49	1049.67	1015.266	0.112750	0.112821	0.06
001K	50	1049.67	1160.304	0.135529	0.135055	-0.35
001K	51	1049.67	1305.342	0.161914	0.160282	-1.01
001K	52	1067.67	145.038	0.012951	0.012962	0.09
001K	53	1067.67	290.076	0.026519	0.026584	0.24
001K	54	1067.67	435.114	0.040812	0.040955	0.35
001K	55	1067.67	580.152	0.055957	0.056189	0.41
001K	56	1067.67	725.190	0.072074	0.072428	0.49
001K	57	1067.67	870.228	0.089502	0.089858	0.40
001K	58	1067.67	1015.266	0.108483	0.108727	0.23
001K	59	1067.67	1160.304	0.129410	0.129379	-0.02

TABLE 5. CONTINUED. KENNEDY.

DATA ID		T RANKINE	P PSIA	RHO EXP LBMOL/FT3	RHO CALC LBMOL/FT3	ERROR PERCENT
001K	60	1067.67	1305.342	0.152986	0.152315	-0.44
001K	61	1067.67	1450.380	0.180073	0.178315	-0.98
001K	62	1103.67	145.038	0.012493	0.012502	0.07
001K	63	1103.67	290.076	0.025498	0.025555	0.22
001K	64	1103.67	435.114	0.039091	0.039222	0.33
001K	65	1103.67	580.152	0.053382	0.053579	0.37
001K	66	1103.67	725.190	0.068393	0.068718	0.48
001K	67	1103.67	870.228	0.084364	0.084755	0.46
001K	68	1103.67	1015.266	0.101409	0.101833	0.42
001K	69	1103.67	1160.304	0.119717	0.120136	0.35
001K	70	1103.67	1305.342	0.139565	0.139908	0.25
001K	71	1103.67	1450.380	0.161387	0.161482	0.06
001K	72	1139.67	145.038	0.012076	0.012077	0.01
001K	73	1139.67	290.076	0.024566	0.024618	0.21
001K	74	1139.67	435.114	0.037551	0.037668	0.31
001K	75	1139.67	580.152	0.051093	0.051280	0.37
001K	76	1139.67	725.190	0.065216	0.065516	0.46
001K	77	1139.67	870.228	0.080078	0.080451	0.46
001K	78	1139.67	1015.266	0.096674	0.096171	0.52
001K	79	1139.67	1160.304	0.112203	0.112786	0.52
001K	80	1139.67	1305.342	0.129895	0.130430	0.41
001K	81	1139.67	1450.380	0.148722	0.149271	0.37
001K	82	1175.67	145.038	0.011677	0.011683	0.05
001K	83	1175.67	290.076	0.023722	0.023759	0.16
001K	84	1175.67	435.114	0.036180	0.036262	0.23
001K	85	1175.67	580.152	0.049048	0.049230	0.37
001K	86	1175.67	725.190	0.062445	0.062704	0.41
001K	87	1175.67	870.228	0.076375	0.076734	0.47
001K	88	1175.67	1015.266	0.090909	0.091378	0.51
001K	89	1175.67	1160.304	0.106094	0.106702	0.57
001K	90	1175.67	1305.342	0.122120	0.122786	0.55
001K	91	1175.67	1450.380	0.139062	0.139726	0.48
001K	92	1211.67	145.038	0.011312	0.011315	0.03
001K	93	1211.67	290.076	0.022938	0.022967	0.13
001K	94	1211.67	435.114	0.034898	0.034980	0.23
001K	95	1211.67	580.152	0.047218	0.047380	0.34
001K	96	1211.67	725.190	0.059972	0.060199	0.38
001K	97	1211.67	870.228	0.073122	0.073468	0.47
001K	98	1211.67	1015.266	0.086792	0.087228	0.50
001K	99	1211.67	1160.304	0.101025	0.101522	0.49
001K	100	1211.67	1305.342	0.115800	0.116399	0.52
001K	101	1211.67	1450.380	0.131321	0.131917	0.45
001K	102	1247.67	145.038	0.010968	0.010972	0.03
001K	103	1247.67	290.076	0.022204	0.022233	0.13
001K	104	1247.67	435.114	0.033727	0.033802	0.22
001K	105	1247.67	580.152	0.045562	0.045698	0.30
001K	106	1247.67	725.190	0.057755	0.057943	0.32
001K	107	1247.67	870.228	0.070235	0.070560	0.46
001K	108	1247.67	1015.266	0.083210	0.083576	0.44
001K	109	1247.67	1160.304	0.096607	0.097020	0.43
001K	110	1247.67	1305.342	0.110452	0.110924	0.43
001K	111	1247.67	1450.380	0.124800	0.125326	0.42
001K	112	1283.67	145.038	0.010645	0.010650	0.04
001K	113	1283.67	290.076	0.021515	0.021550	0.16
001K	114	1283.67	435.114	0.032620	0.032714	0.29
001K	115	1283.67	580.152	0.044041	0.044157	0.26
001K	116	1283.67	725.190	0.055759	0.055894	0.24
001K	117	1283.67	870.228	0.067685	0.067941	0.38
001K	118	1283.67	1015.266	0.080041	0.080318	0.35

TABLE 5. CONTINUED. KENNEDY.

DATA ID		T RANKINE	P PSIA	RHO EXP LBMOL/FT3	RHO CALC LBMOL/FT3	ERROR PERCENT
001K	119	1283.67	1160.304	0.092683	0.093044	0.39
001K	120	1283.67	1305.342	0.105706	0.106142	0.41
001K	121	1283.67	1450.380	0.119141	0.119635	0.41
001K	122	1319.67	145.038	0.010340	0.010347	0.06
001K	123	1319.67	290.076	0.020880	0.020912	0.15
001K	124	1319.67	435.114	0.031624	0.031705	0.26
001K	125	1319.67	580.152	0.042643	0.042737	0.22
001K	126	1319.67	725.190	0.053913	0.054018	0.20
001K	127	1319.67	870.228	0.065401	0.065562	0.25
001K	128	1319.67	1015.266	0.077140	0.077381	0.31
001K	129	1319.67	1160.304	0.089157	0.089490	0.37
001K	130	1319.67	1305.342	0.101469	0.101903	0.43
001K	131	1319.67	1450.380	0.114161	0.114637	0.42
001K	132	1355.67	145.038	0.010056	0.010062	0.06
001K	133	1355.67	290.076	0.020294	0.020314	0.10
001K	134	1355.67	435.114	0.030697	0.030765	0.22
001K	135	1355.67	580.152	0.041342	0.041421	0.19
001K	136	1355.67	725.190	0.052200	0.052291	0.17
001K	137	1355.67	870.228	0.063277	0.063384	0.17
001K	138	1355.67	1015.266	0.074505	0.074710	0.28
001K	139	1355.67	1160.304	0.085995	0.086279	0.33
001K	140	1355.67	1305.342	0.097668	0.098101	0.44
001K	141	1355.67	1450.380	0.109718	0.110188	0.43
001K	142	1391.67	145.038	0.009789	0.009793	0.04
001K	143	1391.67	290.076	0.019739	0.019753	0.07
001K	144	1391.67	435.114	0.029860	0.029885	0.09
001K	145	1391.67	580.152	0.040132	0.040196	0.16
001K	146	1391.67	725.190	0.050608	0.050692	0.16
001K	147	1391.67	870.228	0.061243	0.061379	0.22
001K	148	1391.67	1015.266	0.072104	0.072264	0.22
001K	149	1391.67	1160.304	0.083090	0.083355	0.32
001K	150	1391.67	1305.342	0.094270	0.094659	0.41
001K	151	1391.67	1450.380	0.105770	0.106183	0.39
001K	152	1427.67	145.038	0.009536	0.009539	0.03
001K	153	1427.67	290.076	0.019214	0.019224	0.05
001K	154	1427.67	435.114	0.029023	0.029060	0.13
001K	155	1427.67	580.152	0.039004	0.039053	0.13
001K	156	1427.67	725.190	0.049139	0.049205	0.13
001K	157	1427.67	870.228	0.059397	0.059522	0.21
001K	158	1427.67	1015.266	0.069895	0.070010	0.16
001K	159	1427.67	1160.304	0.080450	0.080673	0.28
001K	160	1427.67	1305.342	0.091220	0.091517	0.33
001K	161	1427.67	1450.380	0.102246	0.102547	0.29
001K	162	1463.67	145.038	0.009296	0.009297	0.02
001K	163	1463.67	290.076	0.018727	0.018725	-0.01
001K	164	1463.67	435.114	0.028259	0.028284	0.09
001K	165	1463.67	580.152	0.037941	0.037981	0.10
001K	166	1463.67	725.190	0.047758	0.047817	0.12
001K	167	1463.67	870.228	0.057688	0.057796	0.19
001K	168	1463.67	1015.266	0.067778	0.067922	0.21
001K	169	1463.67	1160.304	0.078025	0.078199	0.22
001K	170	1463.67	1305.342	0.088429	0.088630	0.23
001K	171	1463.67	1450.380	0.099006	0.099221	0.22
001K	172	1499.67	145.038	0.009067	0.009069	0.02
001K	173	1499.67	290.076	0.018244	0.018252	0.04
001K	174	1499.67	435.114	0.027536	0.027553	0.06
001K	175	1499.67	580.152	0.036939	0.036973	0.09
001K	176	1499.67	725.190	0.046472	0.046516	0.09
001K	177	1499.67	870.228	0.056111	0.056183	0.13

TABLE 5. CONTINUED. KENNEDY.

DATA ID		T RANKINE	P PSIA	RHO EXP LBMOL/FT3	RHO CALC LBMOL/FT3	ERROR PERCENT
001K	178	1499.67	1015.266	0.065885	0.065979	0.14
001K	179	1499.67	1160.304	0.075791	0.075905	0.15
001K	180	1499.67	1305.342	0.085846	0.085964	0.14
001K	181	1499.67	1450.380	0.095992	0.096159	0.17
001K	182	1535.67	145.038	0.008852	0.008851	-0.01
001K	183	1535.67	290.076	0.017804	0.017804	0.00
001K	184	1535.67	435.114	0.026854	0.026861	0.03
001K	185	1535.67	580.152	0.036000	0.036023	0.07
001K	186	1535.67	725.190	0.045259	0.045293	0.08
001K	187	1535.67	870.228	0.054626	0.054673	0.09
001K	188	1535.67	1015.266	0.064095	0.064164	0.11
001K	189	1535.67	1160.304	0.073666	0.073768	0.14
001K	190	1535.67	1305.342	0.083410	0.083488	0.09
001K	191	1535.67	1450.380	0.093156	0.093325	0.18
001K	192	1571.67	145.038	0.008645	0.008644	-0.01
001K	193	1571.67	290.076	0.017376	0.017379	0.02
001K	194	1571.67	435.114	0.026213	0.026206	-0.03
001K	195	1571.67	580.152	0.035114	0.035126	0.03
001K	196	1571.67	725.190	0.044113	0.044141	0.06
001K	197	1571.67	870.228	0.053234	0.053253	0.03
001K	198	1571.67	1015.266	0.062411	0.062462	0.08
001K	199	1571.67	1160.304	0.071687	0.071770	0.12
001K	200	1571.67	1305.342	0.081108	0.081179	0.09
001K	201	1571.67	1450.380	0.090530	0.090690	0.18
001K	202	1607.67	145.038	0.008451	0.008447	-0.05
001K	203	1607.67	290.076	0.016984	0.016974	-0.06
001K	204	1607.67	435.114	0.025599	0.025534	-0.06
001K	205	1607.67	580.152	0.034274	0.034276	0.01
001K	206	1607.67	725.190	0.043030	0.043053	0.05
001K	207	1607.67	870.228	0.051896	0.051914	0.04
001K	208	1607.67	1015.266	0.060814	0.060862	0.08
001K	209	1607.67	1160.304	0.069811	0.069896	0.12
001K	210	1607.67	1305.342	0.078930	0.079018	0.11
001K	211	1607.67	1450.380	0.088070	0.088230	0.18
001K	212	1643.67	145.038	0.008263	0.008258	-0.06
001K	213	1643.67	290.076	0.016594	0.016589	-0.03
001K	214	1643.67	435.114	0.025005	0.024993	-0.05
001K	215	1643.67	580.152	0.033477	0.033471	-0.02
001K	216	1643.67	725.190	0.041998	0.042023	0.06
001K	217	1643.67	870.228	0.050631	0.050650	0.04
001K	218	1643.67	1015.266	0.059306	0.059353	0.08
001K	219	1643.67	1160.304	0.068044	0.068133	0.13
001K	220	1643.67	1305.342	0.076900	0.076990	0.12
001K	221	1643.67	1450.380	0.085762	0.085924	0.19
001K	222	1679.67	145.038	0.008086	0.008079	-0.10
001K	223	1679.67	290.076	0.016237	0.016222	-0.09
001K	224	1679.67	435.114	0.024441	0.024430	-0.04
001K	225	1679.67	580.152	0.032713	0.032705	-0.02
001K	226	1679.67	725.190	0.041024	0.041045	0.05
001K	227	1679.67	870.228	0.049433	0.049452	0.04
001K	228	1679.67	1015.266	0.057880	0.057927	0.08
001K	229	1679.67	1160.304	0.066377	0.066469	0.14
001K	230	1679.67	1305.342	0.074810	0.075079	0.36
001K	231	1679.67	1450.380	0.083611	0.083758	0.17
001K	232	1715.67	145.038	0.007913	0.007906	-0.08
001K	233	1715.67	290.076	0.015880	0.015871	-0.06
001K	234	1715.67	435.114	0.023902	0.023894	-0.03
001K	235	1715.67	580.152	0.031986	0.031975	-0.03
001K	236	1715.67	725.190	0.040095	0.040116	0.05

TABLE 5. CONTINUED. KENNEDY.

DATA ID		T RANKINE	P PSIA	RHO EXP LBMOL/FT3	RHO CALC LBMOL/FT3	ERROR PERCENT
001K	237	1715.67	870.228	0.048297	0.048316	0.04
001K	238	1715.67	1015.266	0.056531	0.056576	0.08
001K	239	1715.67	1160.304	0.064814	0.064895	0.13
001K	240	1715.67	1305.342	0.073169	0.073275	0.15
001K	241	1715.67	1450.380	0.081547	0.081715	0.21
001K	242	1751.67	145.038	0.007748	0.007742	-0.09
001K	243	1751.67	290.076	0.015545	0.015535	-0.07
001K	244	1751.67	435.114	0.023386	0.023382	-0.02
001K	245	1751.67	580.152	0.031293	0.031280	-0.04
001K	246	1751.67	725.190	0.039215	0.039232	0.04
001K	247	1751.67	870.228	0.047231	0.047236	0.01
001K	248	1751.67	1015.266	0.055252	0.055293	0.07
001K	249	1751.67	1160.304	0.063334	0.063404	0.11
001K	250	1751.67	1305.342	0.071450	0.071568	0.16
001K	251	1751.67	1450.380	0.079637	0.079785	0.19
001K	252	1787.67	145.038	0.007591	0.007584	-0.09
001K	253	1787.67	290.076	0.015225	0.015214	-0.07
001K	254	1787.67	435.114	0.022892	0.022892	-0.00
001K	255	1787.67	580.152	0.030630	0.030616	-0.04
001K	256	1787.67	725.190	0.038373	0.038388	0.04
001K	257	1787.67	870.228	0.046206	0.046207	0.00
001K	258	1787.67	1015.266	0.054047	0.054074	0.05
001K	259	1787.67	1160.304	0.061932	0.061988	0.09
001K	260	1787.67	1305.342	0.069853	0.069949	0.14
001K	261	1787.67	1450.380	0.077832	0.077957	0.16
001K	262	1823.67	145.038	0.007439	0.007432	-0.10
001K	263	1823.67	290.076	0.014917	0.014906	-0.07
001K	264	1823.67	435.114	0.022448	0.022423	-0.11
001K	265	1823.67	580.152	0.029994	0.029982	-0.04
001K	266	1823.67	725.190	0.037567	0.037563	0.04
001K	267	1823.67	870.228	0.045229	0.045227	-0.01
001K	268	1823.67	1015.266	0.052893	0.052912	0.04
001K	269	1823.67	1160.304	0.060580	0.060640	0.10
001K	270	1823.67	1305.342	0.068325	0.068410	0.12
001K	271	1823.67	1450.380	0.076124	0.076222	0.13
001K	272	1859.67	145.038	0.007292	0.007287	-0.08
001K	273	1859.67	290.076	0.014621	0.014611	-0.07
001K	274	1859.67	435.114	0.021964	0.021974	0.04
001K	275	1859.67	580.152	0.029384	0.029375	-0.03
001K	276	1859.67	725.190	0.036794	0.036813	0.05
001K	277	1859.67	870.228	0.044294	0.044290	-0.01
001K	278	1859.67	1015.266	0.051787	0.051804	0.03
001K	279	1859.67	1160.304	0.059306	0.059356	0.08
001K	280	1859.67	1305.342	0.066876	0.066945	0.10
001K	281	1859.67	1450.380	0.074489	0.074572	0.11
001K	282	1895.67	145.038	0.007154	0.007147	-0.10
001K	283	1895.67	290.076	0.014337	0.014328	-0.07
001K	284	1895.67	435.114	0.021555	0.021543	-0.06
001K	285	1895.67	580.152	0.028803	0.028793	-0.04
001K	286	1895.67	725.190	0.036059	0.036076	0.05
001K	287	1895.67	870.228	0.043396	0.043394	-0.01
001K	288	1895.67	1015.266	0.050734	0.050745	0.02
001K	289	1895.67	1160.304	0.058094	0.058130	0.06
001K	290	1895.67	1305.342	0.065487	0.065548	0.09
001K	291	1895.67	1450.380	0.072923	0.073000	0.11
001K	292	1931.67	145.038	0.007019	0.007012	-0.10
001K	293	1931.67	290.076	0.014064	0.014055	-0.06
001K	294	1931.67	435.114	0.021135	0.021129	-0.02
001K	295	1931.67	580.152	0.028245	0.028234	-0.04

TABLE 5. CONTINUED. KENNEDY.

DATA ID		T RANKINE	P PSIA	RHO EXP LBMOL/FT3	RHO CALC LBMOL/FT3	ERROR PERCENT
001K	296	1931.67	725.190	0.035354	0.035370	0.05
001K	297	1931.67	870.228	0.042534	0.042536	0.00
001K	298	1931.67	1015.266	0.049716	0.049732	0.03
001K	299	1931.67	1160.304	0.056930	0.056958	0.05
001K	300	1931.67	1305.342	0.064155	0.064214	0.09
001K	301	1931.67	1450.380	0.071436	0.071500	0.09
001K	302	1967.67	145.038	0.006888	0.006883	-0.08
001K	303	1967.67	290.076	0.013801	0.013793	-0.06
001K	304	1967.67	435.114	0.020743	0.020732	-0.05
001K	305	1967.67	580.152	0.027708	0.027698	-0.04
001K	306	1967.67	725.190	0.034675	0.034692	0.05
001K	307	1967.67	870.228	0.041705	0.041713	0.02
001K	308	1967.67	1015.266	0.048738	0.048761	0.05
001K	309	1967.67	1160.304	0.055813	0.055836	0.04
001K	310	1967.67	1305.342	0.062887	0.062938	0.08
001K	311	1967.67	1450.380	0.070008	0.070067	0.08
001K	312	2003.67	145.038	0.006763	0.006758	-0.08
001K	313	2003.67	290.076	0.013553	0.013541	-0.09
001K	314	2003.67	435.114	0.020365	0.020350	-0.08
001K	315	2003.67	580.152	0.027191	0.027133	-0.03
001K	316	2003.67	725.190	0.034022	0.034041	0.06
001K	317	2003.67	870.228	0.040913	0.040924	0.03
001K	318	2003.67	1015.266	0.047804	0.047831	0.06
001K	319	2003.67	1160.304	0.054747	0.054762	0.03
001K	320	2003.67	1305.342	0.061668	0.061717	0.08
001K	321	2003.67	1450.380	0.068650	0.068695	0.07
001K	322	2039.67	145.038	0.006641	0.006638	-0.06
001K	323	2039.67	290.076	0.013308	0.013298	-0.08
001K	324	2039.67	435.114	0.019990	0.019981	-0.04
001K	325	2039.67	580.152	0.026693	0.026687	-0.02
001K	326	2039.67	725.190	0.033396	0.033415	0.06
001K	327	2039.67	870.228	0.040150	0.040165	0.04
001K	328	2039.67	1015.266	0.046912	0.046937	0.05
001K	329	2039.67	1160.304	0.053704	0.053731	0.05
001K	330	2039.67	1305.342	0.060495	0.060546	0.08
001K	331	2039.67	1450.380	0.067344	0.067382	0.06
001K	332	2075.67	145.038	0.006526	0.006522	-0.07
001K	333	2075.67	290.076	0.013073	0.013064	-0.07
001K	334	2075.67	435.114	0.019639	0.019627	-0.06
001K	335	2075.67	580.152	0.026213	0.026210	-0.01
001K	336	2075.67	725.190	0.032796	0.032813	0.05
001K	337	2075.67	870.228	0.039420	0.039436	0.04
001K	338	2075.67	1015.266	0.046052	0.046078	0.06
001K	339	2075.67	1160.304	0.052716	0.052740	0.05
001K	340	2075.67	1305.342	0.059377	0.059422	0.08
001K	341	2075.67	1450.380	0.066099	0.066122	0.03
001K	342	2111.67	145.038	0.014415	0.006410	-55.53
001K	343	2111.67	290.076	0.012845	0.012838	-0.06
001K	344	2111.67	435.114	0.019289	0.019285	-0.02
001K	345	2111.67	580.152	0.025751	0.025750	-0.01
001K	346	2111.67	725.190	0.032217	0.032233	0.05
001K	347	2111.67	870.228	0.038716	0.038734	0.05
001K	348	2111.67	1015.266	0.045224	0.045252	0.06
001K	349	2111.67	1160.304	0.051764	0.051788	0.05
001K	350	2111.67	1305.342	0.058299	0.058341	0.07
001K	351	2111.67	1450.380	0.064862	0.064911	0.08
001K	352	2147.67	145.038	0.006305	0.006301	-0.05
001K	353	2147.67	290.076	0.012621	0.012620	-0.01
001K	354	2147.67	435.114	0.018859	0.018955	0.51

TABLE 5. CONTINUED. KENNEDY.

DATA ID		T RANKINE	P PSIA	RHO EXP LBMOL/FT3	RHO CALC LBMOL/FT3	ERROR PERCENT
001K	355	2147.67	580.152	0.025304	0.025306	0.01
001K	356	2147.67	725.190	0.031659	0.031674	0.05
001K	357	2147.67	870.228	0.038037	0.038058	0.05
001K	358	2147.67	1015.266	0.044424	0.044457	0.07
001K	359	2147.67	1160.304	0.050846	0.050872	0.05
001K	360	2147.67	1305.342	0.057259	0.057303	0.08
001K	361	2147.67	1450.380	0.063683	0.063748	0.10
001K	362	2183.67	145.038	0.006201	0.006197	-0.07
001K	363	2183.67	290.076	0.012413	0.012409	-0.03
001K	364	2183.67	435.114	0.018646	0.018636	-0.05
001K	365	2183.67	580.152	0.024876	0.024878	0.01
001K	366	2183.67	725.190	0.031119	0.031135	0.05
001K	367	2183.67	870.228	0.037381	0.037406	0.07
001K	368	2183.67	1015.266	0.043658	0.043691	0.08
001K	369	2183.67	1160.304	0.049952	0.049990	0.07
001K	370	2183.67	1305.342	0.056256	0.056303	0.08
001K	371	2183.67	1450.380	0.062569	0.062629	0.10
001K	372	2219.67	145.038	0.006101	0.006096	-0.08
001K	373	2219.67	290.076	0.012208	0.012205	-0.02
001K	374	2219.67	435.114	0.018331	0.018328	-0.01
001K	375	2219.67	580.152	0.024460	0.024465	0.02
001K	376	2219.67	725.190	0.030597	0.030614	0.06
001K	377	2219.67	870.228	0.036747	0.036777	0.08
001K	378	2219.67	1015.266	0.042923	0.042952	0.07
001K	379	2219.67	1160.304	0.049097	0.049139	0.09
001K	380	2219.67	1305.342	0.055288	0.055339	0.09
001K	381	2219.67	1450.380	0.061493	0.061551	0.09
001K	382	2255.67	145.038	0.005999	0.005998	-0.02
001K	383	2255.67	290.076	0.012009	0.012008	-0.01
001K	384	2255.67	435.114	0.018035	0.018031	-0.03
001K	385	2255.67	580.152	0.024058	0.024065	0.03
001K	386	2255.67	725.190	0.030093	0.030112	0.06
001K	387	2255.67	870.228	0.036138	0.036169	0.09
001K	388	2255.67	1015.266	0.042213	0.042238	0.06
001K	389	2255.67	1160.304	0.048263	0.048319	0.11
001K	390	2255.67	1305.342	0.054352	0.054410	0.11
001K	391	2255.67	1450.380	0.060422	0.060512	0.15
001K	392	2291.67	145.038	0.005905	0.005903	-0.04
001K	393	2291.67	290.076	0.011817	0.011818	0.01
001K	394	2291.67	435.114	0.017740	0.017743	0.02
001K	395	2291.67	580.152	0.023669	0.023679	0.04
001K	396	2291.67	725.190	0.029605	0.029625	0.07
001K	397	2291.67	870.228	0.035553	0.035582	0.08
001K	398	2291.67	1015.266	0.041505	0.041549	0.11
001K	399	2291.67	1160.304	0.047458	0.047526	0.15
001K	400	2291.67	1305.342	0.053447	0.053513	0.12
001K	401	2291.67	1450.380	0.059407	0.059509	0.17

THE AVERAGE ABSOLUTE ERROR IN PERCENT IS 0.31
FOR 401 DATA POINTS.

TABLE 6. THE PREDICTION OF EXPERIMENTAL DENSITY DATA OF KEYES AND SMITH. PROC. AM. ACAD. ARTS AND SCI., 258(1934.

DATA ID		T RANKINE	P PSIA	RHO EXP LBMOL/FT3	RHO CALC LBMOL/FT3	ERROR PERCENT
002K	1	545.67	62.063	3.453388	3.459388	0.17
002K	2	545.67	324.939	3.456499	3.460155	0.11
002K	3	545.67	682.358	3.460219	3.461201	0.03
002K	4	545.67	1120.520	3.464846	3.462475	-0.07
002K	5	545.67	1558.696	3.469402	3.463734	-0.16
002K	6	545.67	1996.843	3.473966	3.464982	-0.26
002K	7	545.67	2435.004	3.478447	3.466228	-0.35
002K	8	545.67	2873.137	3.482901	3.467458	-0.44
002K	9	545.67	3311.282	3.487295	3.468681	-0.53
002K	10	545.67	3749.429	3.491697	3.469891	-0.62
002K	11	545.67	4187.570	3.496019	3.471095	-0.71
002K	12	545.67	4625.730	3.500315	3.472287	-0.80
002K	13	581.67	61.960	3.427279	3.436846	0.28
002K	14	581.67	324.851	3.430139	3.437660	0.22
002K	15	581.67	682.270	3.433918	3.438769	0.14
002K	16	581.67	1120.432	3.438342	3.440117	0.05
002K	17	581.67	1558.608	3.442808	3.441455	-0.04
002K	18	581.67	1996.755	3.447194	3.442782	-0.13
002K	19	581.67	2434.931	3.451578	3.444101	-0.22
002K	20	581.67	2873.063	3.455995	3.445407	-0.31
002K	21	581.67	3311.209	3.460361	3.446708	-0.39
002K	22	581.67	3749.385	3.464575	3.447995	-0.48
002K	23	581.67	4187.527	3.468801	3.449274	-0.56
002K	24	581.67	4625.703	3.473043	3.450546	-0.65
002K	25	581.67	5063.852	3.477221	3.451812	-0.73
002K	26	626.67	62.475	3.381586	3.391099	0.28
002K	27	626.67	325.351	3.384429	3.392068	0.23
002K	28	626.67	682.755	3.388290	3.393381	0.15
002K	29	626.67	1120.916	3.392756	3.394975	0.07
002K	30	626.67	1559.078	3.397232	3.396560	-0.02
002K	31	626.67	1997.240	3.401732	3.398130	-0.11
002K	32	626.67	2435.372	3.406172	3.399688	-0.19
002K	33	626.67	3311.665	3.414992	3.402765	-0.36
002K	34	626.67	4187.973	3.423674	3.405792	-0.52
002K	35	626.67	5064.266	3.432198	3.408772	-0.68
002K	36	671.67	62.666	3.324335	3.333576	0.28
002K	37	671.67	325.571	3.327233	3.334782	0.23
002K	38	671.67	683.020	3.331563	3.336407	0.15
002K	39	671.67	1121.181	3.335999	3.338377	0.07
002K	40	671.67	1559.343	3.340964	3.340330	-0.02
002K	41	671.67	1997.489	3.345606	3.342269	-0.10
002K	42	671.67	2435.651	3.350359	3.344181	-0.18
002K	43	671.67	3311.958	3.359548	3.347961	-0.34
002K	44	671.67	4188.277	3.368626	3.351668	-0.50
002K	45	671.67	5064.590	3.377533	3.355310	-0.66
002K	46	761.67	102.522	3.180632	3.192213	0.36
002K	47	761.67	326.747	3.184052	3.193889	0.31
002K	48	761.67	684.136	3.188914	3.196525	0.24
002K	49	761.67	1122.269	3.194790	3.199718	0.15
002K	50	761.67	1560.401	3.200495	3.202861	0.07
002K	51	761.67	1998.518	3.205837	3.205957	0.00
002K	52	761.67	2436.665	3.211693	3.209009	-0.08
002K	53	761.67	3312.928	3.222671	3.214987	-0.24
002K	54	761.67	4189.203	3.233426	3.220801	-0.39
002K	55	761.67	5065.480	3.243937	3.226466	-0.54
002K	56	851.67	240.332	2.999573	3.013924	0.48
002K	57	851.67	685.341	3.007576	3.019639	0.40
002K	58	851.67	1123.459	3.015302	3.025162	0.33
002K	59	851.67	1561.606	3.022778	3.030521	0.26

TABLE 6. CONTINUED. KEYES, AND SMITH.

DATA ID		T RANKINE	P PSIA	RHO EXP LBMOL/FT3	RHO CALC LBMOL/FT3	ERROR PERCENT
002K	60	851.67	1999.738	3.030257	3.035761	0.18
002K	61	851.67	2437.885	3.037683	3.040872	0.10
002K	62	851.67	3314.148	3.051950	3.050755	-0.04
002K	63	851.67	4190.426	3.065674	3.060224	-0.18
002K	64	851.67	5066.703	3.079068	3.069313	-0.32
002K	65	941.67	573.409	2.771319	2.783577	0.44
002K	66	941.67	683.255	2.774200	2.786226	0.43
002K	67	941.67	1121.357	2.786129	2.796953	0.39
002K	68	941.67	1559.475	2.797588	2.807178	0.34
002K	69	941.67	1997.578	2.808804	2.816948	0.29
002K	70	941.67	2435.695	2.819651	2.826315	0.24
002K	71	941.67	3311.915	2.840302	2.843962	0.13
002K	72	941.67	4188.176	2.859841	2.860369	0.02
002K	73	941.67	5064.426	2.878553	2.875717	-0.10
002K	74	1031.67	1269.469	2.471990	2.466121	-0.24
002K	75	1031.67	1561.959	2.487291	2.483578	-0.15
002K	76	1031.67	1999.973	2.508924	2.507333	-0.06
002K	77	1031.67	2438.017	2.529092	2.528791	-0.01
002K	78	1031.67	3314.148	2.565641	2.566504	0.03
002K	79	1031.67	4190.133	2.598472	2.599050	0.02
002K	80	1031.67	5066.438	2.628258	2.627612	-0.02
002K	81	1067.67	1656.383	2.315985	2.294660	-0.92
002K	82	1067.67	1997.769	2.342318	2.326921	-0.66
002K	83	1067.67	2435.724	2.372389	2.362311	-0.42
002K	84	1067.67	2873.710	2.399491	2.392896	-0.27
002K	85	1067.67	3311.708	2.424069	2.419930	-0.17
002K	86	1067.67	4187.750	2.468260	2.466315	-0.08
002K	87	1067.67	5063.852	2.506495	2.505430	-0.04
002K	88	1085.67	1911.015	2.227225	2.196980	-1.36
002K	89	1085.67	1998.577	2.236829	2.208494	-1.27
002K	90	1085.67	2436.459	2.276958	2.258304	-0.82
002K	91	1085.67	2874.371	2.311399	2.298965	-0.54
002K	92	1085.67	3312.312	2.341743	2.333556	-0.35
002K	93	1085.67	4188.242	2.394217	2.390674	-0.15
002K	94	1085.67	5064.266	2.438992	2.437205	-0.07
002K	95	1103.67	2145.086	2.120034	2.078967	-1.94
002K	96	1103.67	2437.209	2.160769	2.128958	-1.47
002K	97	1103.67	2875.003	2.208229	2.187422	-0.94
002K	98	1103.67	3312.855	2.247839	2.233996	-0.62
002K	99	1103.67	3750.752	2.282242	2.272959	-0.41
002K	100	1103.67	4188.676	2.312774	2.306618	-0.27
002K	101	1103.67	4626.645	2.340434	2.336328	-0.18
002K	102	1103.67	5064.590	2.365730	2.362986	-0.12
002K	103	1121.67	2476.889	2.010234	1.958883	-2.55
002K	104	1121.67	2875.870	2.079570	2.046383	-1.60
002K	105	1121.67	3313.604	2.136215	2.114674	-1.01
002K	106	1121.67	3751.413	2.181993	2.167727	-0.65
002K	107	1121.67	4189.250	2.220882	2.211414	-0.43
002K	108	1121.67	4627.156	2.254975	2.248730	-0.28
002K	109	1121.67	5065.086	2.285534	2.281390	-0.18
002K	110	1139.67	2785.560	1.862714	1.897367	-2.97
002K	111	1139.67	2873.004	1.891999	1.841216	-2.68
002K	112	1139.67	2877.516	1.893556	1.842834	-2.68
002K	113	1139.67	3314.927	1.993811	1.961702	-1.61
002K	114	1139.67	3752.604	2.061652	2.040707	-1.02
002K	115	1139.67	4190.359	2.114240	2.100667	-0.64
002K	116	1139.67	4628.219	2.158072	2.149323	-0.41
002K	117	1139.67	5066.102	2.195999	2.190441	-0.25
002K	118	1157.67	3137.600	1.671416	1.640926	-1.82

TABLE 6. CONTINUED. KEYES, AND SMITH.

DATA ID		T RANKINE	P PSIA	RHO EXP LBMOL/FT3	RHO CALC LBMOL/FT3	ERROR PERCENT
002K	119	1157.67	3312.105	1.772704	1.733478	-2.21
002K	120	1157.67	3486.935	1.835553	1.800038	-1.93
002K	121	1157.67	3661.810	1.883040	1.852429	-1.63
002K	122	1157.67	3836.816	1.921942	1.895844	-1.36
002K	123	1164.87	3226.852	1.457501	1.519708	4.27
002K	124	1164.87	3313.354	1.606056	1.591427	-0.91
002K	125	1164.87	3487.744	1.723244	1.690964	-1.87
002K	126	1164.87	3662.486	1.792998	1.761762	-1.74
002K	127	1164.87	3837.372	1.844886	1.817172	-1.50
002K	128	1164.87	4012.321	1.886962	1.862843	-1.28
002K	129	1164.87	4099.816	1.902360	1.883024	-1.33

THE AVERAGE ABSOLUTE ERROR IN PERCENT IS 0.58
FOR 129 DATA POINTS.

TABLE 7. THE PREDICTION OF EXPERIMENTAL DENSITY DATA OF KEYES, SMITH AND GERRY, PROC. AM. ACAD. ARTS SCI., V 70,319(1936.

DATA ID		T RANKINE	P PSIA	RHO EXP LBMOL/FT3	RHO CALC LBMOL/FT3	ERROR PERCENT
004K	1	842.67	202.621	0.024773	0.024655	-0.48
004K	2	844.47	204.252	0.024773	0.024797	0.10
004K	3	846.27	205.119	0.024773	0.024836	0.26
004K	4	848.07	205.795	0.024773	0.024850	0.31
004K	5	849.87	206.339	0.024773	0.024845	0.29
004K	6	851.67	206.838	0.024773	0.024835	0.25
004K	7	851.67	194.288	0.023121	0.023181	0.26
004K	8	869.67	212.790	0.024773	0.024868	0.38
004K	9	869.67	199.740	0.023121	0.023204	0.36
004K	10	874.17	288.228	0.034682	0.034644	-0.11
004K	11	887.67	301.484	0.035571	0.035537	0.04
004K	12	887.67	295.194	0.034682	0.034745	0.18
004K	13	887.67	218.551	0.024773	0.024883	0.44
004K	14	887.67	205.046	0.023121	0.023216	0.41
004K	15	901.17	385.607	0.046243	0.046142	-0.22
004K	16	905.67	389.192	0.046243	0.046243	0.00
004K	17	905.67	389.501	0.046243	0.046286	0.09
004K	18	905.67	310.185	0.035571	0.035621	0.14
004K	19	905.67	303.638	0.034682	0.034782	0.29
004K	20	905.67	224.151	0.024773	0.024885	0.45
004K	21	905.67	210.189	0.023121	0.023214	0.40
004K	22	923.67	401.259	0.046243	0.046338	0.21
004K	23	923.67	401.346	0.046243	0.046350	0.23
004K	24	923.67	318.738	0.035571	0.035648	0.22
004K	25	923.67	311.815	0.034682	0.034784	0.30
004K	26	923.67	229.662	0.024773	0.024884	0.45
004K	27	923.67	215.259	0.023121	0.023209	0.38
004K	28	941.67	578.665	0.069364	0.069510	0.21
004K	29	941.67	573.927	0.069364	0.068768	-0.86
004K	30	941.67	514.127	0.060316	0.060067	-0.41
004K	31	941.67	412.707	0.046243	0.046369	0.27
004K	32	941.67	412.957	0.046243	0.046401	0.34
004K	33	941.67	327.114	0.035571	0.035665	0.26
004K	34	941.67	319.928	0.034682	0.034797	0.33
004K	35	941.67	235.350	0.024773	0.024908	0.55
004K	36	941.67	220.241	0.023121	0.023200	0.34
004K	37	959.67	596.560	0.069364	0.069457	0.13
004K	38	959.67	594.752	0.069364	0.069197	-0.24
004K	39	959.67	529.823	0.060316	0.060148	-0.28
004K	40	959.67	424.052	0.046243	0.046403	0.35
004K	41	959.67	424.273	0.046243	0.046431	0.41
004K	42	959.67	335.315	0.035571	0.035671	0.28
004K	43	959.67	327.688	0.034682	0.034778	0.28
004K	44	959.67	240.523	0.024773	0.024879	0.43
004K	45	959.67	225.195	0.023121	0.023193	0.31
004K	46	966.87	722.538	0.087802	0.087189	-0.70
004K	47	966.87	717.586	0.086705	0.086408	-0.34
004K	48	966.87	715.557	0.086705	0.086089	-0.71
004K	49	968.67	720.069	0.086705	0.086432	-0.31
004K	50	977.67	739.557	0.087802	0.087641	-0.18
004K	51	977.67	732.709	0.086705	0.086592	-0.13
004K	52	977.67	732.694	0.086705	0.086589	-0.13
004K	53	977.67	731.195	0.086705	0.086361	-0.40
004K	54	977.67	545.092	0.060316	0.060196	-0.20
004K	55	977.67	434.899	0.046243	0.046392	0.32
004K	56	977.67	435.281	0.046243	0.046438	0.42
004K	57	977.67	343.384	0.035571	0.035671	0.28
004K	58	977.67	335.447	0.034682	0.034769	0.25
004K	59	977.67	246.092	0.024773	0.024895	0.51

TABLE 7. CONTINUED. KEYES, SMITH AND GERRY.

DATA ID		T RANKINE	P PSIA	RHO EXP LBMOL/FT3	RHO CALC LBMOL/FT3	ERROR PERCENT
004K	60	977.67	230.118	0.023121	0.023186	0.28
004K	61	995.67	764.335	0.087802	0.087860	0.07
004K	62	995.67	757.355	0.086705	0.086841	0.16
004K	63	995.67	757.032	0.086705	0.086794	0.10
004K	64	995.67	755.650	0.086705	0.086593	-0.13
004K	65	995.67	633.242	0.069364	0.069650	0.41
004K	66	995.67	631.773	0.069364	0.069456	0.13
004K	67	995.67	559.995	0.060316	0.060222	-0.16
004K	68	995.67	445.965	0.046243	0.046422	0.39
004K	69	995.67	446.112	0.046243	0.046439	0.43
004K	70	995.67	351.320	0.035571	0.035664	0.26
004K	71	995.67	343.251	0.034682	0.034773	0.26
004K	72	995.67	251.120	0.024773	0.024865	0.37
004K	73	995.67	234.997	0.023121	0.023179	0.25
004K	74	997.47	936.608	0.115607	0.114667	-0.81
004K	75	997.47	935.021	0.115607	0.114395	-1.05
004K	76	1013.67	968.808	0.115607	0.115212	-0.34
004K	77	1013.67	967.338	0.115607	0.114972	-0.55
004K	78	1013.67	788.247	0.087802	0.087994	0.22
004K	79	1013.67	780.722	0.086705	0.086944	0.28
004K	80	1013.67	574.647	0.060316	0.060238	-0.13
004K	81	1013.67	456.399	0.046243	0.046392	0.32
004K	82	1013.67	456.781	0.046243	0.046435	0.42
004K	83	1013.67	359.138	0.035571	0.035653	0.23
004K	84	1013.67	350.703	0.034682	0.034747	0.19
004K	85	1013.67	256.425	0.024773	0.024865	0.37
004K	86	1013.67	239.832	0.023121	0.023170	0.21
004K	87	1031.67	1002.595	0.115607	0.115535	-0.06
004K	88	1031.67	1001.493	0.115607	0.115364	-0.21
004K	89	1031.67	811.673	0.087802	0.088098	0.34
004K	90	1031.67	803.384	0.086705	0.086991	0.33
004K	91	1031.67	804.016	0.086705	0.087075	0.43
004K	92	1031.67	802.620	0.086705	0.086889	0.21
004K	93	1031.67	668.441	0.069364	0.069756	0.57
004K	94	1031.67	666.720	0.069364	0.069546	0.26
004K	95	1031.67	589.006	0.060316	0.060240	-0.13
004K	96	1031.67	466.864	0.046243	0.046378	0.29
004K	97	1031.67	467.261	0.046243	0.046422	0.39
004K	98	1031.67	366.884	0.035571	0.035641	0.20
004K	99	1031.67	358.271	0.034682	0.034740	0.17
004K	100	1031.67	261.627	0.024773	0.024857	0.34
004K	101	1031.67	244.638	0.023121	0.023162	0.18
004K	102	1049.67	1360.631	0.173410	0.170935	-1.43
004K	103	1049.67	833.952	0.087802	0.088089	0.33
004K	104	1049.67	825.826	0.086705	0.087046	0.39
004K	105	1040.67	1331.561	0.173410	0.170235	-1.83
004K	106	1040.67	1330.018	0.173410	0.169918	-2.01
004K	107	1041.57	1333.927	0.173410	0.170195	-1.85
004K	108	1042.47	1339.483	0.173410	0.170807	-1.50
004K	109	1049.67	825.488	0.086705	0.087003	0.34
004K	110	1049.67	603.071	0.060316	0.060225	-0.15
004K	111	1049.67	477.283	0.046243	0.046370	0.28
004K	112	1049.67	477.577	0.046243	0.046402	0.34
004K	113	1049.67	374.540	0.035571	0.035627	0.16
004K	114	1049.67	365.663	0.034682	0.034721	0.11
004K	115	1049.67	266.682	0.024773	0.024838	0.26
004K	116	1049.67	249.414	0.023121	0.023153	0.14
004K	117	1055.07	1488.564	0.198183	0.194399	-1.91
004K	118	1067.67	1532.639	0.198183	0.194892	-1.66

TABLE 7. CONTINUED. KEYES, SMITH AND GERRY.

DATA ID		T RANKINE	P PSIA	RHO EXP LBMOL/FT3	RHO CALC LBMOL/FT3	ERROR PERCENT
004K	119	1067.67	1415.287	0.173410	0.171684	-1.00
004K	120	1067.67	1417.463	0.173410	0.172089	-0.76
004K	121	1067.67	1415.890	0.173410	0.171796	-0.93
004K	122	1067.67	1067.127	0.115607	0.115885	0.24
004K	123	1067.67	1066.495	0.115607	0.115797	0.16
004K	124	1067.67	856.233	0.087802	0.088118	0.36
004K	125	1067.67	847.077	0.086705	0.086987	0.33
004K	126	1067.67	847.136	0.086705	0.086994	0.33
004K	127	1067.67	848.150	0.086705	0.087119	0.48
004K	128	1067.67	847.151	0.086705	0.086996	0.34
004K	129	1067.67	701.773	0.069364	0.069731	0.53
004K	130	1067.67	700.847	0.069364	0.069625	0.38
004K	131	1067.67	616.959	0.060316	0.060208	-0.18
004K	132	1067.67	487.247	0.046243	0.046325	0.18
004K	133	1067.67	487.747	0.046243	0.046377	0.29
004K	134	1067.67	382.124	0.035571	0.035611	0.11
004K	135	1067.67	373.159	0.034682	0.034718	0.10
004K	136	1067.67	271.914	0.024773	0.024839	0.27
004K	137	1067.67	254.206	0.023121	0.023149	0.12
004K	138	1071.27	1674.887	0.231213	0.224437	-2.93
004K	139	1085.67	1740.256	0.231213	0.226501	-2.04
004K	140	1085.67	1597.362	0.198183	0.196045	-1.08
004K	141	1085.67	1469.782	0.173410	0.172473	-0.54
004K	142	1085.67	877.646	0.087802	0.088074	0.31
004K	143	1085.67	868.593	0.086705	0.086995	0.33
004K	144	1085.67	868.505	0.086705	0.086985	0.32
004K	145	1085.67	630.700	0.060316	0.060191	-0.21
004K	146	1085.67	497.579	0.046243	0.046327	0.18
004K	147	1085.67	497.770	0.046243	0.046346	0.22
004K	148	1085.67	389.663	0.035571	0.035596	0.07
004K	149	1085.67	380.522	0.034682	0.034706	0.07
004K	150	1085.67	276.867	0.024773	0.024816	0.17
004K	151	1085.67	258.952	0.023121	0.023142	0.09
004K	152	1090.17	1919.260	0.277456	0.267745	-3.50
004K	153	1103.67	1993.683	0.277456	0.270211	-2.61
004K	154	1103.67	1818.325	0.231213	0.228193	-1.31
004K	155	1103.67	1660.528	0.198183	0.196955	-0.62
004K	156	1103.67	1523.351	0.173410	0.173160	-0.14
004K	157	1103.67	1522.954	0.173410	0.173094	-0.18
004K	158	1103.67	1522.396	0.173410	0.173003	-0.23
004K	159	1103.67	1129.293	0.115607	0.116109	0.43
004K	160	1103.67	1129.161	0.115607	0.116092	0.42
004K	161	1103.67	891.283	0.086705	0.087166	0.53
004K	162	1103.67	890.402	0.086705	0.087065	0.41
004K	163	1103.67	734.604	0.069364	0.069731	0.53
004K	164	1103.67	733.561	0.069364	0.069618	0.37
004K	165	1111.77	2231.414	0.346820	0.330975	-4.57
004K	166	1121.67	2301.574	0.346820	0.333922	-3.72
004K	167	1121.67	2090.062	0.277456	0.272620	-1.74
004K	168	1121.67	1893.467	0.231213	0.229307	-0.82
004K	169	1121.67	1721.753	0.198183	0.197589	-0.30
004K	170	1121.67	1574.040	0.173410	0.173448	0.02
004K	171	1135.17	2621.885	0.462427	0.432372	-6.50
004K	172	1139.67	2665.784	0.462427	0.435385	-5.85
004K	173	1139.67	2426.936	0.346820	0.338125	-2.51
004K	174	1139.67	2183.400	0.277456	0.274285	-1.14
004K	175	1139.67	1967.229	0.231213	0.230233	-0.42
004K	176	1139.67	1781.729	0.198183	0.198098	-0.04
004K	177	1139.67	1624.022	0.173410	0.173712	0.17

TABLE 7. CONTINUED. KEYES, SMITH AND GERRY.

DATA ID		T RANKINE	P PSIA	RHO EXP LBMOL/FT3	RHO CALC LBMOL/FT3	ERROR PERCENT
004K	178	1139.67	1623.316	0.173410	0.173608	0.11
004K	179	1139.67	1624.330	0.173410	0.173757	0.20
004K	180	1139.67	1188.946	0.115607	0.116184	0.50
004K	181	1139.67	1188.079	0.115607	0.116081	0.41
004K	182	1139.67	933.184	0.086705	0.087172	0.54
004K	183	1139.67	932.169	0.086705	0.087062	0.41
004K	184	1139.67	766.981	0.069364	0.069744	0.55
004K	185	1139.67	765.761	0.069364	0.069620	0.37
004K	186	1147.77	2852.855	0.554912	0.514321	-7.31
004K	187	1157.67	3233.597	1.734098	1.696316	-2.18
004K	188	1157.67	2967.973	0.554912	0.523398	-5.68
004K	189	1157.67	2839.745	0.462427	0.444818	-3.81
004K	190	1157.67	2548.138	0.346820	0.340830	-1.73
004K	191	1157.67	2274.150	0.277456	0.275456	-0.72
004K	192	1160.37	3097.786	0.693640	0.661057	-4.70
004K	195	1175.67	3936.868	1.734098	1.709716	-1.41
004K	197	1175.67	3393.877	0.867050	0.860794	-0.72
004K	198	1175.67	3318.749	0.693640	0.674065	-2.82
004K	199	1175.67	3176.398	0.554912	0.534878	-3.61
004K	200	1175.67	3008.123	0.462427	0.450131	-2.66
004K	201	1175.67	2665.725	0.346820	0.342579	-1.22
004K	202	1175.67	2359.023	0.277456	0.275593	-0.67
004K	203	1175.67	2108.257	0.231213	0.231227	0.01
004K	204	1175.67	1905.827	0.198183	0.199937	0.89
004K	205	1175.67	1720.842	0.173410	0.174016	0.35
004K	206	1175.67	1720.210	0.173410	0.173931	0.30
004K	207	1175.67	1721.033	0.173410	0.174042	0.36
004K	208	1175.67	1246.924	0.115607	0.116211	0.52
004K	209	1175.67	1246.322	0.115607	0.116144	0.46
004K	210	1175.67	974.069	0.086705	0.087152	0.52
004K	211	1175.67	973.276	0.086705	0.087071	0.42
004K	212	1175.67	798.137	0.069364	0.069687	0.47
004K	213	1175.67	797.388	0.069364	0.069615	0.36
004K	214	1193.67	4663.168	1.734098	1.720631	-0.78
004K	215	1193.67	3856.421	1.156065	1.251822	8.28
004K	216	1193.67	3714.511	0.867050	0.917760	5.85
004K	218	1211.67	4275.895	1.156065	1.190921	3.02
004K	217	1211.67	5403.227	1.734098	1.728244	-0.34
004K	219	1211.67	4032.233	0.867050	0.874290	0.84
004K	220	1211.67	3831.599	0.693640	0.681606	-1.73
004K	221	1211.67	3578.862	0.554912	0.543959	-1.97
004K	222	1211.67	3333.474	0.462427	0.455644	-1.47
004K	223	1211.67	2893.872	0.346820	0.344849	-0.57
004K	224	1211.67	2534.191	0.277456	0.277365	-0.03
004K	225	1211.67	2243.714	0.231213	0.231765	0.24
004K	226	1211.67	2008.511	0.198183	0.198993	0.41
004K	227	1211.67	1814.076	0.173410	0.174121	0.41
004K	228	1211.67	1813.548	0.173410	0.174056	0.37
004K	229	1211.67	1815.532	0.173410	0.174301	0.51
004K	230	1211.67	1303.256	0.115607	0.116180	0.50
004K	231	1211.67	1303.197	0.115607	0.116174	0.49
004K	232	1211.67	1014.278	0.086705	0.087133	0.49
004K	233	1211.67	1013.514	0.086705	0.087059	0.41
004K	234	1211.67	829.264	0.069364	0.069673	0.45
004K	235	1211.67	828.647	0.069364	0.069616	0.36
004K	236	1229.67	4699.945	1.156065	1.165588	0.82
004K	237	1229.67	4343.340	0.867050	0.858418	-1.00
004K	238	1247.67	5128.516	1.156065	1.154785	-0.11
004K	239	1247.67	4661.988	0.867050	0.857011	-1.16

TABLE 7. CONTINUED. KEYES, SMITH AND GERRY.

DATA ID		T RANKINE	P PSIA	RHO EXP LBMOL/FT3	RHO CALC LBMOL/FT3	ERROR PERCENT
004K	240	1247.67	4329.035	0.693640	0.682468	-1.61
004K	241	1247.67	3964.323	0.554912	0.546486	-1.52
004K	242	1247.67	3645.452	0.462427	0.457928	-0.97
004K	243	1247.67	3112.351	0.346820	0.345882	-0.27
004K	244	1247.67	2698.425	0.277456	0.277785	0.12
004K	245	1247.67	2373.500	0.231213	0.231896	0.30
004K	246	1247.67	2115.267	0.198183	0.199019	0.42
004K	247	1247.67	1905.019	0.173410	0.174182	0.45
004K	248	1247.67	1905.078	0.173410	0.174189	0.45
004K	249	1247.67	1905.137	0.173410	0.174196	0.45
004K	250	1247.67	1358.529	0.115607	0.116145	0.47
004K	251	1247.67	1358.500	0.115607	0.116143	0.46
004K	252	1247.67	1053.475	0.086705	0.087075	0.43
004K	253	1247.67	1053.122	0.086705	0.087042	0.39
004K	254	1247.67	859.789	0.069364	0.069639	0.40
004K	255	1247.67	859.230	0.069364	0.069590	0.33
004K	256	1265.67	4975.309	0.867050	0.854950	-1.40
004K	257	1283.67	5286.477	0.867050	0.853789	-1.53
004K	258	1283.67	4818.031	0.693640	0.683881	-1.41
004K	259	1283.67	4343.383	0.554912	0.548845	-1.09
004K	260	1283.67	3949.171	0.462427	0.459434	-0.65
004K	261	1283.67	3324.040	0.346820	0.346471	-0.10
004K	262	1283.67	2857.940	0.277456	0.278019	0.20
004K	263	1283.67	2499.786	0.231213	0.231936	0.31
004K	264	1283.67	2218.554	0.198183	0.198903	0.36
004K	265	1283.67	1993.933	0.173410	0.174209	0.46
004K	266	1283.67	1993.669	0.173410	0.174181	0.44
004K	267	1283.67	1992.757	0.173410	0.174083	0.39
004K	268	1283.67	1413.098	0.115607	0.116123	0.45
004K	269	1283.67	1413.230	0.115607	0.116140	0.46
004K	270	1283.67	1092.244	0.086705	0.087027	0.37
004K	271	1283.67	1092.111	0.086705	0.087016	0.36
004K	272	1283.67	889.946	0.069364	0.069604	0.35
004K	273	1283.67	889.814	0.069364	0.069593	0.33
004K	274	1319.67	5293.277	0.693640	0.683823	-1.42
004K	275	1319.67	4709.402	0.554912	0.549520	-0.97
004K	276	1319.67	4242.875	0.462427	0.460020	-0.52
004K	277	1319.67	3529.673	0.346820	0.346768	-0.01
004K	278	1319.67	3012.606	0.277456	0.278041	0.21
004K	279	1319.67	2622.928	0.231213	0.231904	0.30
004K	280	1319.67	2320.371	0.198183	0.198855	0.34
004K	281	1319.67	2080.833	0.173410	0.174186	0.45
004K	282	1319.67	2080.730	0.173410	0.174175	0.44
004K	283	1319.67	2079.320	0.173410	0.174034	0.36
004K	284	1319.67	1466.549	0.115607	0.116077	0.41
004K	285	1319.67	1467.240	0.115607	0.116139	0.46
004K	286	1319.67	1130.851	0.086705	0.087007	0.35

THE AVERAGE ABSOLUTE ERROR IN PERCENT IS 0.73
FOR 283 DATA POINTS.

TABLE 8. THE PREDICTION OF EXPERIMENTAL DENSITY DATA OF KELL AND WALLEY, PHIL. TRANS. ROY. SOC.(LONDON), 258A, 565(1965).

DATA ID		T RANKINE	P PSIA	RHO EXP LBMOL/FT3	RHO CALC LBMOL/FT3	ERROR PERCENT
003K	1	491.67	76.870	3.466608	3.412975	-1.60
003K	2	509.67	76.870	3.467884	3.452994	-0.43
003K	3	527.66	76.870	3.462670	3.462022	-0.02
003K	4	536.67	76.870	3.458656	3.461755	0.09
003K	5	536.67	76.870	3.458652	3.461755	0.09
003K	6	536.68	76.870	3.458636	3.461749	0.09
003K	7	545.87	76.870	3.453673	3.459359	0.16
003K	8	491.67	182.748	3.469892	3.413616	-1.62
003K	9	509.67	182.748	3.469083	3.453363	-0.45
003K	10	527.66	182.748	3.463821	3.462349	-0.04
003K	11	536.67	182.748	3.459768	3.462069	0.07
003K	12	536.67	182.748	3.459771	3.462069	0.07
003K	13	536.68	182.748	3.459771	3.462068	0.07
003K	14	545.87	182.748	3.454795	3.459670	0.14
003K	15	491.67	290.076	3.471190	3.414249	-1.64
003K	16	509.67	290.076	3.470319	3.453738	-0.48
003K	17	527.66	290.076	3.464999	3.462667	-0.07
003K	18	536.67	290.076	3.460946	3.462386	0.04
003K	19	536.67	290.076	3.460937	3.462386	0.04
003K	20	536.68	290.076	3.460931	3.462388	0.04
003K	21	545.87	290.076	3.455928	3.459987	0.12
003K	22	491.67	397.404	3.472497	3.414893	-1.66
003K	23	509.67	397.404	3.471531	3.454112	-0.50
003K	24	527.66	397.404	3.466159	3.462992	-0.09
003K	25	536.67	397.404	3.462070	3.462705	0.02
003K	26	536.67	397.404	3.462073	3.462705	0.02
003K	27	536.68	397.404	3.462070	3.462702	0.02
003K	28	545.87	397.404	3.457058	3.460300	0.09
003K	29	491.67	610.755	3.475061	3.416141	-1.70
003K	30	509.67	610.755	3.473945	3.454844	-0.55
003K	31	527.66	610.755	3.468486	3.463638	-0.14
003K	32	536.67	610.755	3.464366	3.463332	-0.03
003K	33	536.67	610.755	3.464373	3.463332	-0.03
003K	34	536.68	610.755	3.464366	3.463331	-0.03
003K	35	545.87	610.755	3.459324	3.460921	0.05
003K	36	491.67	823.961	3.477651	3.417375	-1.73
003K	37	509.67	823.961	3.476371	3.455582	-0.60
003K	38	527.66	823.961	3.470801	3.464283	-0.19
003K	39	536.67	823.961	3.466655	3.463955	-0.08
003K	40	536.67	823.961	3.466655	3.463955	-0.08
003K	41	536.68	823.961	3.466648	3.463956	-0.08
003K	42	545.87	823.961	3.461599	3.461541	-0.00
003K	43	491.67	1037.167	3.480205	3.418562	-1.77
003K	44	509.67	1037.167	3.478766	3.456313	-0.65
003K	45	527.66	1037.167	3.473088	3.464917	-0.24
003K	46	536.67	1037.167	3.468888	3.464581	-0.12
003K	47	536.67	1037.167	3.468885	3.464581	-0.12
003K	48	536.68	1037.167	3.468892	3.464575	-0.12
003K	49	545.87	1037.167	3.463808	3.462161	-0.05
003K	50	491.67	1465.029	3.485318	3.420958	-1.85
003K	51	509.67	1465.029	3.483571	3.457757	-0.74
003K	52	527.66	1465.029	3.477706	3.466137	-0.33
003K	53	536.67	1465.029	3.473442	3.465821	-0.22
003K	54	536.67	1465.029	3.473454	3.465821	-0.22
003K	55	536.68	1465.029	3.473440	3.465819	-0.22
003K	56	545.87	1465.029	3.468333	3.463396	-0.14
003K	57	491.67	1893.036	3.490408	3.423278	-1.92
003K	58	509.67	1893.036	3.488351	3.459200	-0.84
003K	59	527.66	1893.036	3.482285	3.467446	-0.43

TABLE 8. CONTINUED. KELL AND WHALLEY.

DATA ID		T RANKINE	P PSIA	RHO EXP LBMOL/FT3	RHO CALC LBMOL/FT3	ERROR PERCENT
003K	60	536.67	1893.036	3.477940	3.467053	-0.31
003K	61	536.67	1893.036	3.477971	3.467053	-0.31
003K	62	536.68	1893.036	3.477950	3.467052	-0.31
003K	63	545.87	1893.036	3.472779	3.464615	-0.24
003K	64	491.67	3049.859	3.504003	3.429213	-2.13
003K	65	509.67	3049.859	3.501190	3.462991	-1.09
003K	66	527.66	3049.859	3.494579	3.470799	-0.68
003K	67	536.67	3049.859	3.490060	3.470334	-0.57
003K	68	536.67	3049.859	3.490074	3.470334	-0.57
003K	69	536.68	3049.859	3.490064	3.470333	-0.57
003K	70	545.87	3049.859	3.484719	3.467878	-0.48
003K	71	491.67	4742.016	3.523414	3.437267	-2.44
003K	72	509.67	4742.016	3.519470	3.468352	-1.45
003K	73	527.66	4742.016	3.512146	3.475573	-1.04
003K	74	536.67	4742.016	3.507337	3.475011	-0.92
003K	75	536.67	4742.016	3.507340	3.475011	-0.92
003K	76	536.68	4742.016	3.507347	3.475007	-0.92
003K	77	545.87	4742.016	3.501812	3.472534	-0.84
003K	78	491.67	6432.285	3.542324	3.444671	-2.76
003K	79	509.67	6432.285	3.537311	3.473496	-1.80
003K	80	527.66	6432.285	3.529247	3.480198	-1.39
003K	81	536.67	6432.285	3.524238	3.479556	-1.27
003K	82	536.67	6432.285	3.524244	3.479556	-1.27
003K	83	536.68	6432.285	3.524234	3.479556	-1.27
003K	84	545.87	6432.285	3.518484	3.477055	-1.18
003K	85	491.67	8123.723	3.560727	3.451568	-3.07
003K	86	509.67	8123.723	3.554790	3.478456	-2.15
003K	87	527.66	8123.723	3.546070	3.484693	-1.73
003K	88	536.67	8123.723	3.540810	3.483974	-1.61
003K	89	536.67	8123.723	3.540817	3.483974	-1.61
003K	90	536.68	8123.723	3.540795	3.483972	-1.60
003K	91	545.87	8123.723	3.534863	3.481461	-1.51
003K	92	491.67	9814.859	3.578628	3.458043	-3.37
003K	93	509.67	9814.859	3.571813	3.483235	-2.48
003K	94	527.66	9814.859	3.562447	3.489055	-2.06
003K	95	536.67	9814.859	3.556948	3.488276	-1.93
003K	96	536.67	9814.859	3.556944	3.488276	-1.93
003K	97	536.68	9814.859	3.556952	3.488276	-1.93
003K	98	545.87	9814.859	3.550800	3.485753	-1.83
003K	99	491.67	11505.707	3.596067	3.464143	-3.67
003K	100	509.67	11505.707	3.588377	3.487864	-2.80
003K	101	527.66	11505.707	3.578424	3.493301	-2.38
003K	102	536.67	11505.707	3.572700	3.492471	-2.25
003K	103	536.67	11505.707	3.572700	3.492471	-2.25
003K	104	536.68	11505.707	3.572718	3.492466	-2.25
003K	105	545.87	11505.707	3.566396	3.489945	-2.14
003K	106	491.67	13196.277	3.613068	3.469935	-3.96
003K	107	509.67	13196.277	3.604592	3.492351	-3.11
003K	108	527.66	13196.277	3.594077	3.497444	-2.69
003K	109	536.67	13196.277	3.588142	3.496561	-2.55
003K	110	536.67	13196.277	3.588154	3.496561	-2.55
003K	111	536.68	13196.277	3.588154	3.496557	-2.55
003K	112	545.87	13196.277	3.581673	3.494032	-2.45
003K	113	491.67	14886.547	3.629610	3.475448	-4.25
003K	114	509.67	14886.547	3.620408	3.496693	-3.42
003K	115	527.66	14886.547	3.609371	3.501476	-2.99
003K	116	536.67	14886.547	3.603233	3.500549	-2.85
003K	117	536.67	14886.547	3.603244	3.500549	-2.85
003K	118	536.68	14886.547	3.603241	3.500549	-2.85

TABLE 8. CONTINUED. KELL AND WHALLEY.

DATA ID		T RANKINE	P PSIA	RHO EXP LBMOL/FT3	RHO CALC LBMOL/FT3	ERROR PERCENT
003K	119	545.87	14886.547	3.596597	3.498026	-2.74
003K	120	563.67	76.870	3.441860	3.450313	0.25
003K	121	581.68	76.870	3.427354	3.436879	0.28
003K	122	599.67	76.870	3.410579	3.420348	0.29
003K	123	617.67	76.870	3.391732	3.401388	0.28
003K	124	635.67	76.870	3.371054	3.380447	0.28
003K	125	653.68	76.870	3.348559	3.357793	0.28
003K	126	671.68	76.870	3.324474	3.333630	0.28
003K	127	563.67	290.076	3.444122	3.450948	0.20
003K	128	581.68	290.076	3.429581	3.437542	0.23
003K	129	599.67	290.076	3.412807	3.421054	0.24
003K	130	617.67	290.076	3.393961	3.402145	0.24
003K	131	635.67	290.076	3.373324	3.381266	0.24
003K	132	653.68	290.076	3.350917	3.358689	0.23
003K	133	671.68	290.076	3.326853	3.334605	0.23
003K	134	563.67	610.755	3.447450	3.451900	0.13
003K	135	581.68	610.755	3.432897	3.438538	0.16
003K	136	599.67	610.755	3.416130	3.422112	0.18
003K	137	617.67	610.755	3.397346	3.403278	0.17
003K	138	635.67	610.755	3.376739	3.382494	0.17
003K	139	653.68	610.755	3.354397	3.360023	0.17
003K	140	671.68	610.755	3.330408	3.336061	0.17
003K	141	563.67	1037.167	3.451874	3.453160	0.04
003K	142	581.68	1037.167	3.437250	3.439849	0.08
003K	143	599.67	1037.167	3.420517	3.423507	0.09
003K	144	617.67	1037.167	3.401764	3.404778	0.09
003K	145	635.67	1037.167	3.381231	3.384113	0.09
003K	146	653.68	1037.167	3.358970	3.361784	0.08
003K	147	671.68	1037.167	3.335112	3.337989	-0.09
003K	148	563.67	1465.029	3.456312	3.454414	-0.05
003K	149	581.68	1465.029	3.441671	3.441160	-0.01
003K	150	599.67	1465.029	3.424920	3.424891	-0.00
003K	151	617.67	1465.029	3.406209	3.406265	0.00
003K	152	635.67	1465.029	3.385745	3.385725	-0.00
003K	153	653.68	1465.029	3.363559	3.363537	-0.00
003K	154	671.68	1465.029	3.339823	3.339898	0.00
003K	155	563.67	1893.036	3.460707	3.455658	-0.15
003K	156	581.68	1893.036	3.446018	3.442460	-0.10
003K	157	599.67	1893.036	3.429303	3.426273	-0.09
003K	158	617.67	1893.036	3.410598	3.407746	-0.08
003K	159	635.67	1893.036	3.390211	3.387326	-0.09
003K	160	653.68	1893.036	3.368097	3.365274	-0.08
003K	161	671.68	1893.036	3.344485	3.341796	-0.08
003K	162	563.67	3049.859	3.472456	3.458975	-0.39
003K	163	581.68	3049.859	3.457712	3.445924	-0.34
003K	164	599.67	3049.859	3.441007	3.429948	-0.32
003K	165	617.67	3049.859	3.422387	3.411634	-0.31
003K	166	635.67	3049.859	3.402149	3.391580	-0.31
003K	167	653.68	3049.859	3.380273	3.369392	-0.31
003K	168	671.68	3049.859	3.356912	3.346828	-0.30
003K	169	563.67	4742.016	3.489298	3.463716	-0.73
003K	170	581.68	4742.016	3.474369	3.450674	-0.68
003K	171	599.67	4742.016	3.457709	3.435196	-0.65
003K	172	617.67	4742.016	3.439162	3.417306	-0.64
003K	173	635.67	4742.016	3.419160	3.397642	-0.63
003K	174	653.68	4742.016	3.397566	3.376461	-0.62
003K	175	671.68	4742.016	3.374595	3.353969	-0.61
003K	176	563.67	6432.285	3.505689	3.468327	-1.07
003K	177	581.68	6432.285	3.490667	3.455685	-1.00

TABLE 8. CONTINUED. KELL AND WHALLEY.

DATA ID		T RANKINE	P PSIA	RHO EXP LBMOL/FT3	RHO CALC LBMOL/FT3	ERROR PERCENT
003K	178	599.67	6432.285	3.473965	3.440295	-0.97
003K	179	617.67	6432.285	3.455537	3.422759	-0.95
003K	180	635.67	6432.285	3.435707	3.403514	-0.94
003K	181	653.68	6432.285	3.414376	3.382813	-0.92
003K	182	671.68	6432.285	3.391726	3.360860	-0.91
003K	183	563.67	8123.723	3.521808	3.472820	-1.39
003K	184	581.68	8123.723	3.506670	3.460381	-1.32
003K	185	599.67	8123.723	3.489941	3.445265	-1.28
003K	186	617.67	8123.723	3.471576	3.428070	-1.25
003K	187	635.67	8123.723	3.451909	3.409225	-1.24
003K	188	653.68	8123.723	3.430817	3.388976	-1.22
003K	189	671.68	8123.723	3.408472	3.367531	-1.20
003K	190	563.67	9814.859	3.537480	3.477204	-1.70
003K	191	581.68	9814.859	3.522229	3.464958	-1.63
003K	192	599.67	9814.859	3.505465	3.450106	-1.58
003K	193	617.67	9814.859	3.487168	3.433242	-1.55
003K	194	635.67	9814.859	3.467646	3.414773	-1.52
003K	195	653.68	9814.859	3.446776	3.394959	-1.50
003K	196	671.68	9814.859	3.424707	3.374000	-1.48
003K	197	563.67	11505.707	3.552827	3.481486	-2.01
003K	198	581.68	11505.707	3.537440	3.469426	-1.92
003K	199	599.67	11505.707	3.520645	3.454833	-1.87
003K	200	617.67	11505.707	3.502410	3.438281	-1.83
003K	201	635.67	11505.707	3.483011	3.420177	-1.80
003K	202	653.68	11505.707	3.462321	3.400777	-1.78
003K	203	671.68	11505.707	3.440509	3.380276	-1.75
003K	204	563.67	13196.277	3.567870	3.485668	-2.30
003K	205	581.68	13196.277	3.552339	3.473791	-2.21
003K	206	599.67	13196.277	3.535529	3.459443	-2.15
003K	207	617.67	13196.277	3.517307	3.443195	-2.11
003K	208	635.67	13196.277	3.498036	3.425441	-2.08
003K	209	653.68	13196.277	3.477508	3.406435	-2.04
003K	210	671.68	13196.277	3.455964	3.386372	-2.01
003K	211	563.67	14886.547	3.582580	3.489758	-2.59
003K	212	581.68	14886.547	3.566924	3.478057	-2.49
003K	213	599.67	14886.547	3.550063	3.463953	-2.43
003K	214	617.67	14886.547	3.531893	3.447995	-2.38
003K	215	635.67	14886.547	3.512733	3.430576	-2.34
003K	216	653.68	14886.547	3.492340	3.411947	-2.30
003K	217	671.68	14886.547	3.471013	3.392303	-2.27

THE AVERAGE ABSOLUTE ERROR IN PERCENT IS 1.03
FOR 217 DATA POINTS.

TABLE 9. THE PREDICTION OF EXPERIMENTAL DENSITY DATA OF OSBORNE, STIMSON AND GINNINGS, RP 1229, NBS, 1939.

DATA ID		T RANKINE	P PSIA	RHO EXP LBMOL/FT3	RHO CALC LBMOL/FT3	ERROR PERCENT
0010	1	491.67	0.089	3.467471	3.412506	-1.59
0010	2	500.67	0.126	3.467920	3.439583	-0.82
0010	3	509.67	0.178	3.466985	3.452724	-0.41
0010	4	518.67	0.247	3.464907	3.459270	-0.16
0010	5	527.67	0.339	3.461830	3.461791	-0.00
0010	6	536.67	0.459	3.457791	3.461527	0.11
0010	7	545.67	0.615	3.452935	3.459206	0.18
0010	8	554.67	0.815	3.447342	3.455285	0.23
0010	9	563.67	1.070	3.441050	3.450083	0.26
0010	10	572.67	1.390	3.434099	3.443820	0.28
0010	11	581.67	1.789	3.426734	3.436655	0.29
0010	12	590.67	2.283	3.418630	3.428720	0.30
0010	13	599.67	2.889	3.409888	3.420105	0.30
0010	14	608.67	3.627	3.400526	3.410892	0.30
0010	15	617.67	4.519	3.390884	3.401138	0.30
0010	16	626.67	5.591	3.380969	3.390886	0.29
0010	17	635.67	6.869	3.370454	3.380187	0.29
0010	18	644.67	8.384	3.359355	3.369055	0.29
0010	19	653.67	10.168	3.348004	3.357531	0.28
0010	20	662.67	12.259	3.336088	3.345622	0.29
0010	21	671.67	14.696	3.323621	3.333358	0.29
0010	22	680.67	17.520	3.311243	3.320735	0.29
0010	23	689.67	20.779	3.298333	3.307768	0.29
0010	24	698.67	24.520	3.284900	3.294464	0.29
0010	25	707.67	28.795	3.270960	3.280824	0.30
0010	26	716.67	33.661	3.256828	3.266857	0.31
0010	27	725.67	39.177	3.242215	3.252555	0.32
0010	28	734.67	45.405	3.227130	3.237917	0.33
0010	29	743.67	52.410	3.211590	3.222943	0.34
0010	30	752.67	60.263	3.196201	3.207626	0.36
0010	31	761.67	69.033	3.180082	3.191959	0.37
0010	32	770.67	78.800	3.163837	3.175935	0.38
0010	33	779.67	89.640	3.146898	3.159547	0.40
0010	34	788.67	101.636	3.129861	3.142778	0.41
0010	35	797.67	114.873	3.112166	3.125620	0.43
0010	36	806.67	129.441	3.094395	3.108064	0.44
0010	37	815.67	145.434	3.076009	3.090093	0.46
0010	38	824.67	162.943	3.057297	3.071692	0.47
0010	39	833.67	182.069	3.038280	3.052841	0.48
0010	40	842.67	202.896	3.018711	3.033529	0.49
0010	41	851.67	225.540	2.998875	3.013732	0.50
0010	42	860.67	250.118	2.978527	2.993428	0.50
0010	43	869.67	276.729	2.957700	2.972598	0.50
0010	44	878.67	305.489	2.936165	2.951213	0.51
0010	45	887.67	336.510	2.914454	2.929254	0.51
0010	46	896.67	369.906	2.892094	2.906683	0.50
0010	47	905.67	405.808	2.869362	2.883474	0.49
0010	48	914.67	444.323	2.845817	2.859595	0.48
0010	49	923.67	485.585	2.821737	2.835005	0.47
0010	50	932.67	529.734	2.797160	2.809665	0.45
0010	51	941.67	576.899	2.771898	2.783536	0.42
0010	52	950.67	627.207	2.745783	2.756563	0.39
0010	53	959.67	680.814	2.719089	2.728702	0.35
0010	54	968.67	737.836	2.691446	2.699876	0.31

TABLE 9. CONTINUED. OSBORNE, STIMSON AND GINNINGS.

DATA ID		T RANKINE	P PSIA	RHO EXP LBMOL/FT3	RHO CALC LBMOL/FT3	ERROR PERCENT
0010	55	977.67	798.456	2.663132	2.670035	0.26
0010	56	986.67	862.788	2.633807	2.639102	0.20
0010	57	995.67	931.017	2.603557	2.606995	0.13
0010	58	1004.67	1003.300	2.572274	2.573609	0.05
0010	59	1013.67	1079.793	2.539873	2.538849	-0.04
0010	60	1022.67	1160.667	2.506104	2.502576	-0.14

THE AVERAGE ABSOLUTE ERROR IN PERCENT IS 0.36
FOR 60 DATA POINTS.

TABLE 10. THE PREDICTION OF EXPERIMENTAL ENTHALPY DEPARTURE OF KEENAN, KEYES, ET AL., "STEAM TABLES" JOHN WILEY, 1969

DATA ID		T RANKINE	P PSIA	H EXP BTU/LBMOL	H CALC BTU/LBMOL	ERROR BTU/LBMOL
0010	607	669.67	14693.316	-943.6636	-941.9373	-1.73
0010	608	659.67	13367.926	-951.8357	-950.4654	-1.37
0010	609	634.67	10221.438	-972.1421	-971.6709	-0.47
0010	610	584.67	4800.901	-1011.7266	-1012.5010	0.77
0010	611	559.67	2713.103	-1030.4971	-1031.0342	0.51
0010	612	559.67	1464.760	-1044.6814	-1044.2903	-0.39
0010	613	529.67	1003.765	-1051.4158	-1050.4797	-0.94
0010	614	509.67	452.594	-1064.0105	-1063.8096	-0.20
0010	615	809.67	14063.938	-872.5852	-870.4755	-2.11
0010	616	784.67	10370.430	-892.8628	-890.8477	-1.97
0010	617	759.67	6793.867	-913.2793	-911.4083	-1.87
0010	618	734.67	3844.042	-933.8367	-932.0481	-1.79
0010	619	719.67	1844.379	-946.2256	-944.4993	-1.73
0010	620	819.67	14805.695	-812.8536	-812.1444	-0.71
0010	621	909.67	13417.594	-820.3423	-819.6976	-0.64
0010	622	859.67	6587.645	-856.3025	-857.7593	-0.56
0010	623	854.67	3255.107	-877.6309	-876.9553	-0.68
0010	624	819.67	1291.138	-889.3406	-888.5513	-0.79
0010	625	1079.67	15720.816	-723.2410	-722.4626	-0.78
0010	626	1059.67	13551.320	-735.8931	-735.4324	-0.46
0010	627	1009.67	8111.238	-768.1299	-768.2896	0.16
0010	628	959.67	2701.859	-801.3379	-801.6829	0.34
0010	629	939.67	576.325	-814.5080	-815.1699	0.26
0010	630	1109.67	14471.504	-668.2925	-667.2910	-1.00
0010	631	1159.67	13594.309	-673.8706	-673.0503	-0.82
0010	632	1109.67	9177.488	-702.2144	-702.1614	-0.05
0010	633	1059.67	4756.168	-731.4307	-731.5964	0.17
0010	634	1034.67	2576.487	-746.4075	-746.3315	-0.08
0010	635	1259.67	13575.477	-603.5767	-603.4705	-0.11
0010	636	1209.67	10162.406	-628.0823	-628.8235	0.74
0010	637	1159.67	6746.594	-653.3943	-654.3323	0.94
0010	638	1134.67	5059.770	-666.4192	-666.9734	0.55
0010	639	1059.67	263.506	-707.5481	-701.5454	-6.00
0010	640	1359.67	15203.273	-535.9185	-535.4595	-0.46
0010	641	1309.67	12459.676	-557.4175	-558.1125	0.70
0010	642	1259.67	9096.359	-579.5823	-581.2179	1.63
0010	643	1209.67	6948.625	-602.6526	-604.4519	1.80
0010	644	1159.67	4277.438	-627.0220	-627.0940	0.07
0010	645	1429.67	14864.297	-478.5188	-477.2067	-1.31
0010	646	1359.67	11806.418	-505.4102	-505.7904	0.38
0010	647	1209.67	7432.641	-546.5171	-548.6789	2.16
0010	648	1209.67	5308.883	-569.1265	-570.5681	1.41
0010	649	1159.67	3303.629	-594.0894	-592.2193	-1.87
0010	650	1459.67	13254.074	-433.5120	-431.1624	-2.35
0010	651	1359.67	9759.488	-469.1648	-469.1058	-0.06
0010	652	1259.67	6297.602	-509.2422	-511.0696	1.83
0010	653	1209.67	4637.918	-532.5540	-535.0713	2.52
0010	654	1559.67	13776.508	-360.8262	-356.3726	-4.45
0010	655	1459.67	11073.219	-391.6736	-387.6797	-3.99
0010	656	1359.67	8342.133	-425.3936	-423.3052	-2.08
0010	657	1259.67	5631.809	-465.3606	-466.1915	0.83
0010	658	1209.67	4320.410	-490.0686	-497.2979	7.23
0010	659	1659.67	14434.461	-304.6919	-301.1206	-3.57
0010	660	1559.67	12200.660	-331.9365	-327.0771	-4.86
0010	661	1459.67	9929.813	-361.1752	-357.0022	-4.17
0010	662	1259.67	5322.492	-433.5464	-434.7329	1.19
0010	663	1209.67	4187.965	-459.0457	-468.0068	8.96
0010	664	1959.67	14775.563	-180.4676	-185.4309	4.96

TABLE 10. CONTINUED. KEENAN,KEYES, ET AL.

DATA ID		T RANKINE	P PSIA	H EXP BTU/LBMOL	H CALC BTU/LBMOL	ERROR BTU/LBMOL
0010	665	1459.67	7780.344	-285.6370	-290.0457	-5.59
0010	666	1259.67	4720.324	-351.2643	-347.0239	-4.64
0010	667	1209.67	3919.446	-376.9893	-370.6135	-6.58
0010	668	2459.67	13176.977	-89.4416	-89.9364	0.50
0010	669	1959.67	9602.172	-121.8621	-127.6167	5.75
0010	670	1459.67	5683.734	-199.5204	-196.9110	-2.61
0010	671	1209.67	3434.606	-271.8816	-264.1967	-7.68
0010	672	2859.67	7812.055	-48.6976	-37.8584	-10.84
0010	673	2459.67	6504.238	-47.6701	-48.5986	0.93
0010	674	1959.67	5006.043	-63.9347	-58.6257	4.69
0010	675	1459.67	3622.923	-106.9013	-107.7632	0.86
0010	676	1209.67	2372.051	-148.3819	-148.8110	0.43
0010	677	2859.67	3104.036	-20.3742	-16.0747	-4.30
0010	678	2459.67	2644.325	-20.1973	-20.4159	0.22
0010	679	1959.67	2069.687	-26.1996	-28.6414	2.44
0010	680	1459.67	1474.617	-43.7233	-45.3820	1.66
0010	681	1209.67	1157.050	-60.9395	-63.5726	2.63
0010	682	1159.67	1089.941	-66.3042	-69.0355	2.73
0010	683	1109.67	1020.638	-72.9688	-75.4407	2.47
0010	684	1059.67	948.245	-81.4961	-82.9641	1.49
0010	685	1009.67	871.408	-92.6945	-91.8527	-0.84
0010	686	2859.67	852.204	-5.7548	-4.5488	-1.21
0010	687	2459.67	730.965	-5.7576	-5.7467	-0.01
0010	688	1959.67	579.491	-7.2624	-8.0341	0.77
0010	689	1459.67	426.617	-12.0220	-12.7609	0.74
0010	690	1159.67	332.746	-16.1158	-19.5117	1.40
0010	691	959.67	267.416	-27.3270	-29.5025	2.18
0010	692	859.67	232.317	-37.0011	-38.7361	1.67
0010	693	2859.67	170.362	-1.1613	-0.9175	-0.24
0010	694	2459.67	146.450	-1.1655	-1.1579	-0.01
0010	695	1959.67	116.563	-1.4548	-1.6164	0.16
0010	696	1459.67	86.623	-2.3993	-2.5679	0.17
0010	697	1159.67	68.573	-3.6057	-3.9294	0.32
0010	698	959.67	56.442	-5.2823	-5.9442	0.66
0010	699	859.67	50.299	-6.9615	-7.8177	0.86
0010	700	759.67	44.034	-10.0181	-11.0083	0.99
0010	701	2859.67	34.070	-0.2327	-0.1840	-0.05
0010	702	2459.67	29.301	-0.2337	-0.2321	-0.00
0010	703	1959.67	23.340	-0.2911	-0.3238	0.03
0010	704	1459.67	17.377	-0.4797	-0.5144	0.03
0010	705	1159.67	13.796	-0.7204	-0.7870	0.07
0010	706	959.67	11.404	-1.0486	-1.1902	0.14
0010	707	859.67	10.206	-1.3731	-1.5649	0.19
0010	708	759.67	9.003	-1.9634	-2.2028	0.24
0010	709	659.67	7.790	-3.0645	-3.4217	0.36
0010	710	2859.67	3.406	-0.0233	-0.0185	-0.00
0010	711	2459.67	2.930	-0.0234	-0.0233	-0.00
0010	712	1959.67	2.334	-0.0292	-0.0324	0.00
0010	713	1459.67	1.739	-0.0480	-0.0515	0.00
0010	714	1159.67	1.381	-0.0720	-0.0786	0.01
0010	715	959.67	1.143	-0.1047	-0.1191	0.01
0010	716	859.67	1.024	-0.1369	-0.1567	0.02
0010	717	759.67	0.904	-0.1954	-0.2202	0.02
0010	718	659.67	0.785	-0.3050	-0.3420	0.04
0010	719	559.67	0.666	-0.4770	-0.6165	0.14

THE AVERAGE ABSOLUTE ERROR IN BTU/LBMOL 1.59
FOR 113 DATA POINTS.

TABLE 11. THE PREDICTION OF EXPERIMENTAL ENTHALPY DEPARTURE OF ANGUS AND NEWITT, PHIL. TRANS. ROY. SOC. (LONDON), V. 259(1966)

DATA ID		T RANKINE	P PSIA	H EXP BTU/LBMOL	H CALC BTU/LBMOL	ERROR BTU/LBMCL
003A	1	1211.67	870.221	-41.9860	-46.3983	4.41
003A	2	1211.67	2900.738	-197.9800	-195.8912	-2.09
003A	3	1571.67	870.221	-20.1830	-21.4478	1.26
003A	4	1571.67	2900.738	-70.5180	-73.8509	3.33
003A	5	1571.67	5801.473	-154.6240	-153.4383	-1.19
003A	6	1571.67	8702.211	-237.6120	-233.7884	-3.82
003A	7	1571.67	11602.945	-311.8660	-305.1855	-6.68
003A	8	1751.67	870.221	-12.9390	-16.0740	3.14
003A	9	1751.67	2900.738	-52.4760	-54.1390	1.66
003A	10	1751.67	5801.473	-107.2850	-108.9571	1.67
003A	11	1751.67	8702.211	-158.7380	-162.3328	3.59
003A	12	1751.67	11602.945	-213.2030	-211.7525	-1.45
003A	13	1211.67	5801.473	-580.6948	-581.5754	0.88
003A	14	1211.67	8702.211	-615.7998	-618.8660	3.07
003A	15	1211.67	11602.945	-630.5999	-632.7881	2.19
003A	16	1211.67	14503.688	-633.6108	-639.6125	6.00

THE AVERAGE ABSOLUTE ERROR IN BTU/LBMCL 2.90
FOR 16 DATA POINTS.

TABLE 12. THE PREDICTION OF EXPERIMENTAL ENTHALPY DEPARTURE OF CALLENDAR AND EGERTON, PHIL. TRANS. ROY. SOC.(LONDON), V252(1960)

DATA ID		T RANKINE	P PSIA	H EXP BTU/LBMOL	H CALC BTU/LBMOL	ERROR BTU/LBMOL
002C	1	851.67	71.053	-10.3990	-11.5198	1.12
002C	2	851.67	142.107	-22.2790	-23.6823	1.40
002C	3	896.67	71.053	-8.4540	-9.5314	1.08
002C	4	896.67	142.107	-17.8140	-19.4692	1.66
002C	5	941.67	71.053	-7.2010	-8.0152	0.81
002C	6	941.67	142.107	-14.9410	-16.2952	1.35
002C	7	941.67	355.267	-41.4010	-43.0612	1.66
002C	8	986.67	71.053	-6.2870	-6.8295	0.54
002C	9	986.67	142.107	-12.7670	-13.8396	1.07
002C	10	986.67	355.267	-34.1270	-36.1226	1.94
002C	11	986.67	710.535	-79.5470	-78.9910	-0.56
002C	12	1031.67	71.053	-5.5350	-5.8896	0.35
002C	13	1031.67	142.107	-11.1150	-11.9046	0.79
002C	14	1031.67	355.267	-28.9350	-30.7935	1.86
002C	15	1031.67	710.535	-64.3950	-65.8514	1.46
002C	16	1031.67	1065.802	-111.3740	-107.7068	-3.67
002C	17	1076.67	71.053	-4.9470	-5.1516	0.13
002C	18	1076.67	142.107	-9.8070	-10.3521	0.55
002C	19	1076.67	355.267	-25.1070	-26.5992	1.49
002C	20	1076.67	710.535	-53.7270	-56.0260	2.30
002C	21	1076.67	1065.802	-88.6470	-89.4708	0.83
002C	22	1076.67	1421.069	-134.0070	-129.3095	-4.70
002C	23	1121.67	71.053	-4.5300	-4.5116	-0.02
002C	24	1121.67	142.107	-8.8500	-9.0876	0.24
002C	25	1121.67	355.267	-21.9900	-23.2309	1.24
002C	26	1121.67	710.535	-45.9300	-48.4071	2.48
002C	27	1121.67	1065.802	-74.0100	-76.1278	2.12
002C	28	1121.67	1421.069	-107.3100	-107.3759	0.07
002C	29	1121.67	1776.337	-148.5300	-143.9931	-4.54
002C	30	1121.67	2131.604	-201.2700	-190.3120	-10.96
002C	31	1166.67	71.053	-4.2840	-3.9985	-0.29
002C	32	1166.67	142.107	-7.8840	-8.0441	0.16
002C	33	1166.67	355.267	-19.5840	-20.4816	0.90
002C	34	1166.67	710.535	-40.1040	-42.3563	2.25
002C	35	1166.67	1065.802	-63.5040	-65.8694	2.36
002C	36	1166.67	1421.069	-89.9640	-91.5910	1.63
002C	37	1166.67	1776.337	-120.3840	-120.1731	-0.21
002C	38	1166.67	2131.604	-156.5640	-152.8566	-3.71
002C	39	1166.67	2486.871	-199.0430	-192.0639	-6.98
002C	40	1166.67	2842.139	-258.8040	-244.1564	-14.65
002C	41	1211.67	71.053	-3.8520	-3.5690	-0.28
002C	42	1211.67	142.107	-7.2720	-7.1730	-0.10
002C	43	1211.67	355.267	-17.5320	-18.2057	0.67
002C	44	1211.67	710.535	-35.5320	-37.4021	1.87
002C	45	1211.67	1065.802	-55.5120	-57.7601	2.25
002C	46	1211.67	1421.069	-77.6520	-79.5336	1.88
002C	47	1211.67	1776.337	-101.9520	-103.0285	1.08
002C	48	1211.67	2131.604	-128.7720	-128.7168	-0.06
002C	49	1211.67	2486.871	-159.3720	-157.3096	-2.06
002C	50	1211.67	2842.139	-194.8320	-189.9823	-4.85
002C	51	1211.67	3197.406	-237.1320	-228.9256	-8.21
002C	52	1256.67	71.053	-3.9570	-3.2060	-0.75
002C	53	1256.67	142.107	-6.8370	-6.4381	-0.40
002C	54	1256.67	355.267	-15.8370	-16.2991	0.46
002C	55	1256.67	710.535	-31.8570	-33.3243	1.47
002C	56	1256.67	1065.802	-49.1370	-51.1766	2.04
002C	57	1256.67	1421.069	-68.0370	-69.9811	1.94
002C	58	1256.67	1776.337	-87.8370	-89.8960	2.06

TABLE 12. CONTINUED. CALLENDAR AND EGERTON.

DATA ID		T RANKINE	P PSIA	H EXP BTU/LBMOL	H CALC BTU/LBMOL	ERROR BTU/LBMOL
002C	59	1256.67	2131.604	-110.1570	-111.1256	0.97
002C	60	1256.67	2486.871	-134.8170	-133.9365	-0.88
002C	61	1256.67	2842.139	-162.5370	-158.7054	-3.83
002C	62	1256.67	3197.406	-188.4570	-185.9381	-2.52
002C	63	1301.67	71.053	-3.2810	-2.3963	-0.98
002C	64	1301.67	142.107	-6.5810	-5.8125	-0.77
002C	65	1301.67	355.267	-14.6810	-14.6847	0.00
002C	66	1301.67	710.535	-28.7210	-29.9088	1.19
002C	67	1301.67	1065.802	-44.0210	-45.7305	1.71
002C	68	1301.67	1421.069	-60.2210	-62.2179	2.00
002C	69	1301.67	1776.337	-77.6810	-79.4516	1.77
002C	70	1301.67	2131.604	-96.0420	-97.5284	1.49
002C	71	1301.67	2486.871	-116.5620	-116.5609	0.00
002C	72	1301.67	2842.139	-138.1620	-136.6985	-1.46
002C	73	1301.67	3197.406	-158.6810	-158.1612	-0.53
002C	74	1346.67	71.053	-3.9860	-2.6301	-1.36
002C	75	1346.67	142.107	-6.3260	-5.2754	-1.05
002C	76	1346.67	355.267	-13.5260	-13.3046	-0.22
002C	77	1346.67	710.535	-26.1260	-27.0148	0.89
002C	78	1346.67	1065.802	-40.1670	-41.1626	1.00
002C	79	1346.67	1421.069	-54.7470	-55.7861	1.04
002C	80	1346.67	1776.337	-69.6860	-70.9273	1.24
002C	81	1346.67	2131.604	-85.3470	-86.6352	1.29
002C	82	1346.67	2486.871	-102.2670	-102.9581	0.69
002C	83	1346.67	2842.139	-120.4470	-119.9545	-0.49
002C	84	1346.67	3197.406	-137.1860	-137.6917	0.51
002C	85	1391.67	71.053	-3.7340	-2.3996	-1.33
002C	86	1391.67	142.107	-6.0740	-4.8107	-1.26
002C	87	1391.67	355.267	-12.7340	-12.1157	-0.62
002C	88	1391.67	710.535	-24.0740	-24.5375	0.46
002C	89	1391.67	1065.802	-36.6740	-37.2840	0.61
002C	90	1391.67	1421.069	-49.6340	-50.3761	0.74
002C	91	1391.67	1776.337	-62.9540	-63.8349	0.88
002C	92	1391.67	2131.604	-76.9940	-77.6832	0.69
002C	93	1391.67	2486.871	-92.1140	-91.9449	-0.17
002C	94	1391.67	2842.139	-108.1340	-106.6443	-1.49
002C	95	1436.67	71.053	-3.8450	-2.1988	-1.65
002C	96	1436.67	142.107	-5.8250	-4.4000	-1.42
002C	97	1436.67	355.267	-11.9450	-11.0830	-0.86
002C	98	1436.67	710.535	-22.3850	-22.3924	0.01
002C	99	1436.67	1065.802	-33.7250	-33.9567	0.23
002C	100	1436.67	1421.069	-45.4250	-45.7682	0.34
002C	101	1436.67	1776.337	-57.6650	-57.8437	0.18
002C	102	1436.67	2131.604	-70.4450	-70.1951	-0.25
002C	103	1436.67	2486.871	-83.9450	-82.8268	-1.12
002C	104	1436.67	2842.139	-97.9850	-95.7536	-2.23
002C	105	1481.67	71.053	-3.9620	-2.0222	-1.94
002C	106	1481.67	142.107	-5.5820	-4.0510	-1.53
002C	107	1481.67	355.267	-11.3420	-10.1798	-1.16
002C	108	1481.67	710.535	-21.0620	-20.5368	-0.53
002C	109	1481.67	1065.802	-31.3220	-31.0760	-0.25
002C	110	1481.67	1421.069	-42.1220	-41.8022	-0.32
002C	111	1481.67	1776.337	-53.2820	-52.7199	-0.56
002C	112	1481.67	2131.604	-64.8020	-63.8328	-0.97
002C	113	1481.67	2486.871	-76.6820	-75.1440	-1.54
002C	114	1481.67	2842.139	-89.1020	-86.6557	-2.45
002C	115	1526.67	71.053	-3.7250	-1.8664	-1.86
002C	116	1526.67	142.107	-5.3450	-3.7381	-1.61

TABLE 12. CONTINUED. CALLENDAR AND EGERTON.

DATA ID		T RANKINE	P PSIA	H EXP BTU/LBMOL	H CALC BTU/LBMOL	ERROR BTU/LBMOL
002C	117	1526.67	355.267	-10.5650	-9.3852	-1.18
002C	118	1526.67	710.535	-19.7450	-18.9052	-0.84
002C	119	1526.67	1065.802	-29.1050	-28.5622	-0.54
002C	120	1526.67	1421.069	-39.0050	-38.3574	-0.65
002C	121	1526.67	1776.337	-48.9050	-48.2923	-0.61
002C	122	1526.67	2131.604	-59.1650	-58.3668	-0.80
002C	123	1526.67	2486.871	-69.7850	-68.5809	-1.20
002C	124	1526.67	2842.139	-80.9450	-78.9332	-2.01
002C	125	1571.67	71.053	-3.3150	-1.7263	-1.59
002C	126	1571.67	142.107	-4.7550	-3.4605	-1.29
002C	127	1571.67	355.267	-9.6150	-8.6819	-0.93
002C	128	1571.67	710.535	-18.2550	-17.4661	-0.79
002C	129	1571.67	1065.802	-26.8960	-26.3530	-0.54
002C	130	1571.67	1421.069	-35.7150	-35.3419	-0.37
002C	131	1571.67	1776.337	-44.7150	-44.4321	-0.28
002C	132	1571.67	2131.604	-53.7150	-53.6224	-0.09
002C	133	1571.67	2486.871	-63.0750	-62.9108	-0.16
002C	134	1571.67	2842.139	-73.1560	-72.2944	-0.86

THE AVERAGE ABSOLUTE ERROR IN BTU/LBMOL 1.45
FOR 134 DATA POINTS.

TABLE 13. THE PREDICTION OF EXPERIMENTAL VAPOR PRESSURE DATA OF OSBORNE, STIMSON AND GINNINGS, RP 1229, NBS, 1939.

DATA ID		T RANKINE	P EXP PSIA	P EXP PSIA	ERROR PERCENT
0010	547	491.67	0.089	0.088	-0.61
0010	548	500.67	0.126	0.127	0.46
0010	551	527.67	0.339	0.339	0.03
0010	553	545.67	0.616	0.615	-0.12
0010	554	554.67	0.816	0.815	-0.07
0010	556	572.67	1.391	1.390	-0.05
0010	561	617.67	4.523	4.524	0.02
0010	564	644.67	8.386	8.390	0.03
0010	566	662.67	12.263	12.266	0.02
0010	568	680.67	17.522	17.524	0.01
0010	570	698.67	24.519	24.517	-0.01
0010	571	707.67	28.793	28.789	-0.02
0010	571	707.67	28.793	28.789	-0.02
0010	572	716.67	33.656	33.649	-0.03
0010	573	725.67	39.171	39.156	-0.04
0010	574	734.67	45.396	45.373	-0.05
0010	575	743.67	52.398	52.369	-0.06
0010	576	752.67	60.247	60.208	-0.06
0010	577	761.67	69.013	68.967	-0.07
0010	578	770.67	78.773	78.722	-0.06
0010	579	779.67	89.605	89.547	-0.06
0010	580	788.67	101.591	101.529	-0.06
0010	581	797.67	114.817	114.745	-0.06
0010	582	806.67	129.371	129.290	-0.06
0010	583	815.67	145.343	145.276	-0.05
0010	584	824.67	162.828	162.770	-0.04
0010	585	833.67	181.924	181.879	-0.02
0010	586	842.67	202.730	202.700	-0.01
0010	587	851.67	225.352	225.351	-0.00
0010	588	860.67	249.894	249.922	0.01
0010	589	869.67	276.465	276.552	0.02
0010	590	878.67	305.179	305.296	0.04
0010	591	887.67	336.150	336.319	0.05
0010	592	896.67	369.497	369.728	0.06
0010	593	905.67	405.341	405.641	0.07
0010	594	914.67	443.805	444.176	0.08
0010	595	923.67	485.018	485.463	0.09
0010	596	932.67	529.106	529.625	0.10
0010	597	941.67	576.206	576.923	0.12
0010	598	950.67	626.453	627.270	0.13
0010	599	959.67	679.985	680.895	0.13
0010	600	968.67	736.947	737.958	0.13
0010	601	977.67	797.483	798.552	0.13
0010	602	986.67	861.745	862.869	0.13
0010	603	995.67	929.885	930.791	0.10
0010	604	1004.67	1002.065	1002.956	0.09
0010	605	1013.67	1078.445	1079.295	0.08
0010	606	1022.67	1159.200	1159.985	0.07
0010	720	1059.67	1541.000	1540.780	-0.01
0010	721	1084.67	1849.700	1846.939	-0.15
0010	722	1109.67	2205.000	2197.001	-0.36
0010	724	1134.67	2616.000	2596.280	-0.75
0010	723	1159.67	3090.000	3050.400	-1.28

THE AVERAGE ABSOLUTE ERROR IN PERCENT IS 0.12
FOR 53 DATA POINTS.